# Full wwPDB EM Validation Report

Mar 16, 2026 – 06:39 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 7N9F / pdb_00007n9f |
| EMDB ID | : | EMD-24258 |
| Title | : | Structure of the in situ yeast NPC |
| Authors | : | Villa, E.; Singh, D.; Ludtke, S.J.; Akey, C.W.; Rout, M.P.; Echeverria, I.; Suslov, S. |
| Deposited on | : | 2021-06-17 |
| Resolution | : | 37.00 Å(reported) |

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

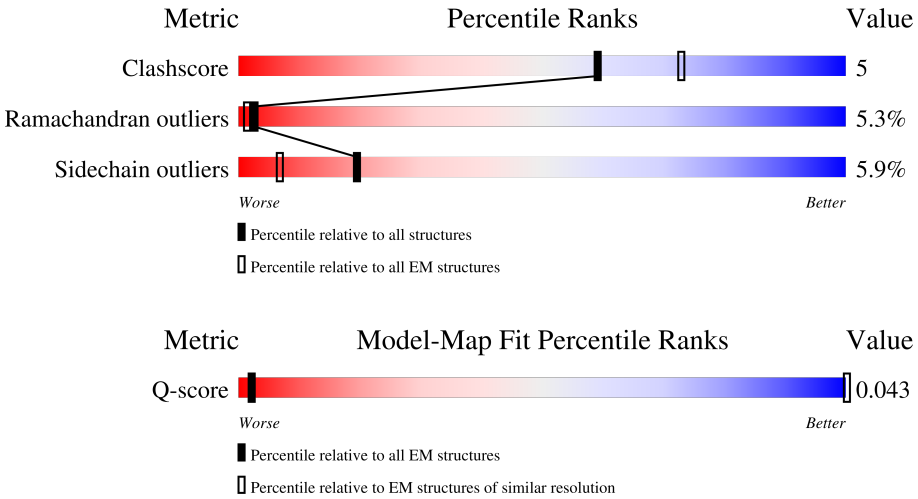
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.49 |

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 37.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.







| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 3 ( 37.00 - 37.00 ) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 0 | 1502 | 28% 36% 7% • 28% |
| 1 | Y | 1502 | 28% 36% 7% • 28% |
| 2 | 1 | 1391 | 32% 39% 8% • 20% |
| 2 | Z | 1391 | 32% 38% 8% • 20% |

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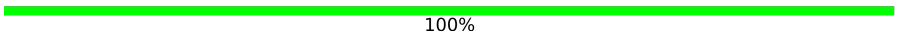
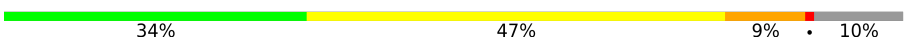
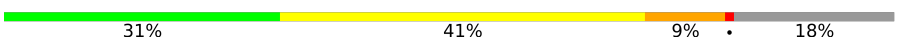
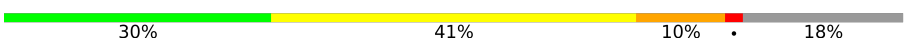
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | 5 | 36 |   |
| 3 | 6 | 36 | |
| 4 | A | 823 | |
| 4 | D | 823 | |
| 4 | G | 823 | |
| 4 | J | 823 | |
| 4 | y | 823 | |
| 4 | z | 823 | |
| 5 | B | 541 | |
| 5 | E | 541 | |
| 5 | H | 541 | |
| 5 | K | 541 | |
| 6 | C | 472 | |
| 6 | F | 472 | |
| 6 | I | 472 | |
| 6 | L | 472 | |
| 7 | M | 1683 |   |
| 7 | O | 1683 | |
| 8 | N | 1655 |   |
| 8 | P | 1655 |   |
| 9 | Q | 839 | |
| 9 | R | 839 | |
| 9 | S | 839 | |
| 9 | T | 839 | |
| 10 | U | 475 | |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 10 | W | 475 | 8% 8% 80% |
| 11 | V | 528 | 6% 9% 82% |
| 11 | X | 528 | 7% 7% 82% |
| 12 | u | 713 | 14% 35% 40% 5% 19% |
| 12 | v | 713 | 35% 37% 7% 21% |
| 13 | w | 1460 | 7% 7% 87% |
| 13 | x | 1460 | 8% 6% 86% |
| 14 | a | 1037 | 38% 47% 11% |
| 14 | h | 1037 | 39% 47% 9% |
| 15 | b | 744 | 43% 41% 6% 9% |
| 15 | i | 744 | 41% 39% 8% 11% |
| 16 | c | 712 | 34% 37% 6% 21% |
| 16 | j | 712 | 35% 38% 5% 21% |
| 17 | d | 297 | 41% 46% 5% 8% |
| 17 | k | 297 | 46% 40% 5% 8% |
| 18 | e | 349 | 37% 41% 8% 13% |
| 18 | l | 349 | 36% 46% 5% 12% |
| 19 | f | 726 | 38% 44% 7% 11% |
| 19 | m | 726 | 35% 47% 7% 11% |
| 20 | g | 1157 | 39% 43% 9% 8% |
| 20 | n | 1157 | 38% 44% 9% 8% |
| 21 | o | 92 | 40% 46% 7% 7% |
| 21 | p | 92 | 34% 54% 7% |
| 21 | q | 92 | 43% 45% 7% |
| 21 | r | 92 | 50% 33% 10% 7% |

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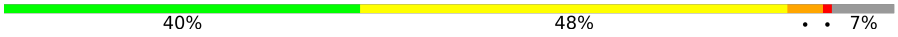
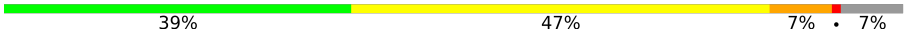
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 21 | s | 92 |   |
| 21 | t | 92 |   |

# 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 212962 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nucleoporin NUP170.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 1085 | Total | C | N | O | S | 0 | 0 |
| | | | 8762 | 5674 | 1424 | 1636 | 28 | | |
| 1 | Y | 1086 | Total | C | N | O | S | 0 | 0 |
| | | | 8770 | 5679 | 1425 | 1637 | 29 | | |

- Molecule 2 is a protein called Nucleoporin NUP157.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | 1113 | Total | C | N | O | S | 0 | 0 |
| | | | 8919 | 5719 | 1479 | 1693 | 28 | | |
| 2 | Z | 1111 | Total | C | N | O | S | 0 | 0 |
| | | | 8906 | 5710 | 1477 | 1691 | 28 | | |

- Molecule 3 is a protein called orphans bound to Nup192 NTD.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 3 | 5 | 36 | Total | C | N | O | 0 | 0 |
| | | | 181 | 108 | 36 | 37 | | |
| 3 | 6 | 36 | Total | C | N | O | 0 | 0 |
| | | | 181 | 108 | 36 | 37 | | |

- Molecule 4 is a protein called Nucleoporin NSP1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | A | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1315 | 814 | 220 | 280 | 1 | | |
| 4 | D | 163 | Total | C | N | O | S | 0 | 0 |
| | | | 1315 | 814 | 220 | 280 | 1 | | |
| 4 | G | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1321 | 817 | 221 | 282 | 1 | | |
| 4 | J | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1321 | 817 | 221 | 282 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 4 | y | 190 | Total<br>946 | C<br>566 | N<br>190 | O<br>190 | 0 | 0 |
| 4 | z | 193 | Total<br>962 | C<br>575 | N<br>193 | O<br>194 | 0 | 0 |

- Molecule 5 is a protein called Nucleoporin NUP57.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | B | 217 | Total<br>1771 | C<br>1115 | N<br>317 | O<br>336 | S<br>3 | 0 | 0 |
| 5 | E | 217 | Total<br>1771 | C<br>1115 | N<br>317 | O<br>336 | S<br>3 | 0 | 0 |
| 5 | H | 217 | Total<br>1771 | C<br>1115 | N<br>317 | O<br>336 | S<br>3 | 0 | 0 |
| 5 | K | 217 | Total<br>1771 | C<br>1115 | N<br>317 | O<br>336 | S<br>3 | 0 | 0 |

- Molecule 6 is a protein called Nucleoporin NUP49/NSP49.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | C | 166 | Total<br>1347 | C<br>863 | N<br>217 | O<br>265 | S<br>2 | 0 | 0 |
| 6 | F | 167 | Total<br>1351 | C<br>865 | N<br>218 | O<br>266 | S<br>2 | 0 | 0 |
| 6 | I | 166 | Total<br>1347 | C<br>863 | N<br>217 | O<br>265 | S<br>2 | 0 | 0 |
| 6 | L | 167 | Total<br>1351 | C<br>865 | N<br>218 | O<br>266 | S<br>2 | 0 | 0 |

- Molecule 7 is a protein called Nucleoporin NUP192.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | M | 1521 | Total<br>11909 | C<br>7694 | N<br>1943 | O<br>2241 | S<br>31 | 0 | 0 |
| 7 | O | 1520 | Total<br>11902 | C<br>7689 | N<br>1942 | O<br>2240 | S<br>31 | 0 | 0 |

- Molecule 8 is a protein called Nucleoporin NUP188.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | N | 1360 | Total<br>10971 | C<br>7162 | N<br>1746 | O<br>2038 | S<br>25 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | P | 1360 | Total<br>10971 | C<br>7162 | N<br>1746 | O<br>2038 | S<br>25 | 0 | 0 |

- Molecule 9 is a protein called Nucleoporin NIC96.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | Q | 688 | Total<br>5184 | C<br>3294 | N<br>894 | O<br>979 | S<br>17 | 0 | 0 |
| 9 | R | 708 | Total<br>5287 | C<br>3357 | N<br>914 | O<br>999 | S<br>17 | 0 | 0 |
| 9 | S | 690 | Total<br>5197 | C<br>3303 | N<br>896 | O<br>981 | S<br>17 | 0 | 0 |
| 9 | T | 708 | Total<br>5287 | C<br>3357 | N<br>914 | O<br>999 | S<br>17 | 0 | 0 |

- Molecule 10 is a protein called Nucleoporin NUP53.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | U | 94 | Total<br>745 | C<br>486 | N<br>120 | O<br>137 | S<br>2 | 0 | 0 |
| 10 | W | 94 | Total<br>745 | C<br>486 | N<br>120 | O<br>137 | S<br>2 | 0 | 0 |

- Molecule 11 is a protein called Nucleoporin ASM4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | V | 94 | Total<br>739 | C<br>475 | N<br>122 | O<br>139 | S<br>3 | 0 | 0 |
| 11 | X | 94 | Total<br>739 | C<br>475 | N<br>122 | O<br>139 | S<br>3 | 0 | 0 |

- Molecule 12 is a protein called Nucleoporin NUP82.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | u | 581 | Total<br>4214 | C<br>2673 | N<br>708 | O<br>821 | S<br>12 | 0 | 0 |
| 12 | v | 564 | Total<br>4063 | C<br>2579 | N<br>681 | O<br>791 | S<br>12 | 0 | 0 |

- Molecule 13 is a protein called Nucleoporin NUP159.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | w | 195 | Total | C | N | O | S | 0 | 0 |
| | | | 1088 | 664 | 206 | 216 | 2 | | |
| 13 | x | 198 | Total | C | N | O | S | 0 | 0 |
| | | | 1106 | 676 | 209 | 219 | 2 | | |

- Molecule 14 is a protein called Nucleoporin NUP120.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | h | 1006 | Total | C | N | O | S | 0 | 0 |
| | | | 8279 | 5346 | 1334 | 1566 | 33 | | |
| 14 | a | 1006 | Total | C | N | O | S | 0 | 0 |
| | | | 8279 | 5346 | 1334 | 1566 | 33 | | |

- Molecule 15 is a protein called Nucleoporin NUP85.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | i | 663 | Total | C | N | O | S | 0 | 0 |
| | | | 5327 | 3431 | 849 | 1019 | 28 | | |
| 15 | b | 675 | Total | C | N | O | S | 0 | 0 |
| | | | 5424 | 3493 | 863 | 1038 | 30 | | |

- Molecule 16 is a protein called Nucleoporin 145c.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | j | 559 | Total | C | N | O | S | 0 | 0 |
| | | | 4520 | 2884 | 750 | 869 | 17 | | |
| 16 | c | 559 | Total | C | N | O | S | 0 | 0 |
| | | | 4520 | 2884 | 750 | 869 | 17 | | |

- Molecule 17 is a protein called Protein transport protein SEC13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | k | 274 | Total | C | N | O | S | 0 | 0 |
| | | | 2160 | 1379 | 369 | 409 | 3 | | |
| 17 | d | 274 | Total | C | N | O | S | 0 | 0 |
| | | | 2160 | 1379 | 369 | 409 | 3 | | |

- Molecule 18 is a protein called Nucleoporin SEH1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | l | 307 | Total | C | N | O | S | 0 | 0 |
| | | | 2438 | 1543 | 422 | 462 | 11 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | e | 303 | Total<br>2407 | C<br>1524 | N<br>415 | O<br>457 | S<br>11 | 0 | 0 |

- Molecule 19 is a protein called Nucleoporin NUP84.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 19 | m | 649 | Total<br>5261 | C<br>3370 | N<br>866 | O<br>1011 | S<br>14 | 0 | 0 |
| 19 | f | 649 | Total<br>5261 | C<br>3370 | N<br>866 | O<br>1011 | S<br>14 | 0 | 0 |

- Molecule 20 is a protein called Nucleoporin NUP133.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | n | 1062 | Total<br>8627 | C<br>5541 | N<br>1393 | O<br>1664 | S<br>29 | 0 | 0 |
| 20 | g | 1062 | Total<br>8627 | C<br>5541 | N<br>1393 | O<br>1664 | S<br>29 | 0 | 0 |

- Molecule 21 is a protein called Dynein light chain 1, cytoplasmic.

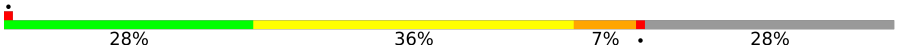
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 21 | o | 86 | Total<br>691 | C<br>453 | N<br>111 | O<br>127 | 0 | 0 |
| 21 | p | 86 | Total<br>691 | C<br>453 | N<br>111 | O<br>127 | 0 | 0 |
| 21 | q | 86 | Total<br>691 | C<br>453 | N<br>111 | O<br>127 | 0 | 0 |
| 21 | r | 86 | Total<br>691 | C<br>453 | N<br>111 | O<br>127 | 0 | 0 |
| 21 | s | 86 | Total<br>691 | C<br>453 | N<br>111 | O<br>127 | 0 | 0 |
| 21 | t | 86 | Total<br>691 | C<br>453 | N<br>111 | O<br>127 | 0 | 0 |

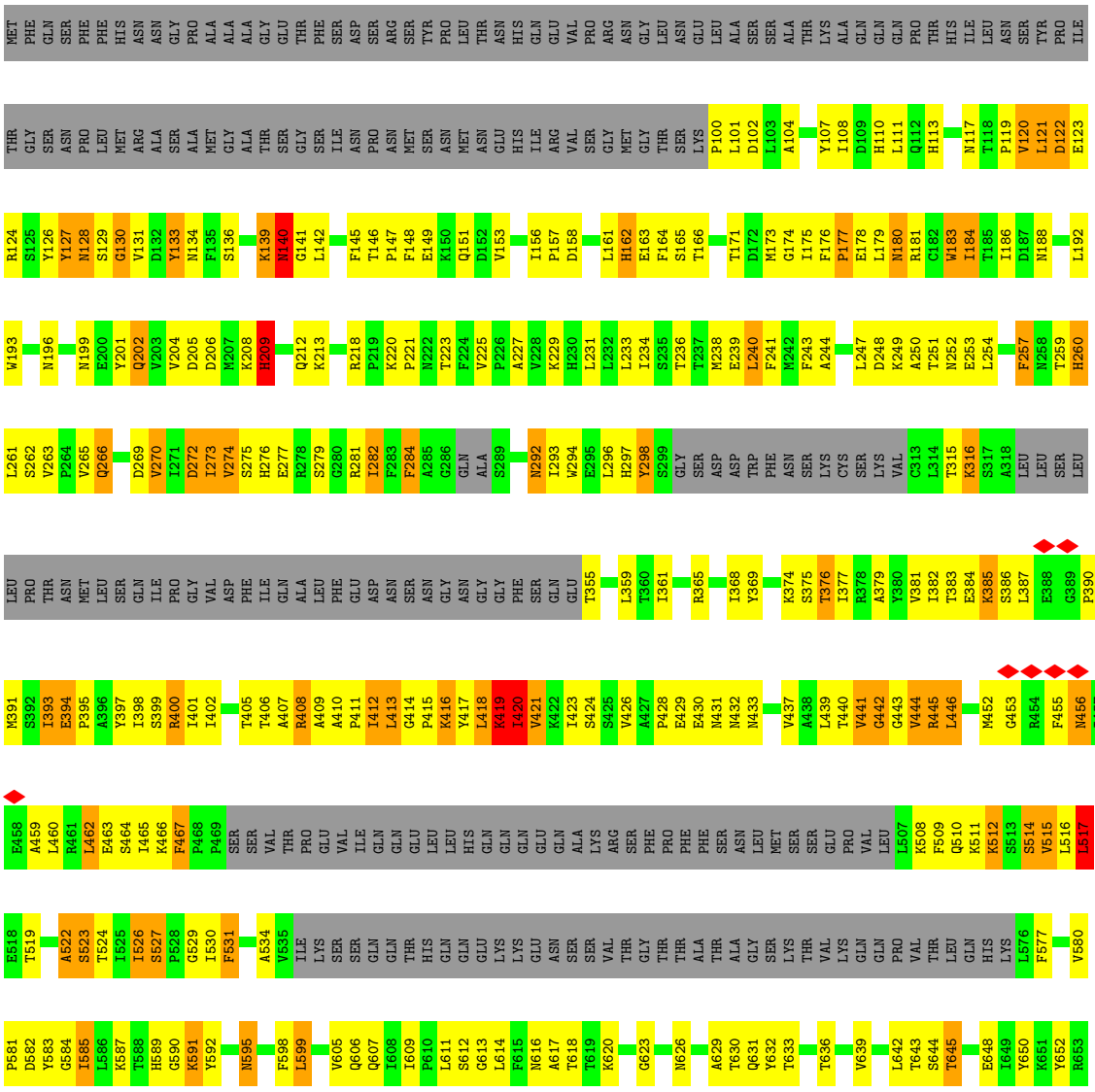
# 3 Residue-property plots (i)

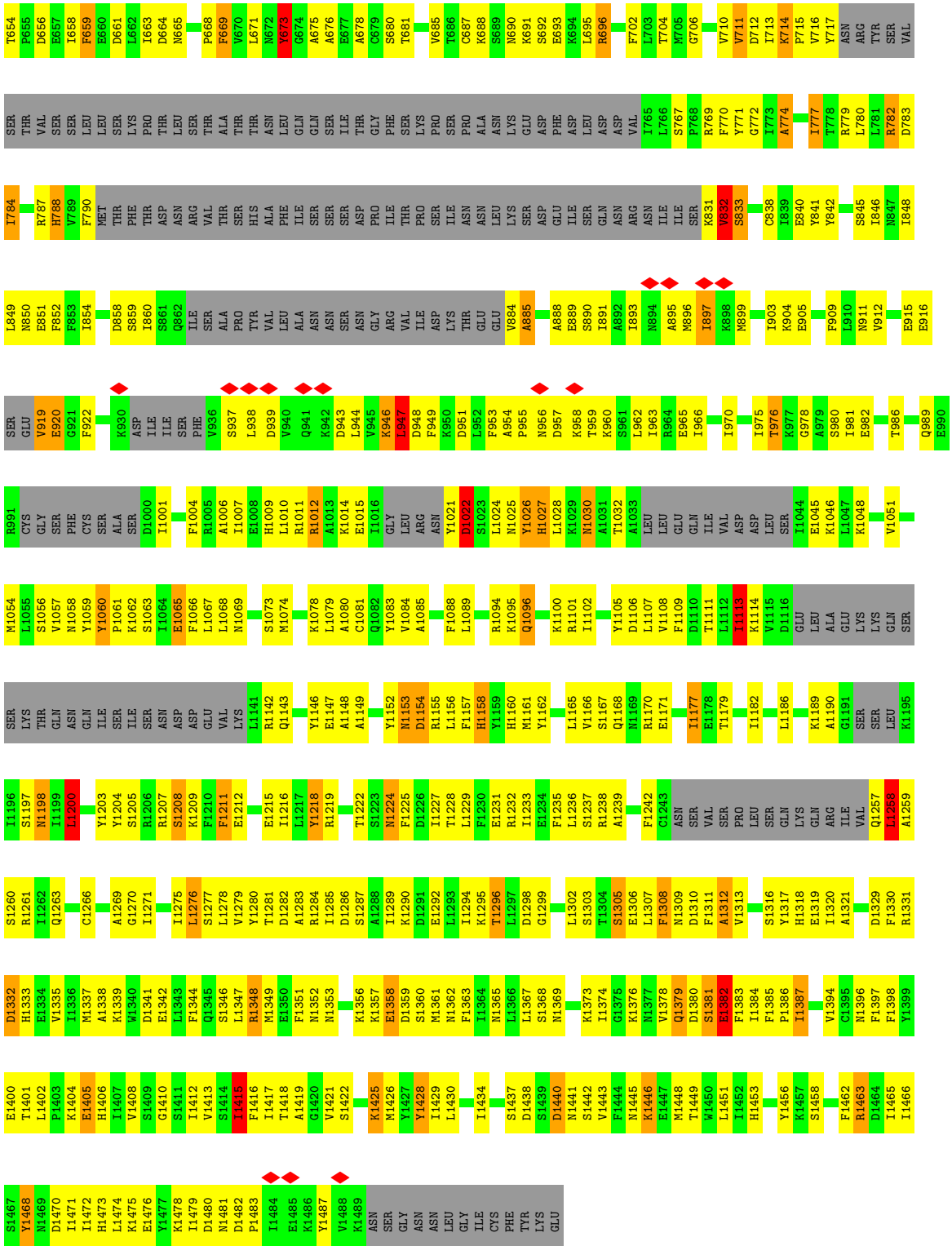
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nucleoporin NUP170

Chain 0:

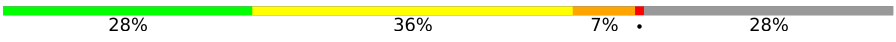


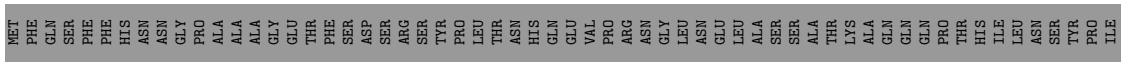



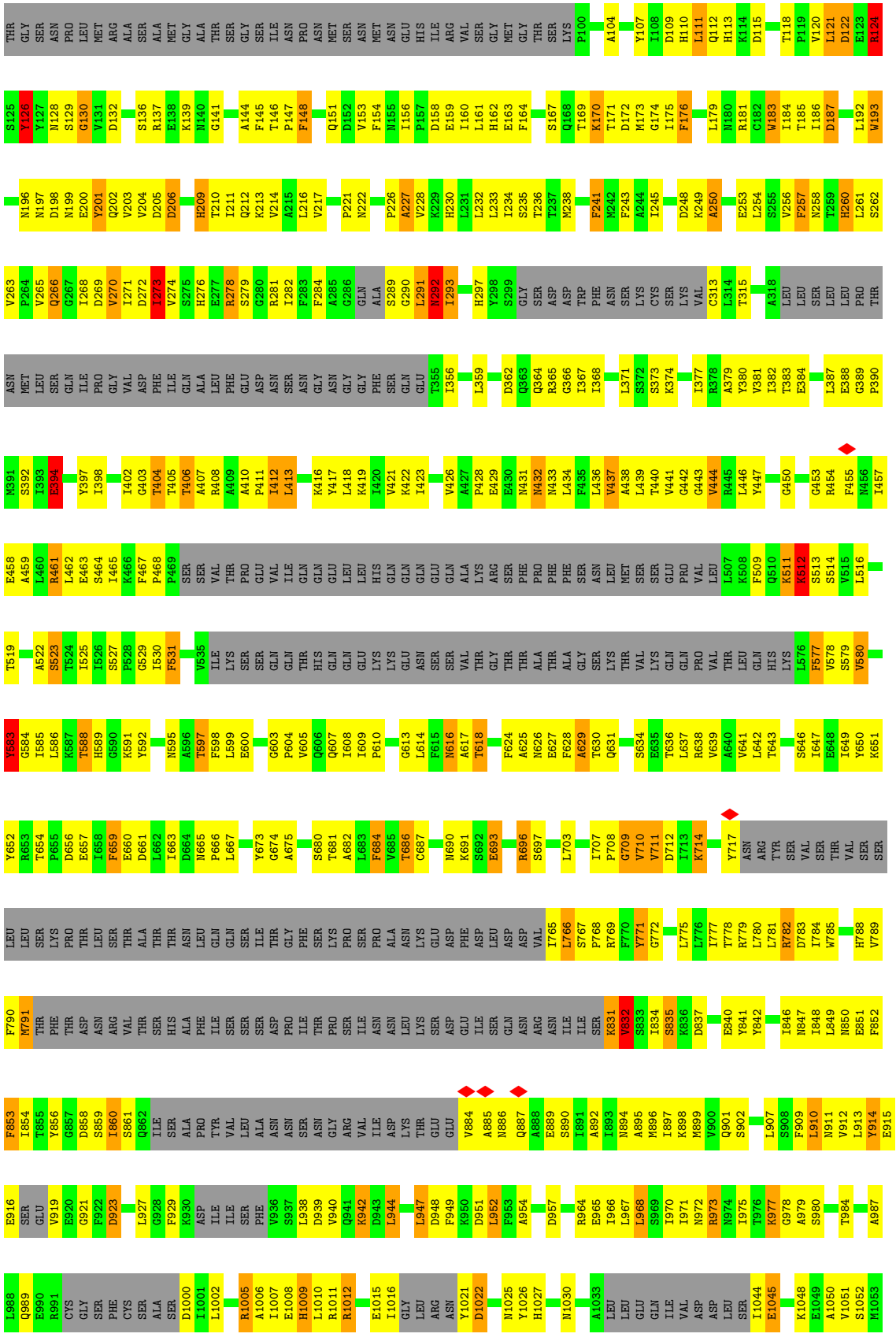


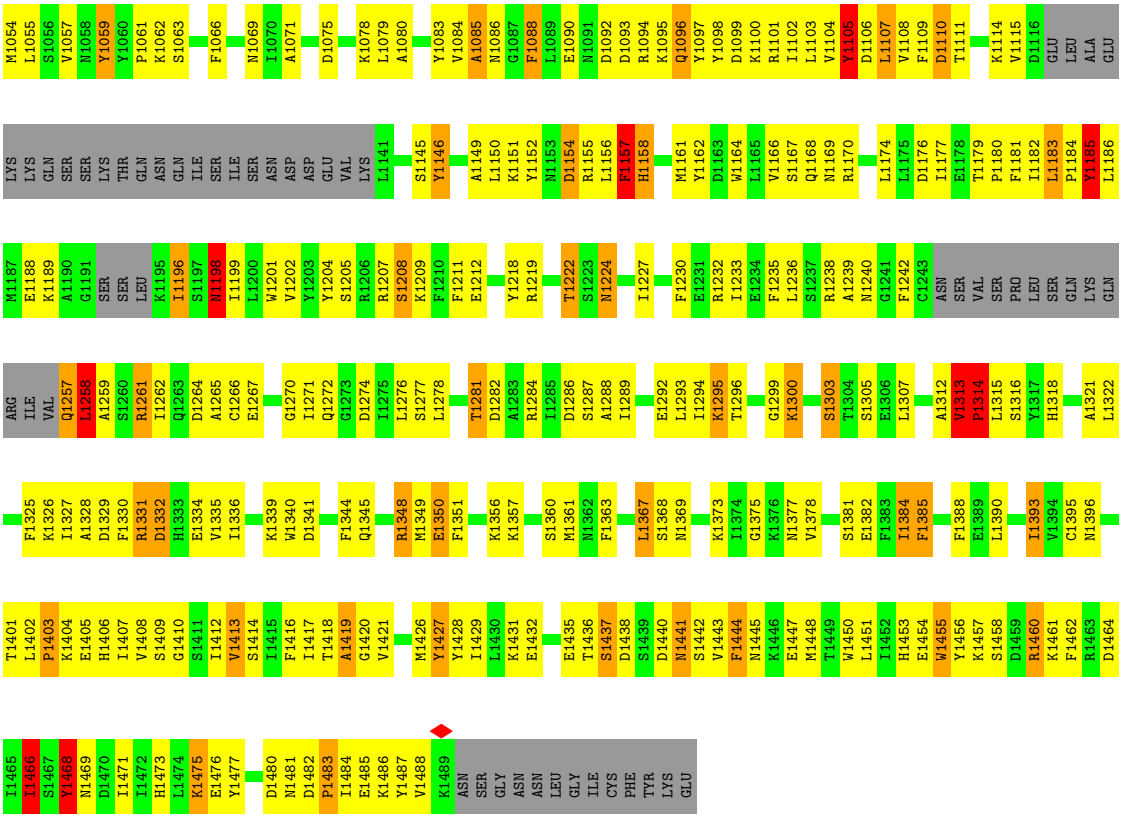
• Molecule 1: Nucleoporin NUP170

Chain Y:



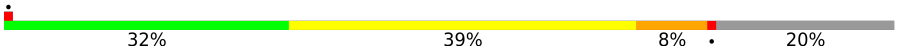



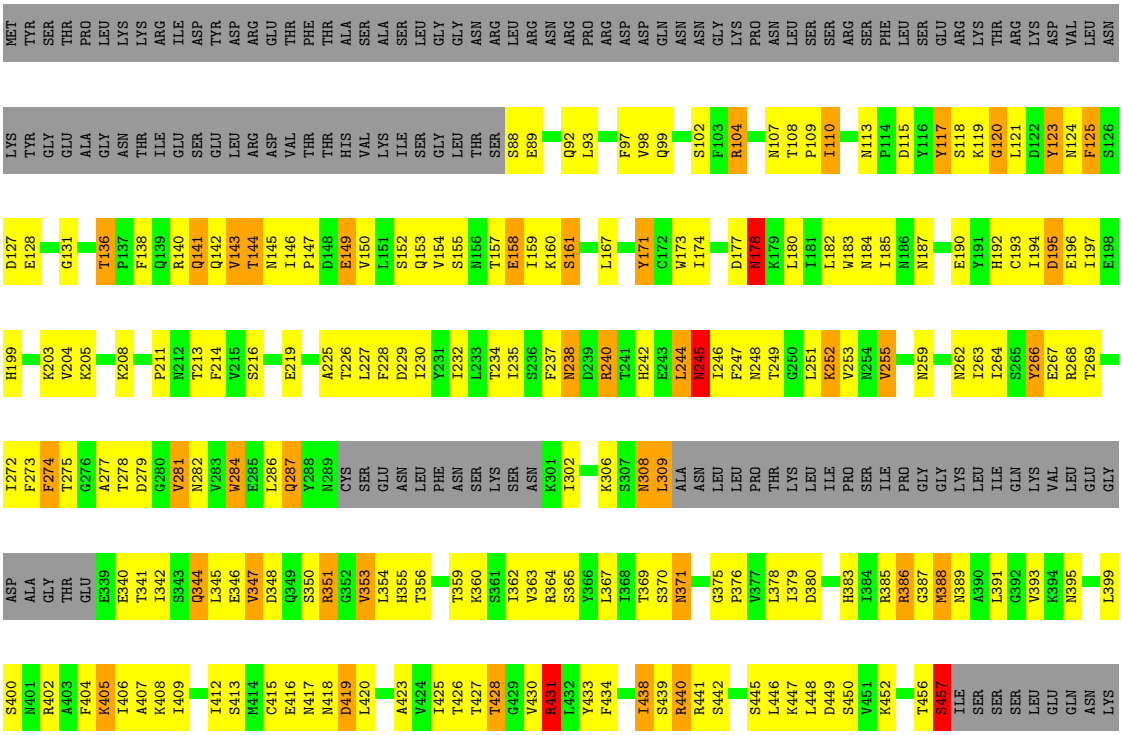


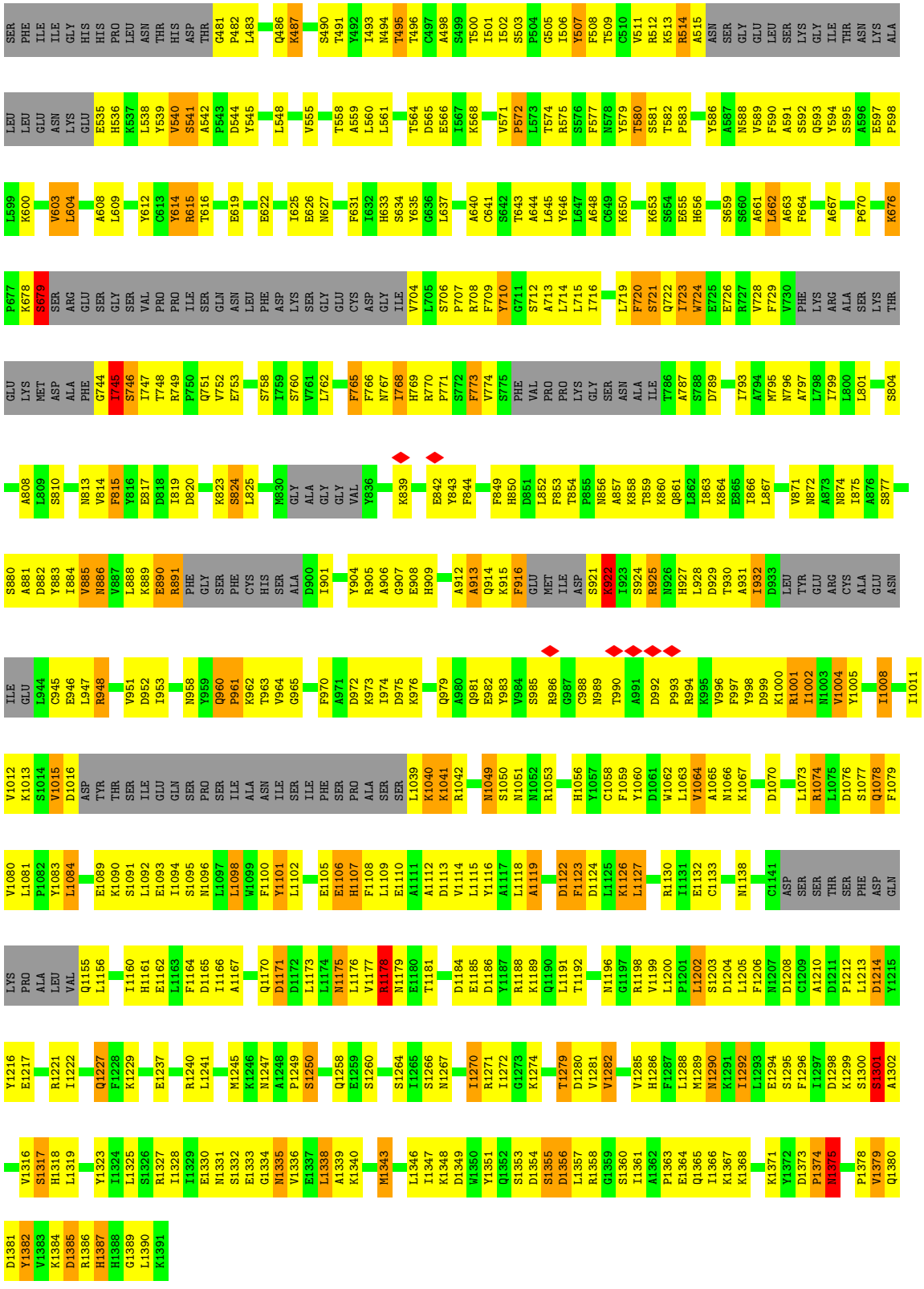


• Molecule 2: Nucleoporin NUP157

Chain 1:

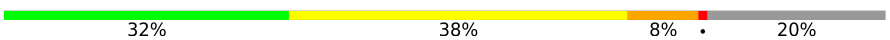


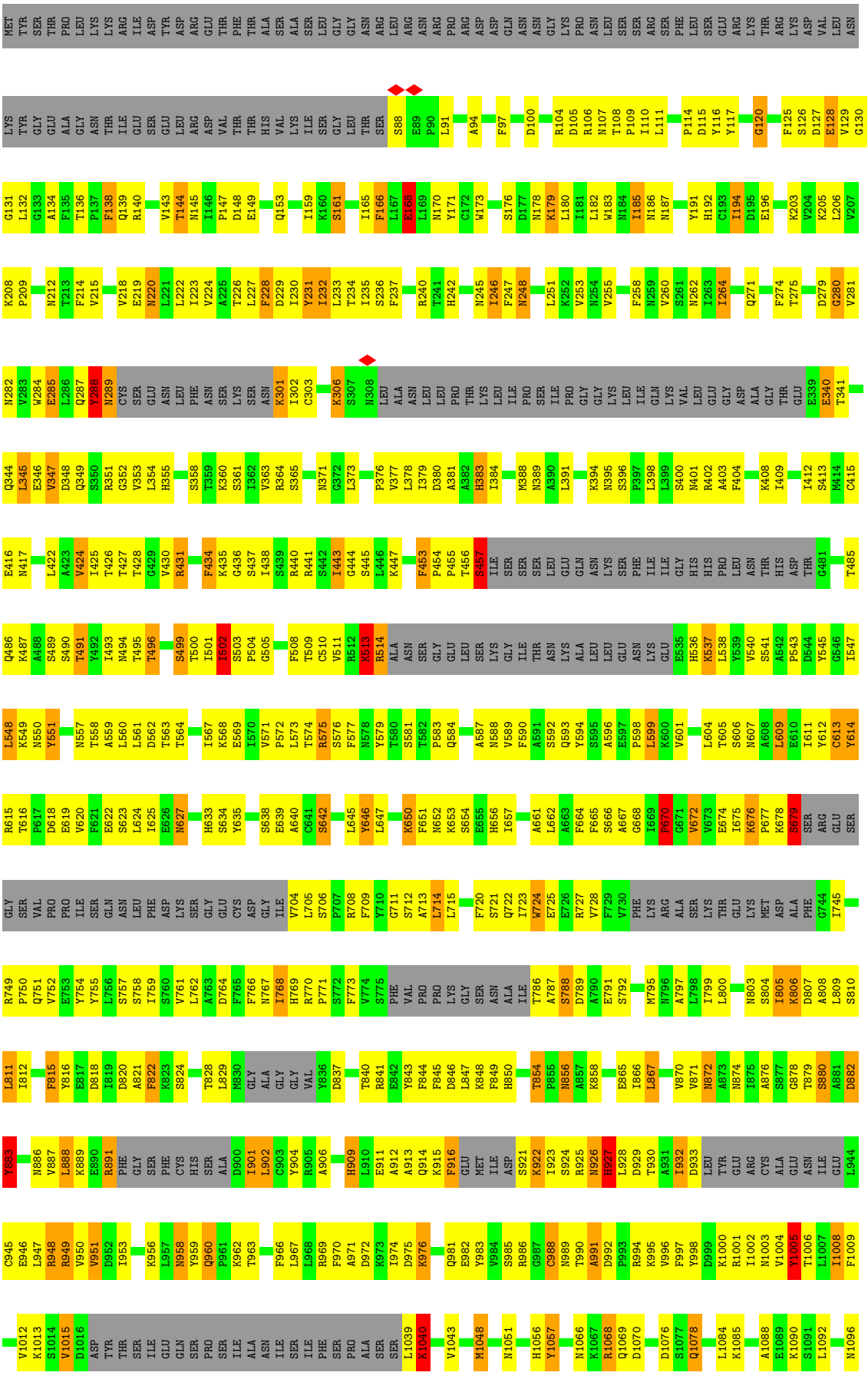



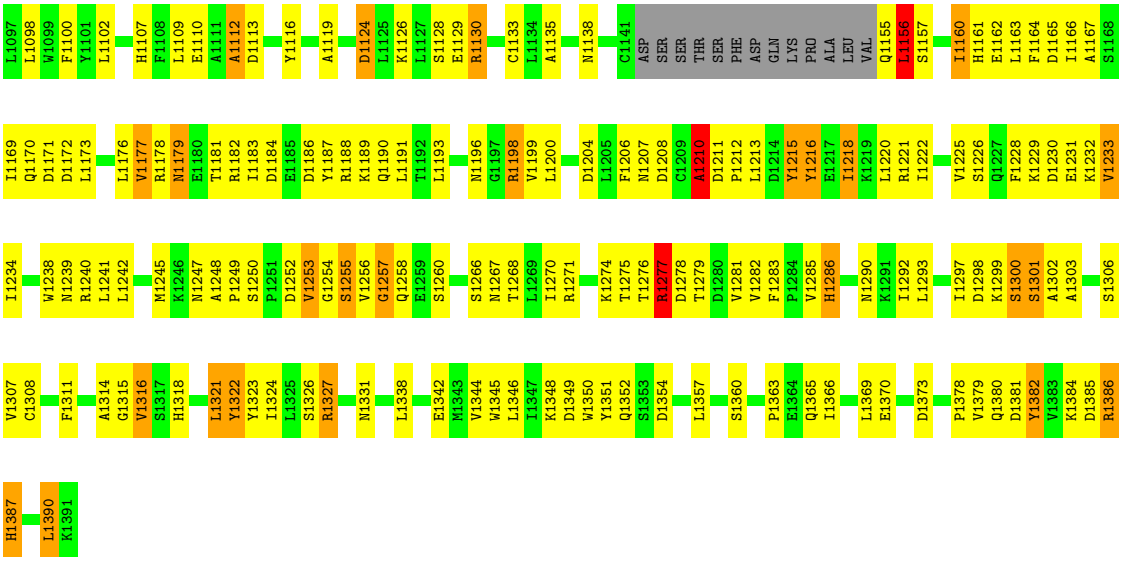


• Molecule 2: Nucleoporin NUP157

Chain Z:

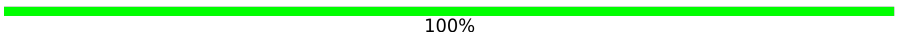







• Molecule 3: orphans bound to Nup192 NTD

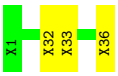
Chain 5:




There are no outlier residues recorded for this chain.

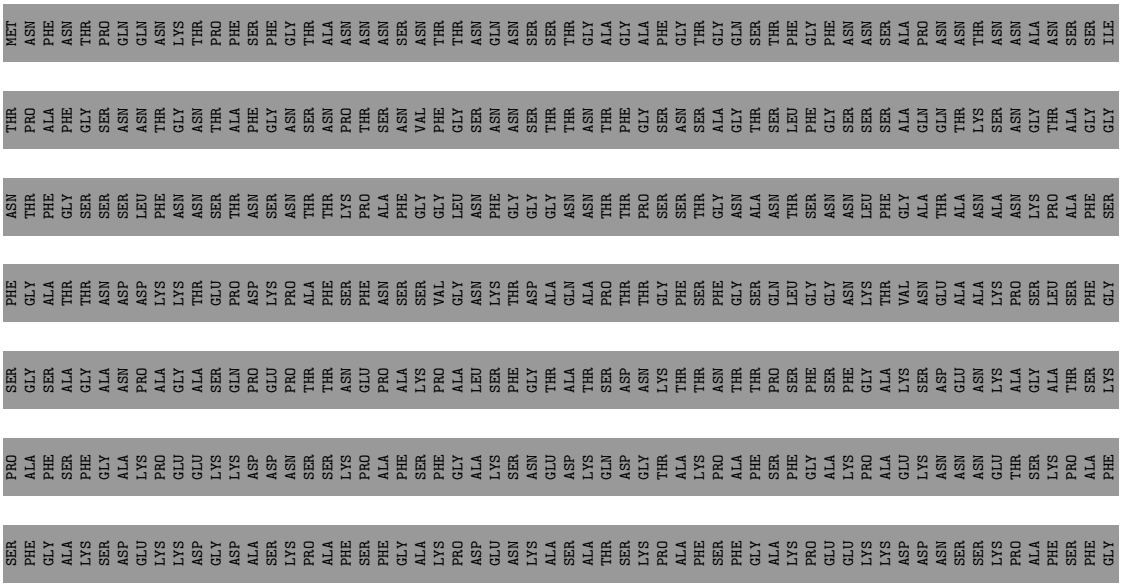
• Molecule 3: orphans bound to Nup192 NTD

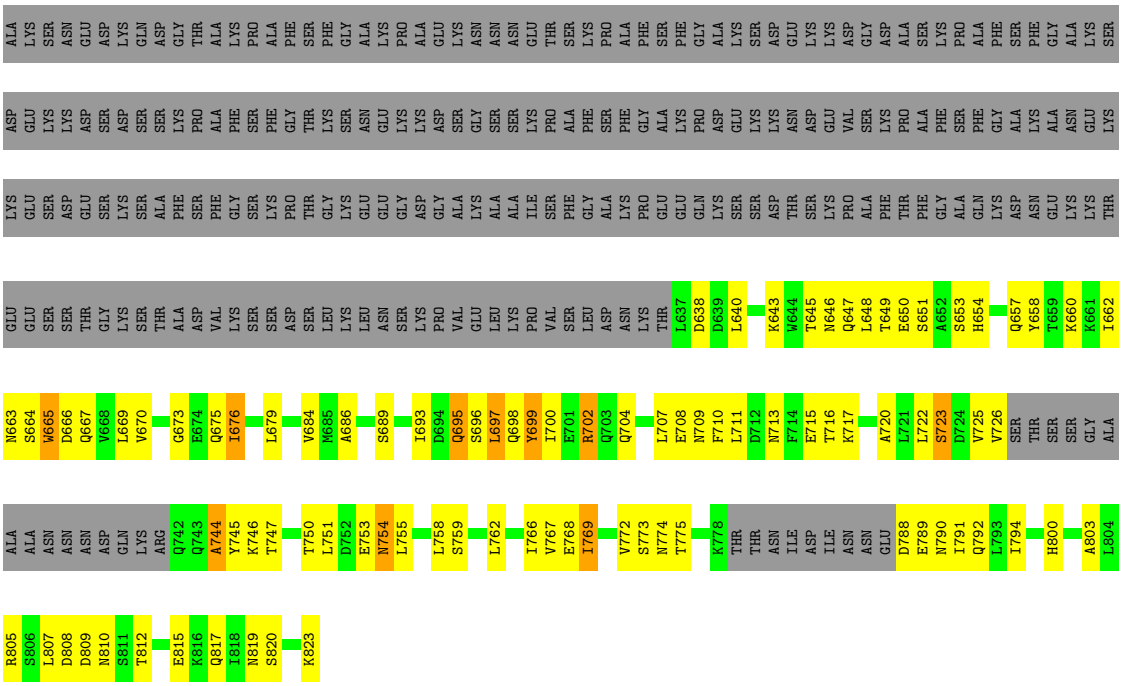
Chain 6:




• Molecule 4: Nucleoporin NSP1

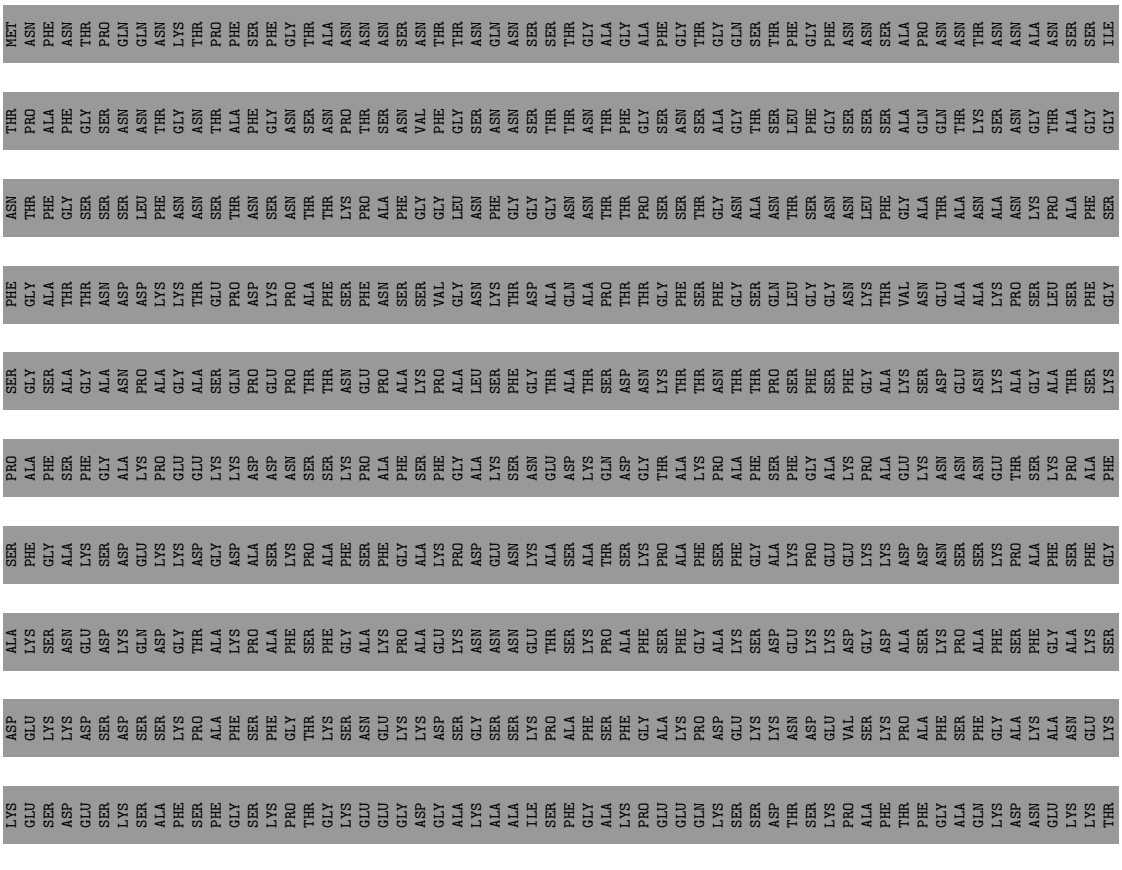
Chain A:

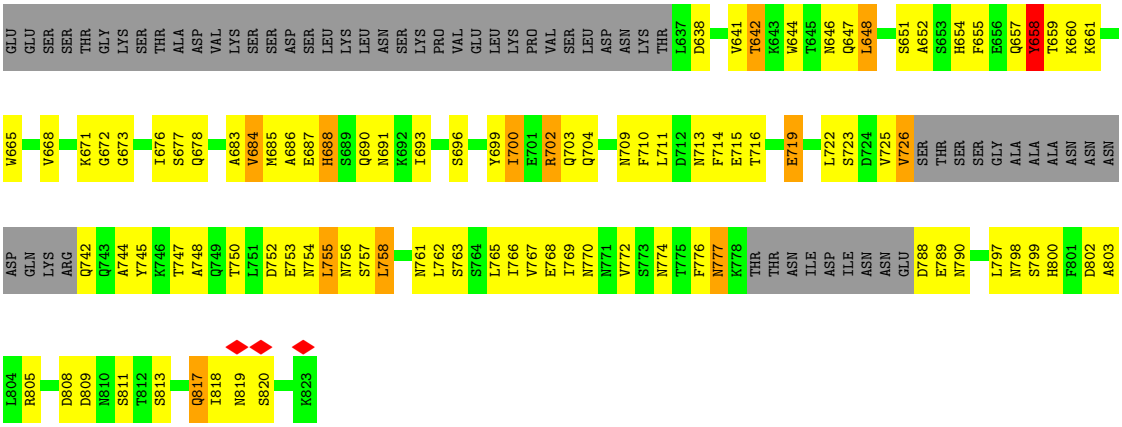





• Molecule 4: Nucleoporin NSP1

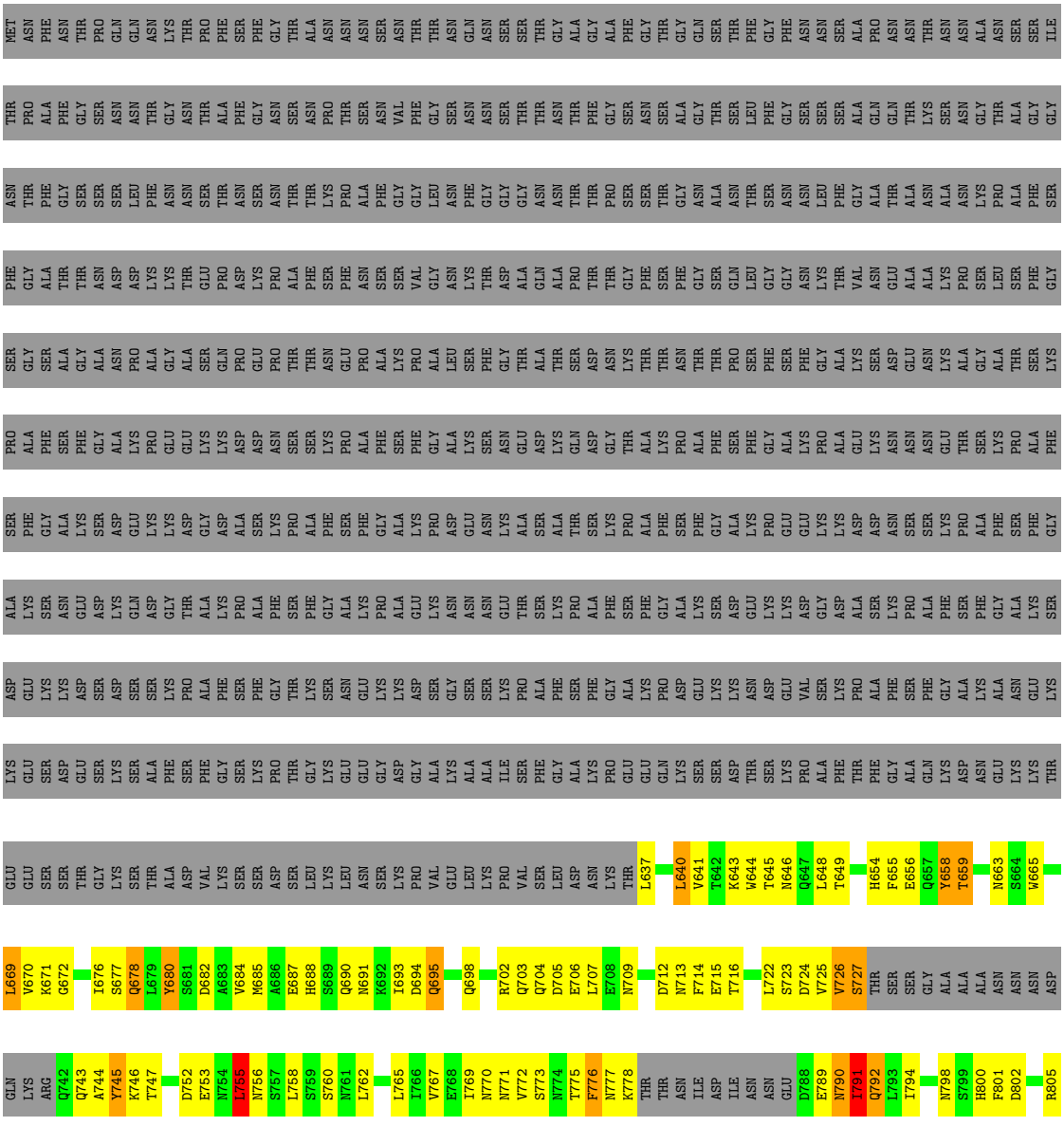
Chain D:





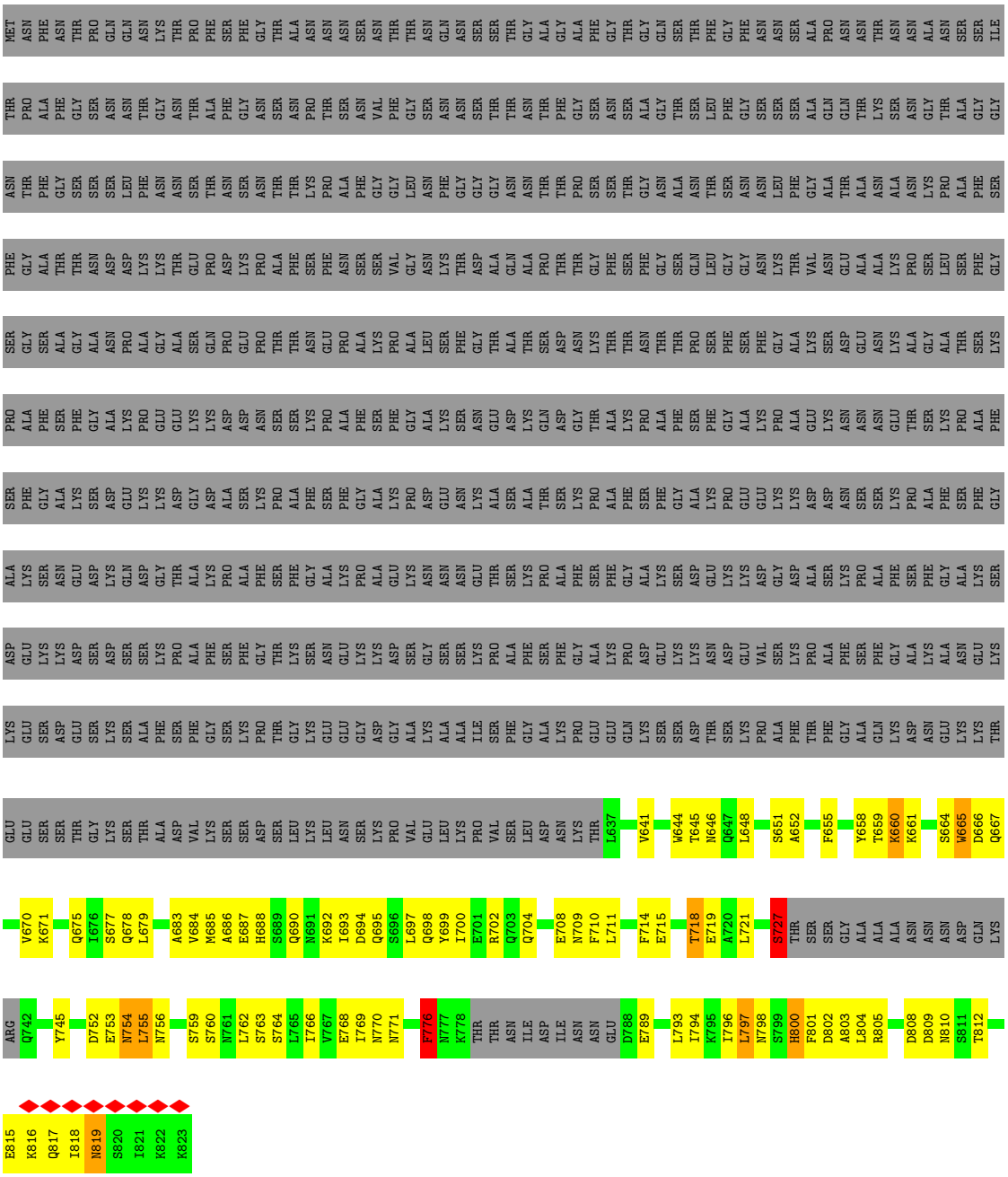
• Molecule 4: Nucleoporin NSP1

Chain G: 8% 9% 80%



• Molecule 4: Nucleoporin NSP1

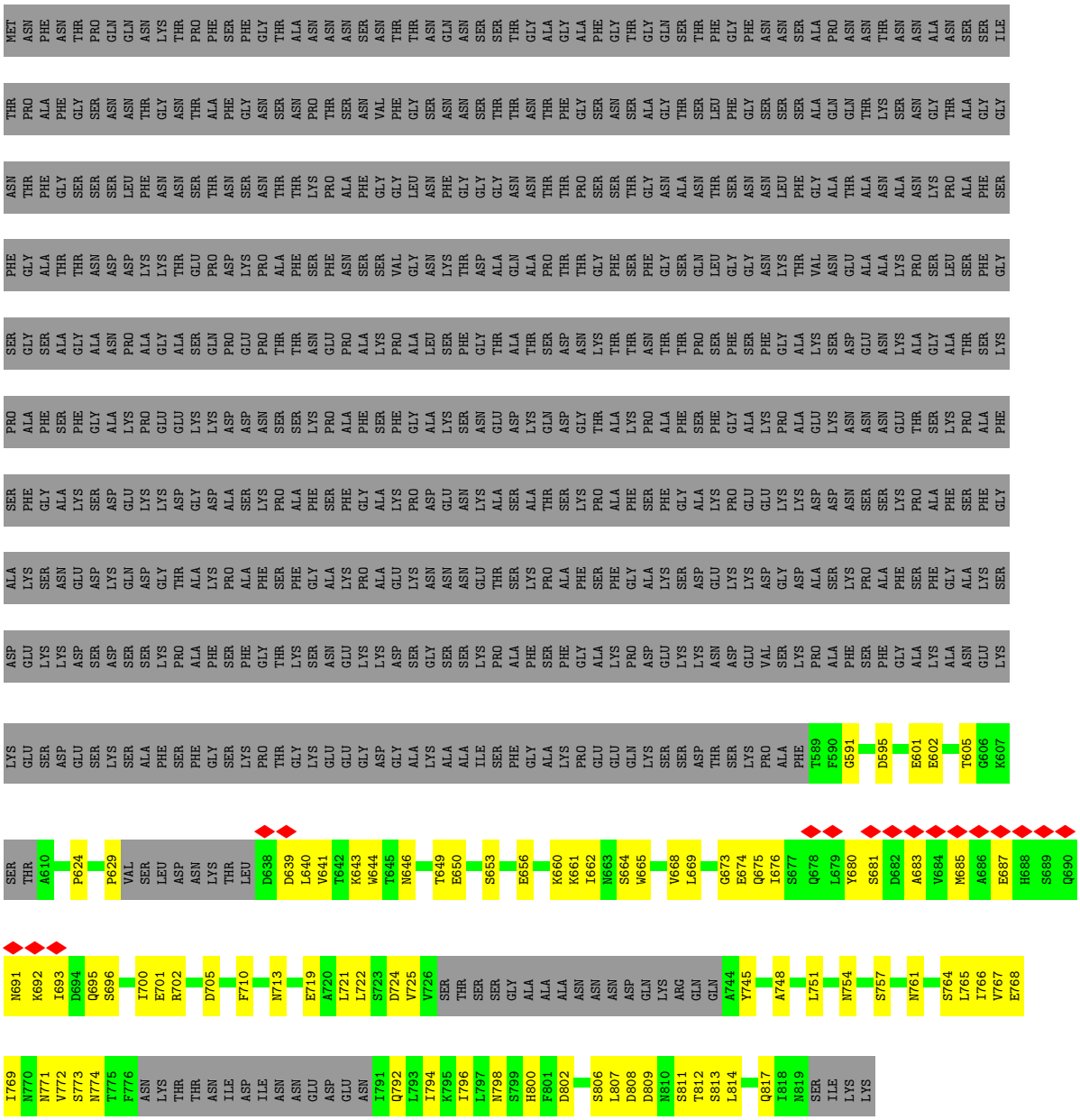
Chain J:





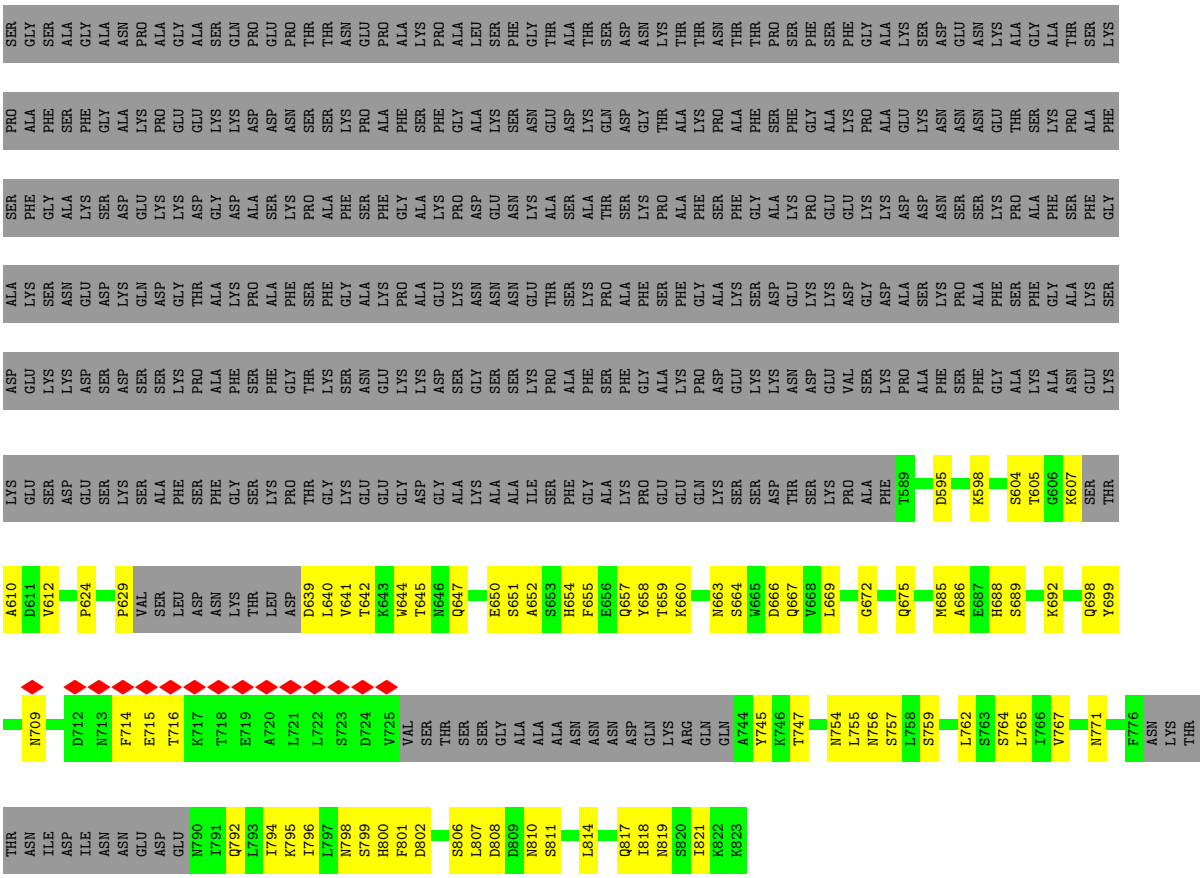

• Molecule 4: Nucleoporin NSP1

Chain y:



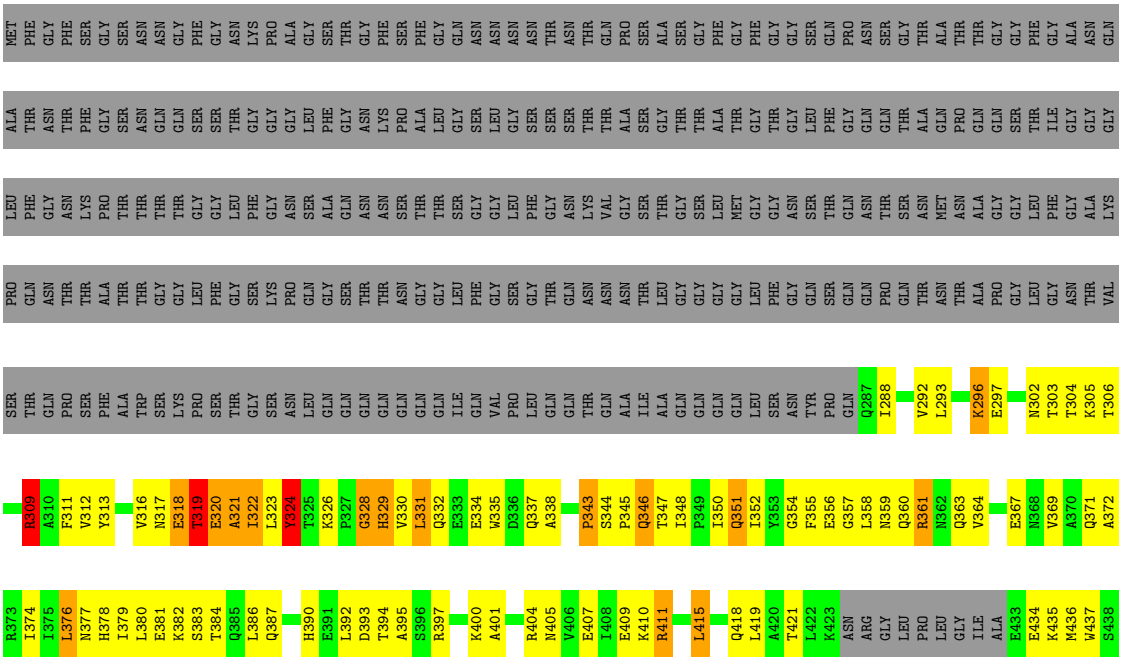
• Molecule 4: Nucleoporin NSP1

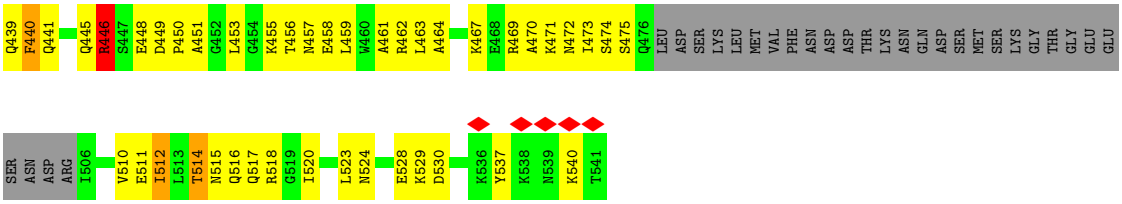
Chain z:



• Molecule 5: Nucleoporin NUP57

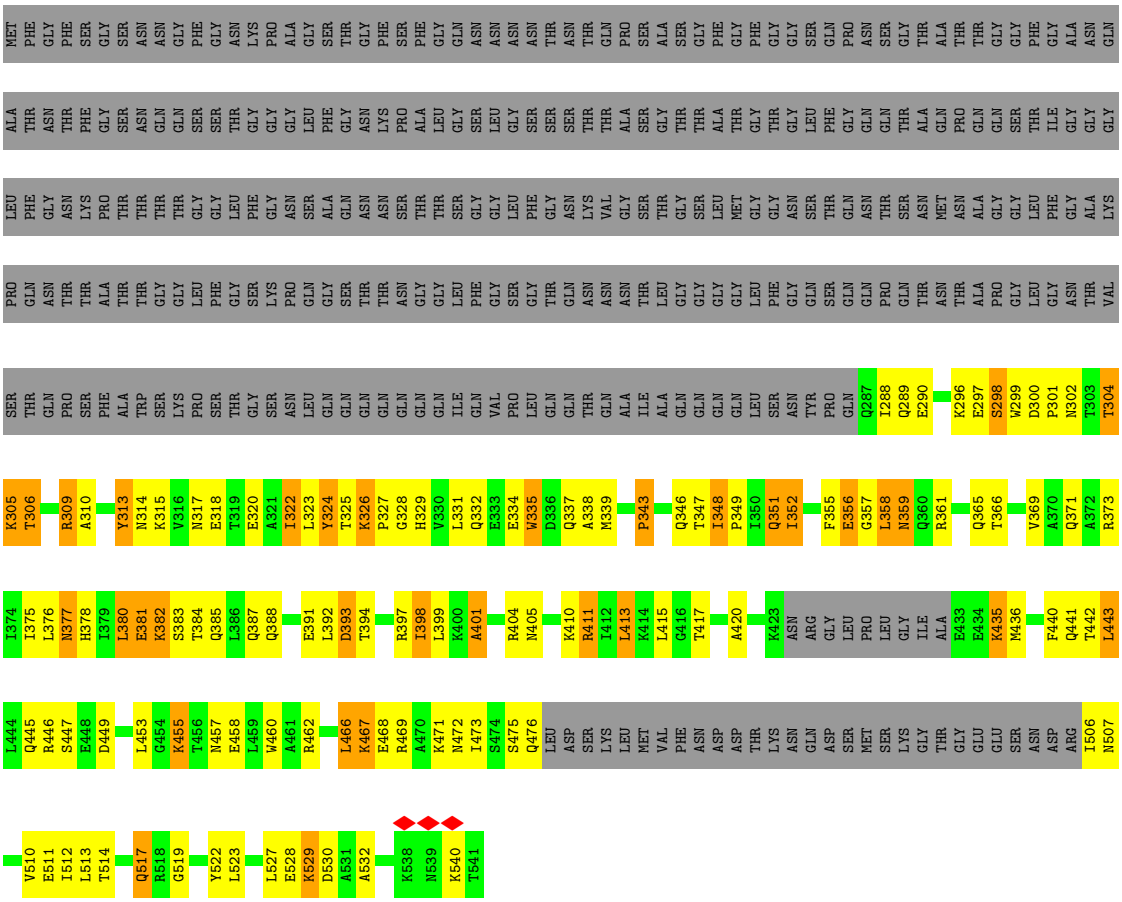
Chain B:





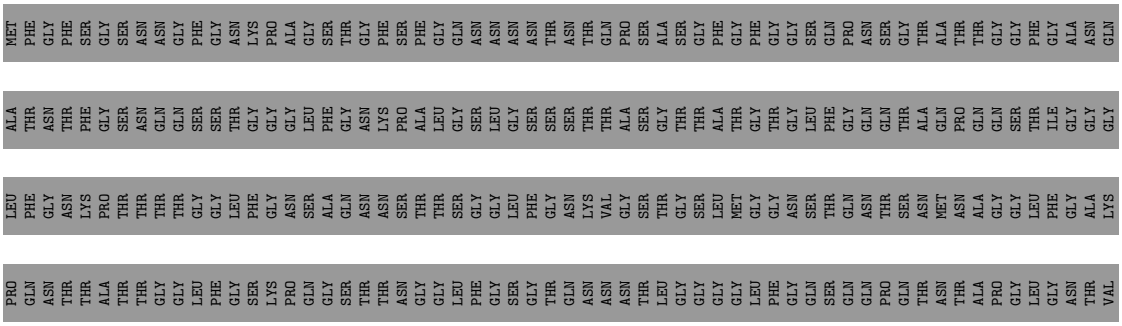

• Molecule 5: Nucleoporin NUP57

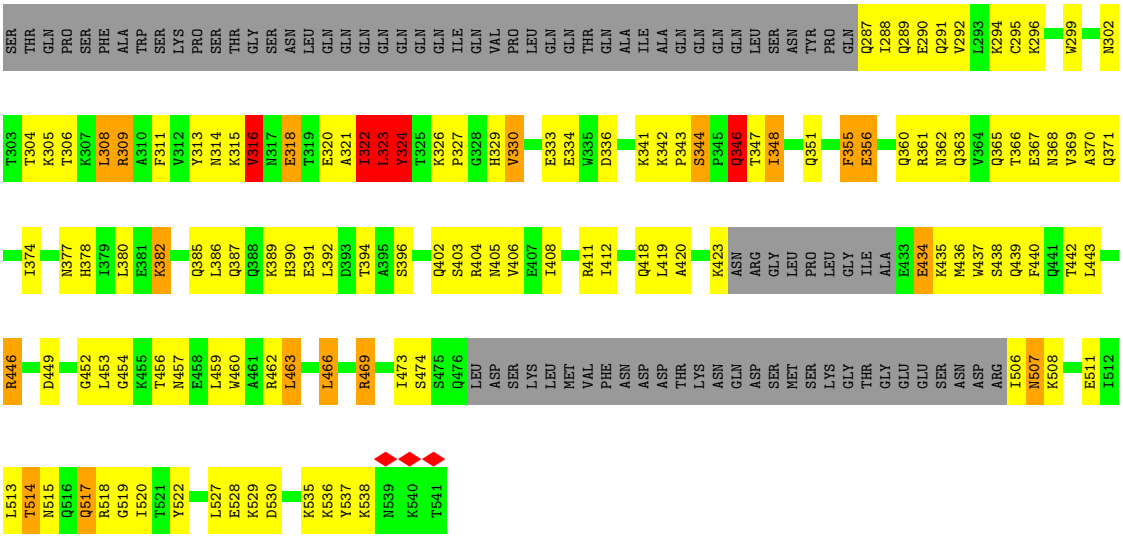
Chain E:




• Molecule 5: Nucleoporin NUP57

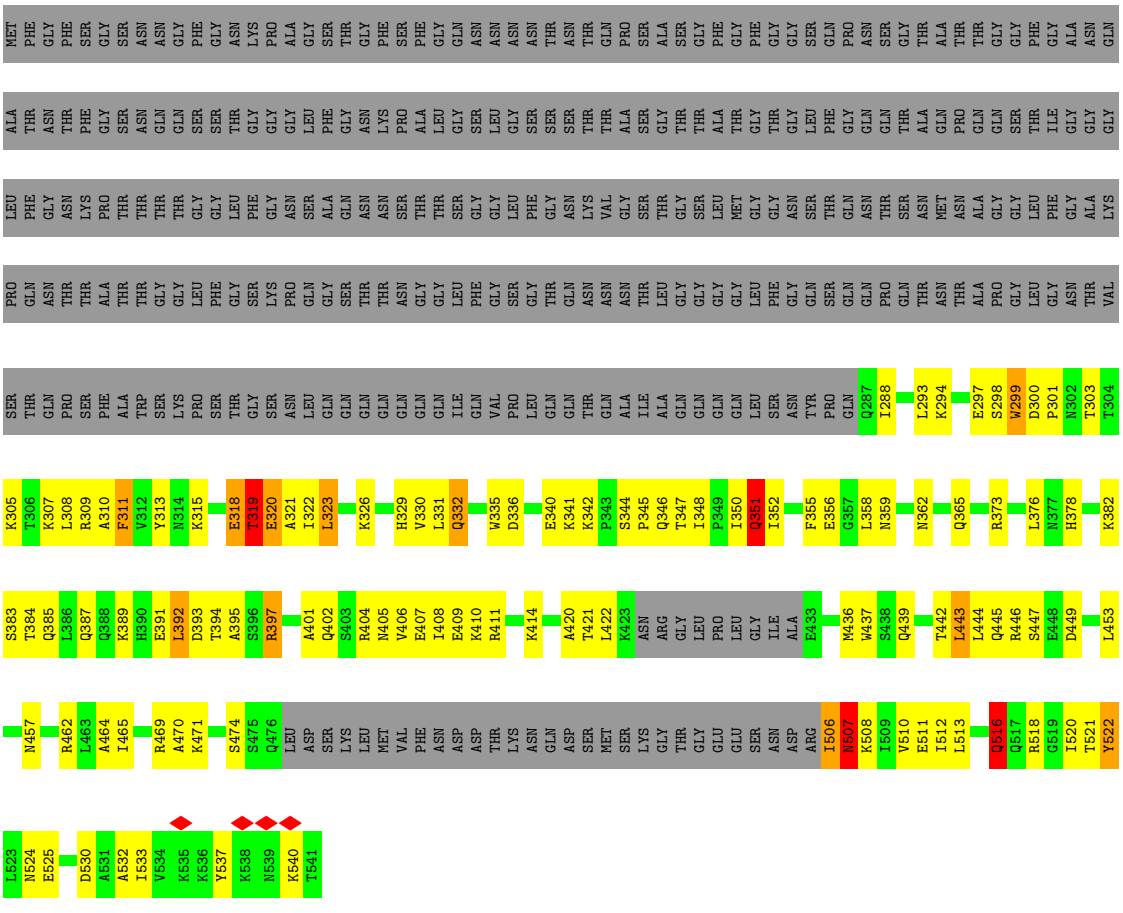
Chain H:





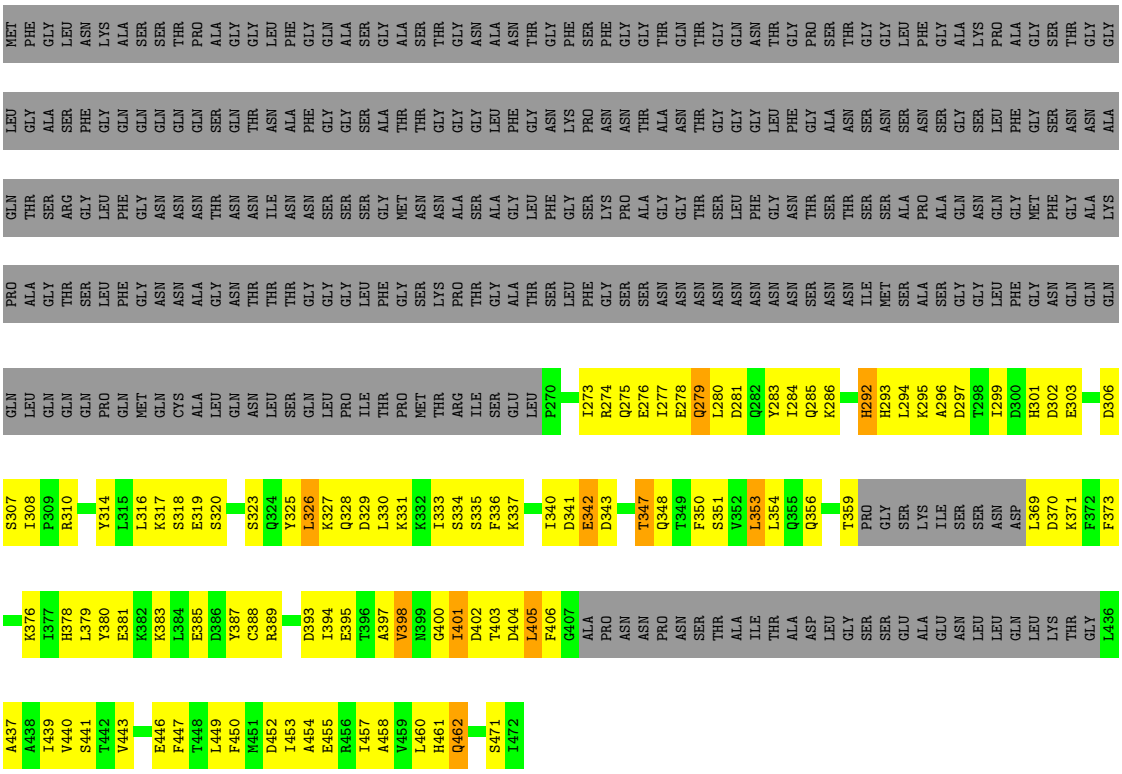
• Molecule 5: Nucleoporin NUP57

Chain K:



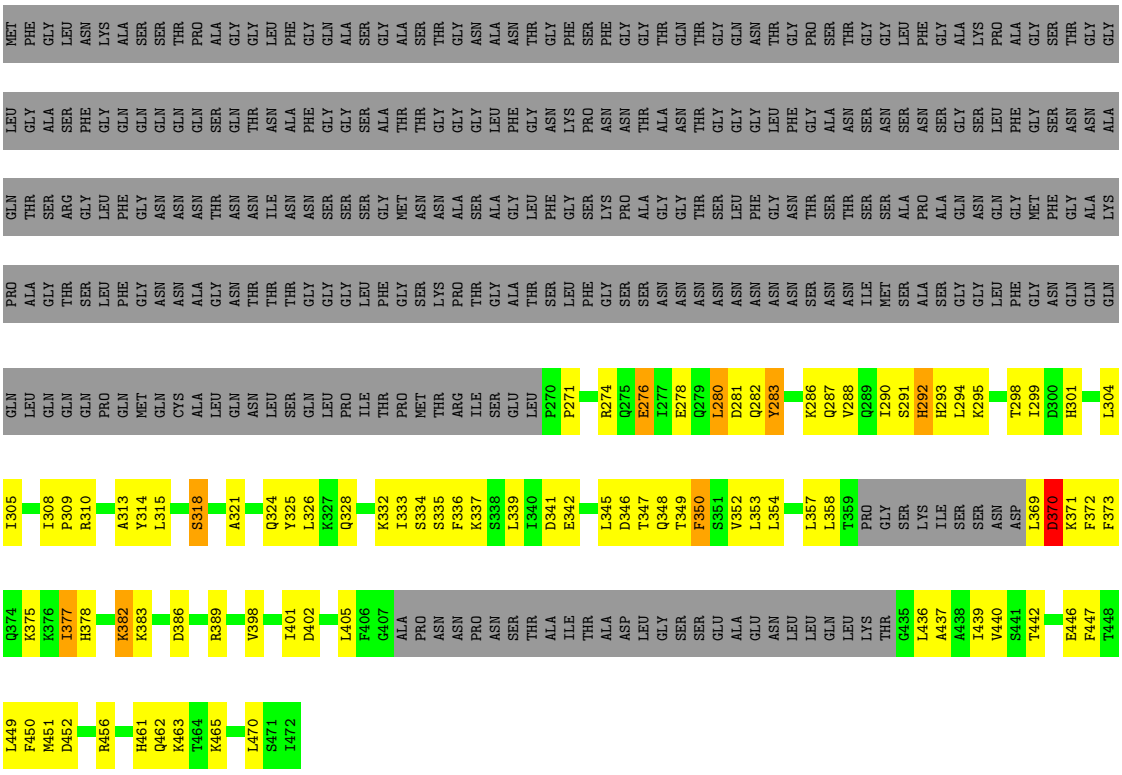
• Molecule 6: Nucleoporin NUP49/NSP49

Chain C:



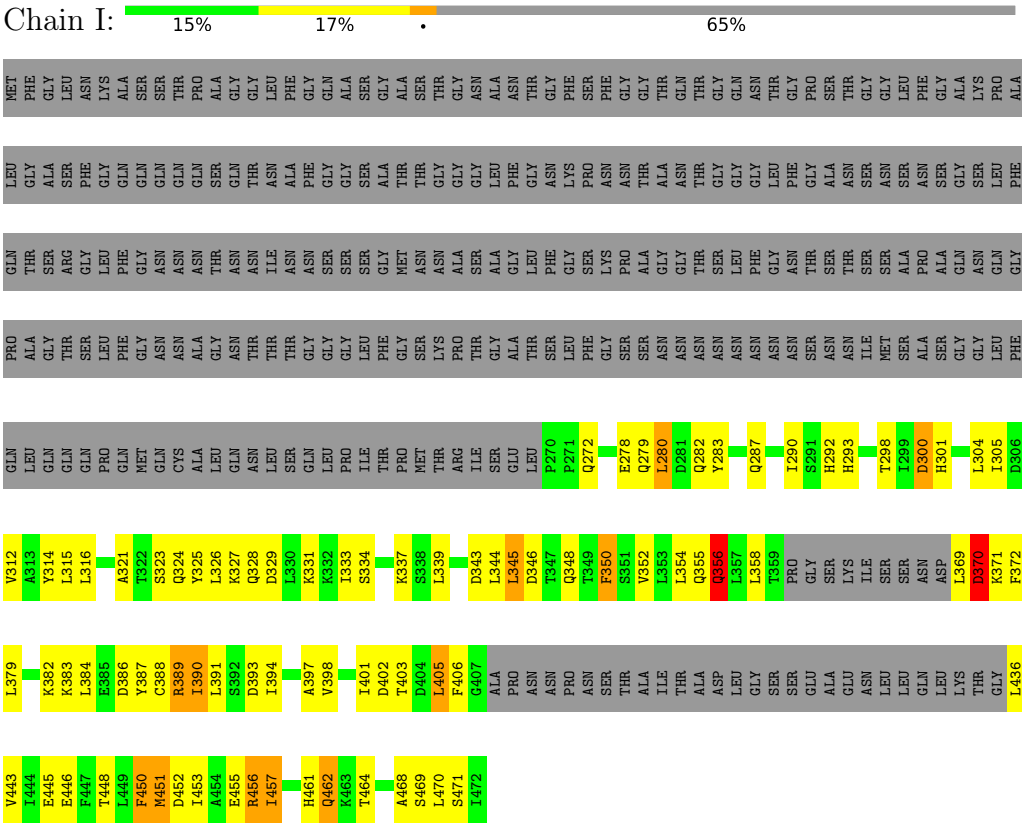
• Molecule 6: Nucleoporin NUP49/NSP49

Chain F:



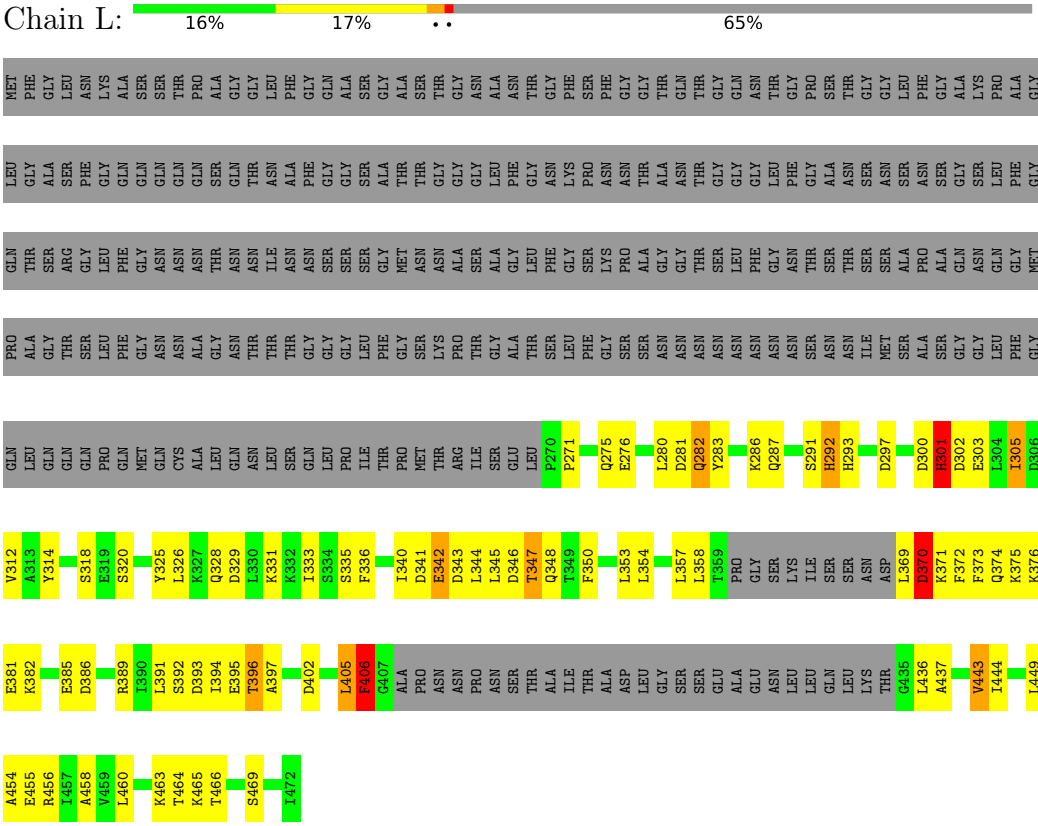
• Molecule 6: Nucleoporin NUP49/NSP49

Chain I:



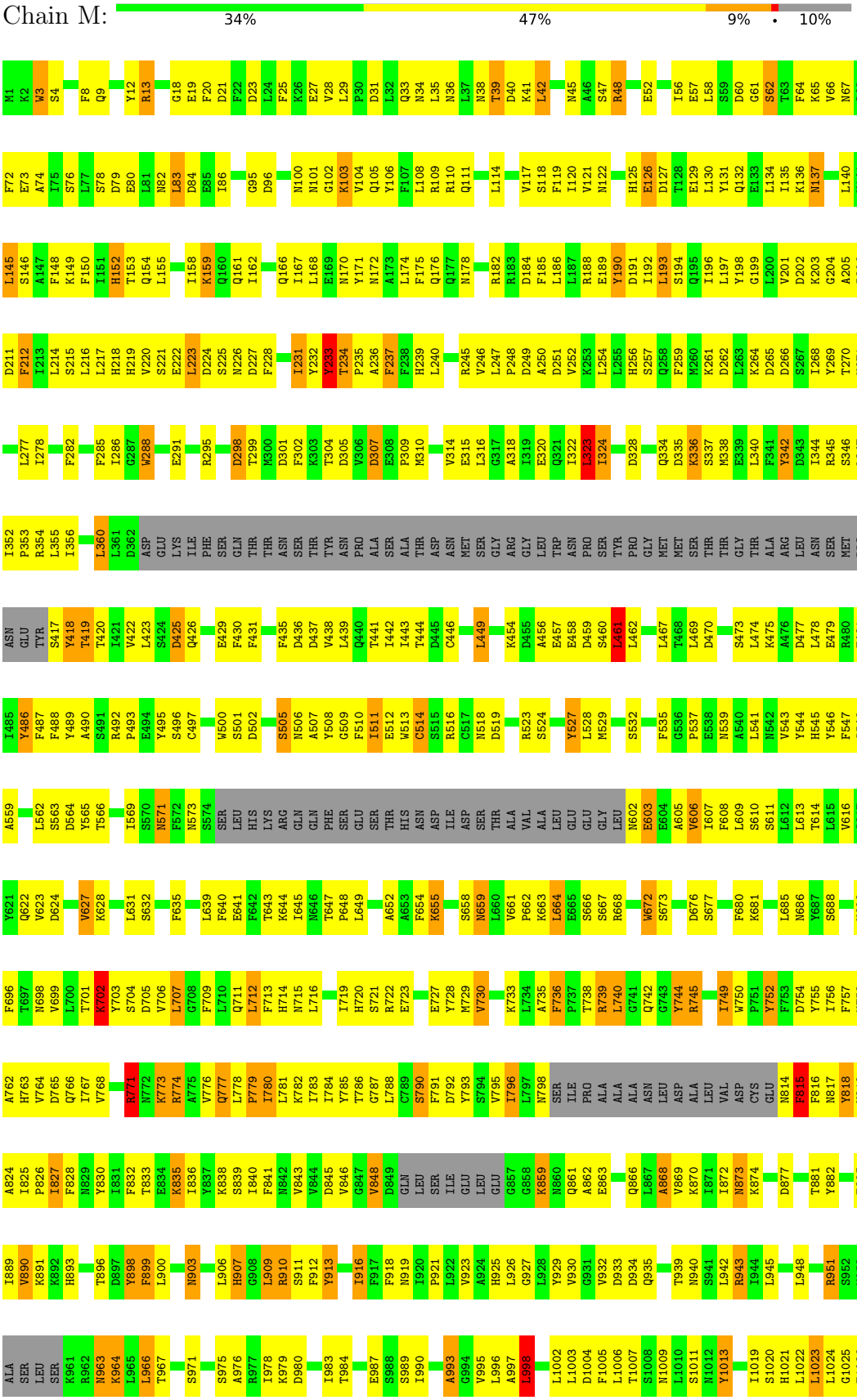

• Molecule 6: Nucleoporin NUP49/NSP49

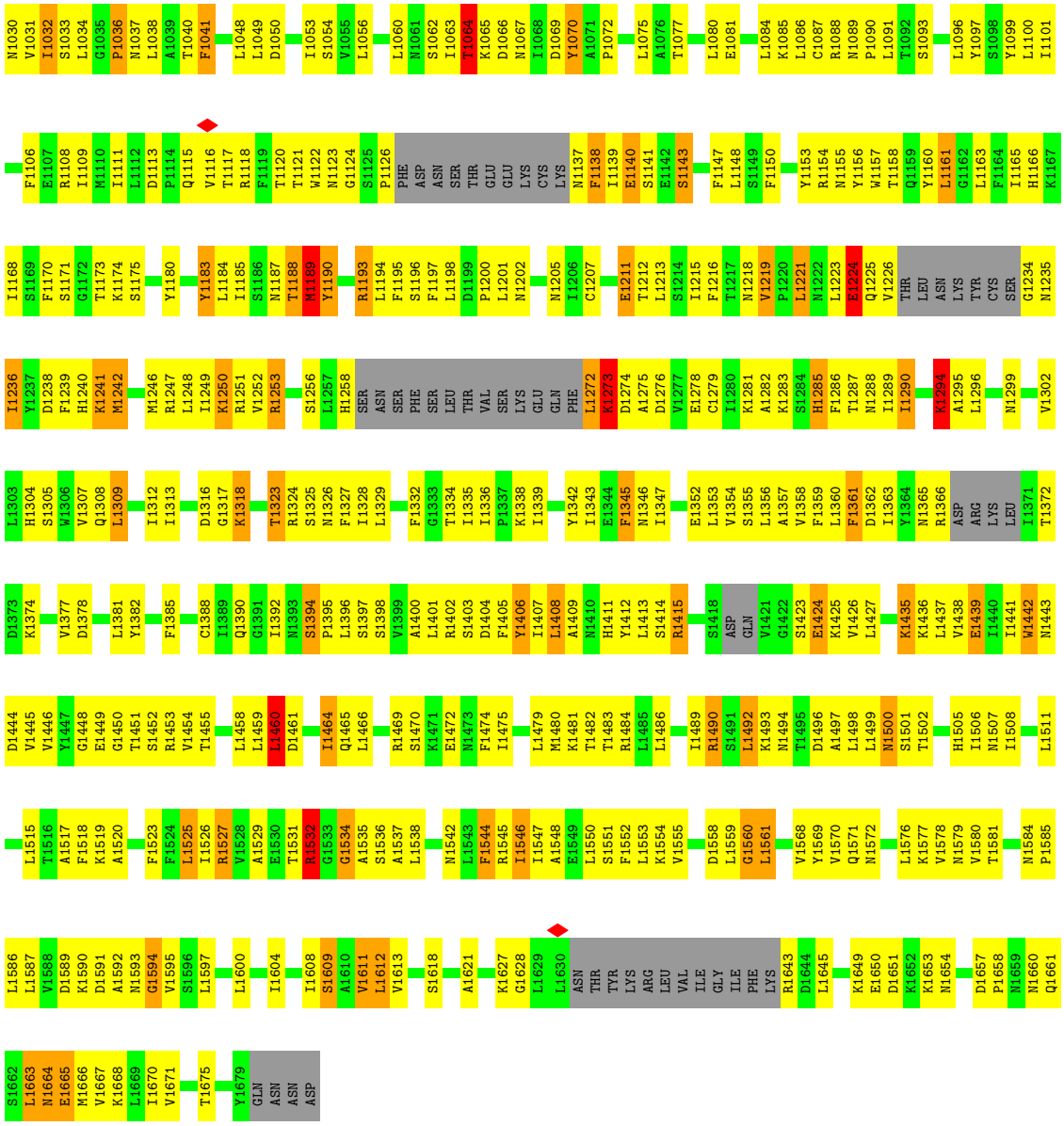
Chain L:



• Molecule 7: Nucleoporin NUP192

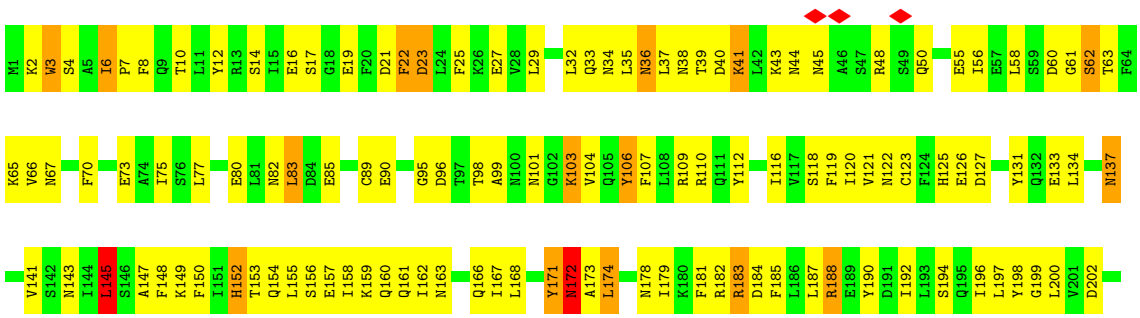
Chain M:

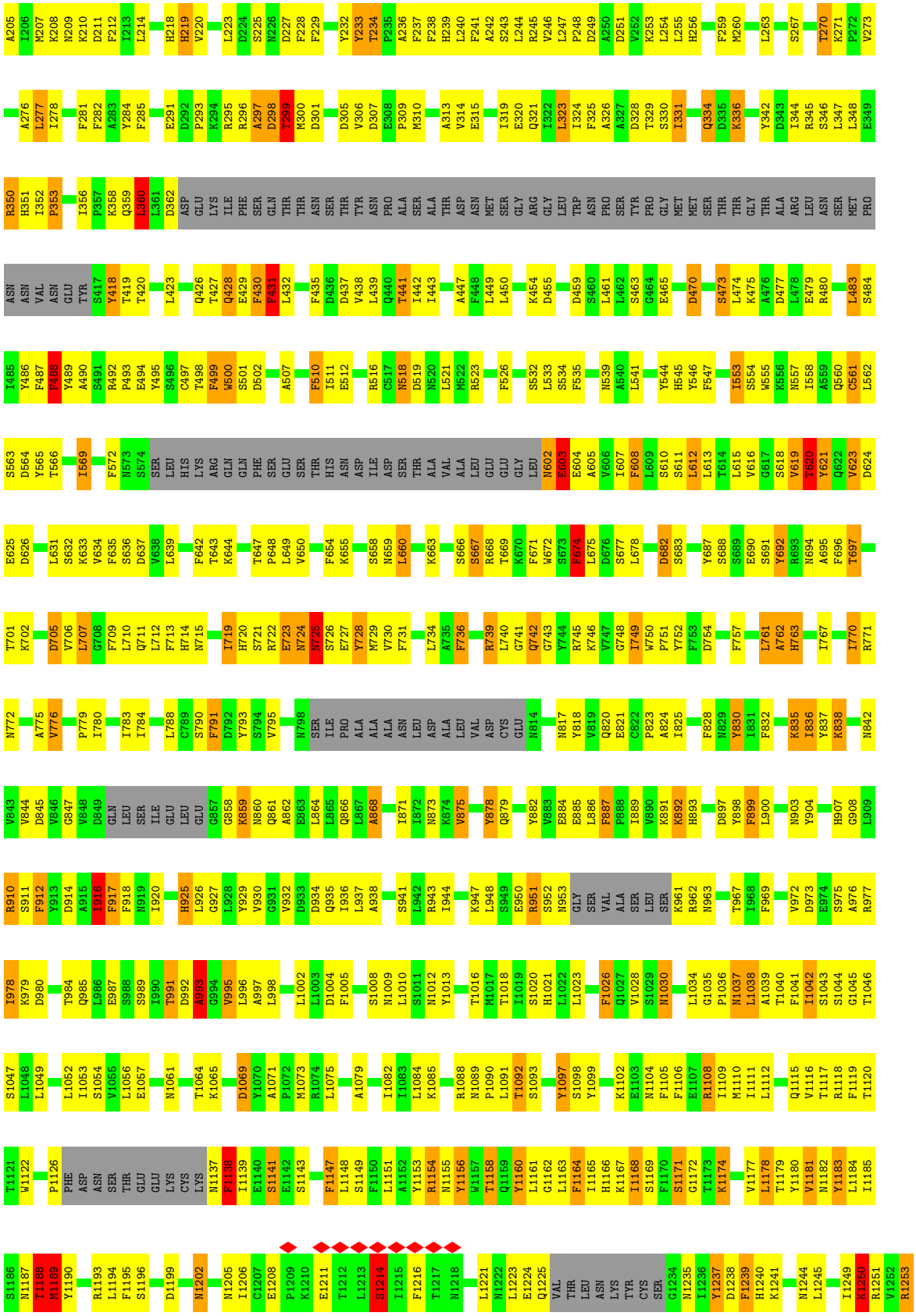


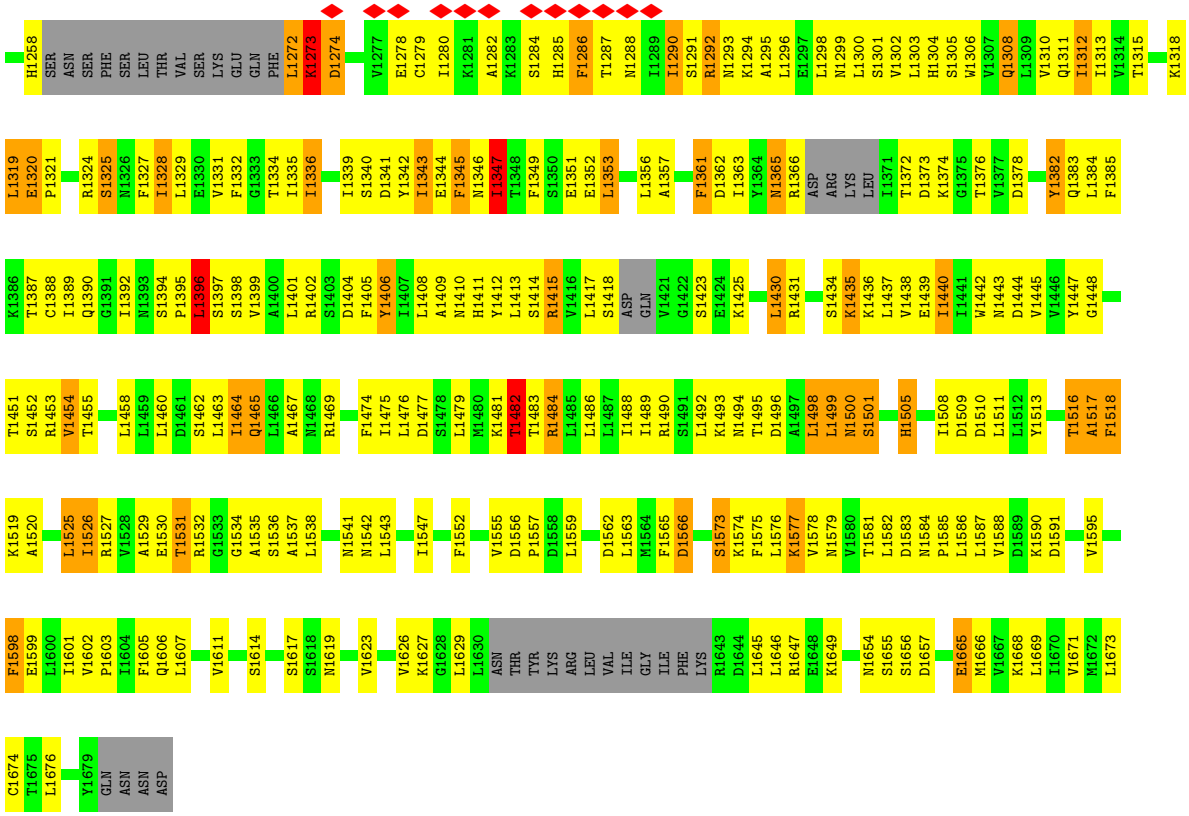


• Molecule 7: Nucleoporin NUP192

Chain O:

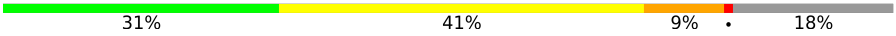


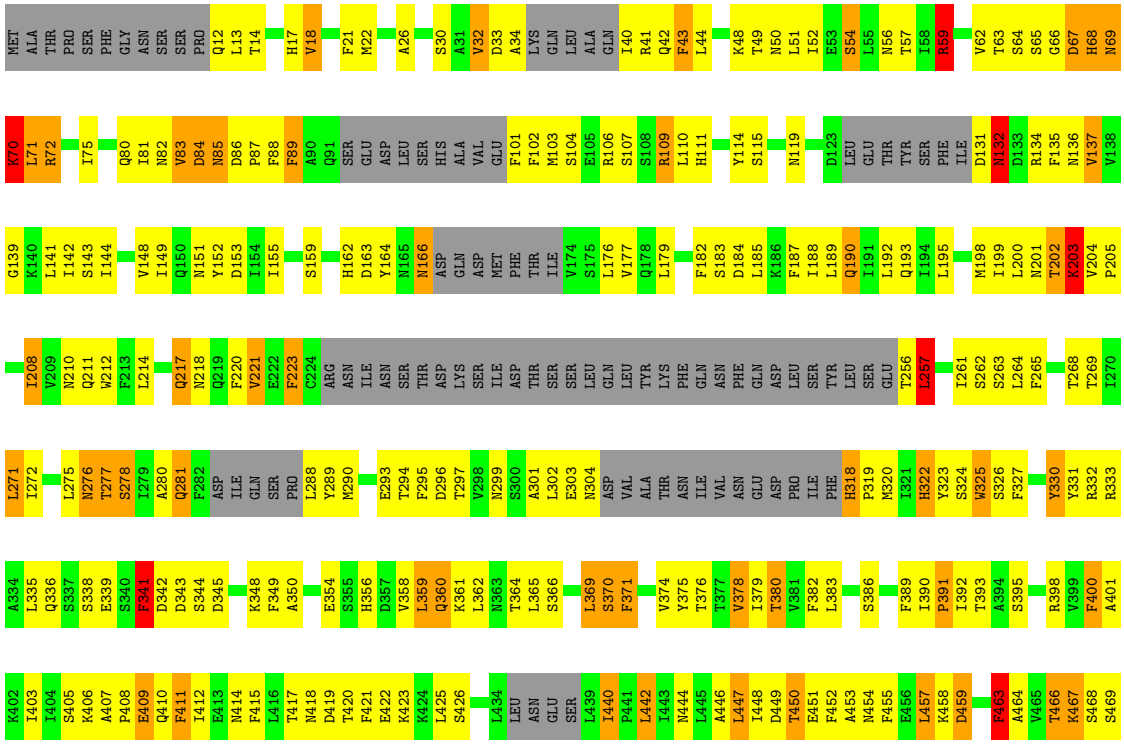


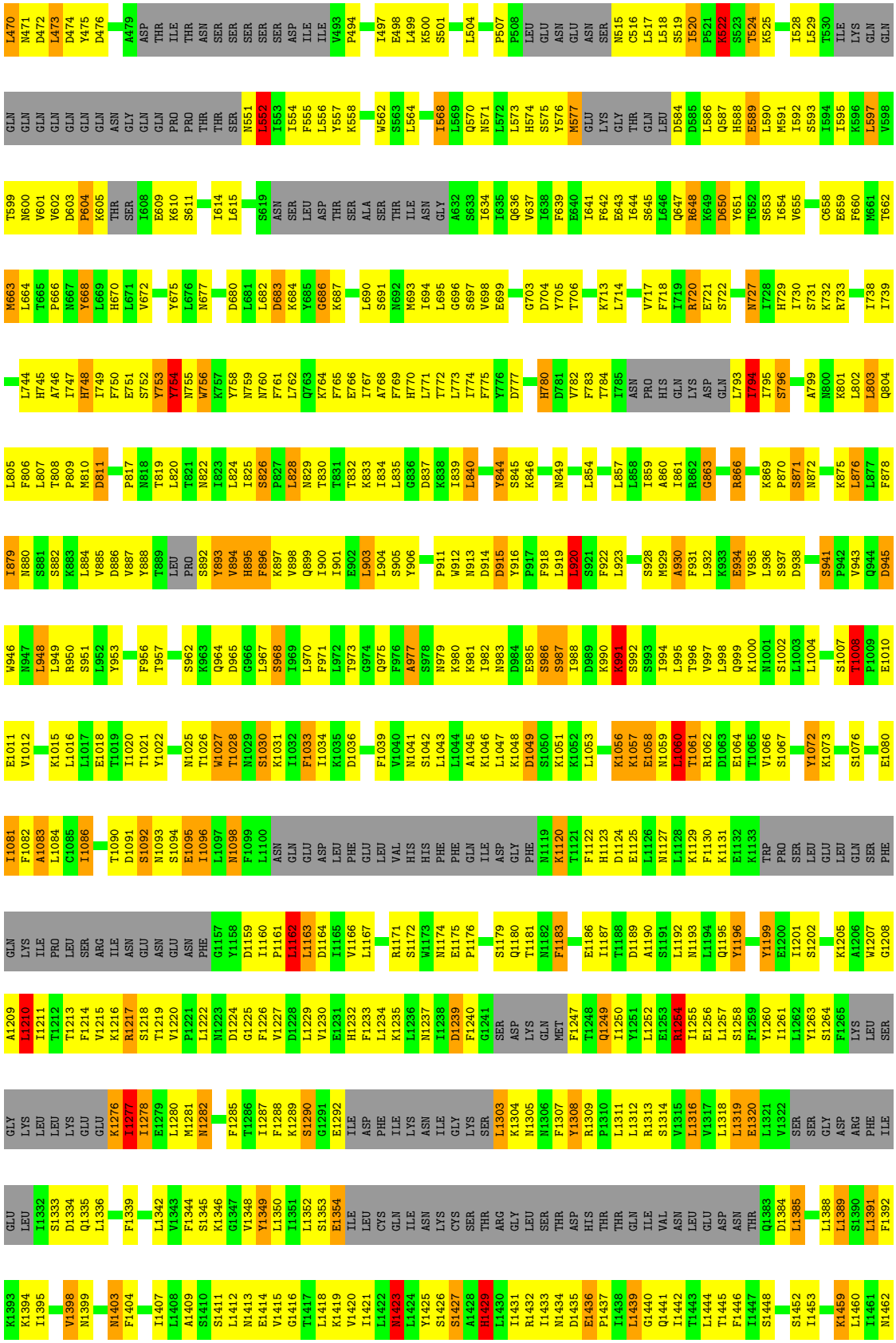


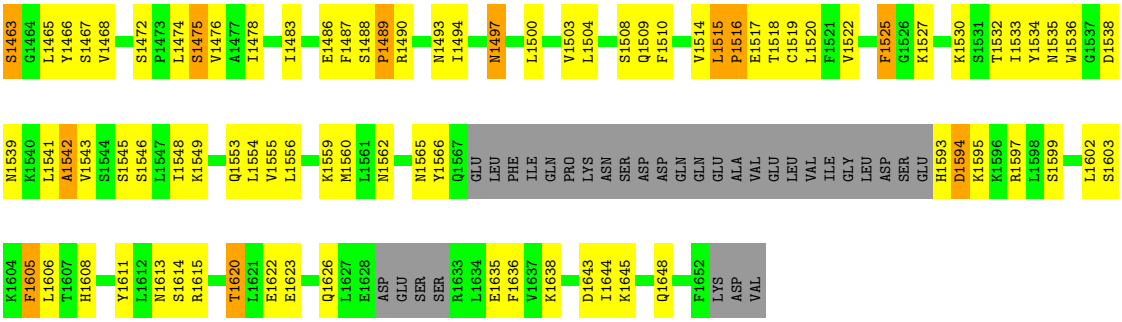
• Molecule 8: Nucleoporin NUP188

Chain N:





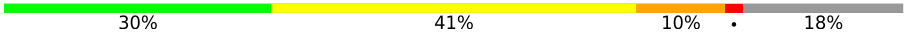


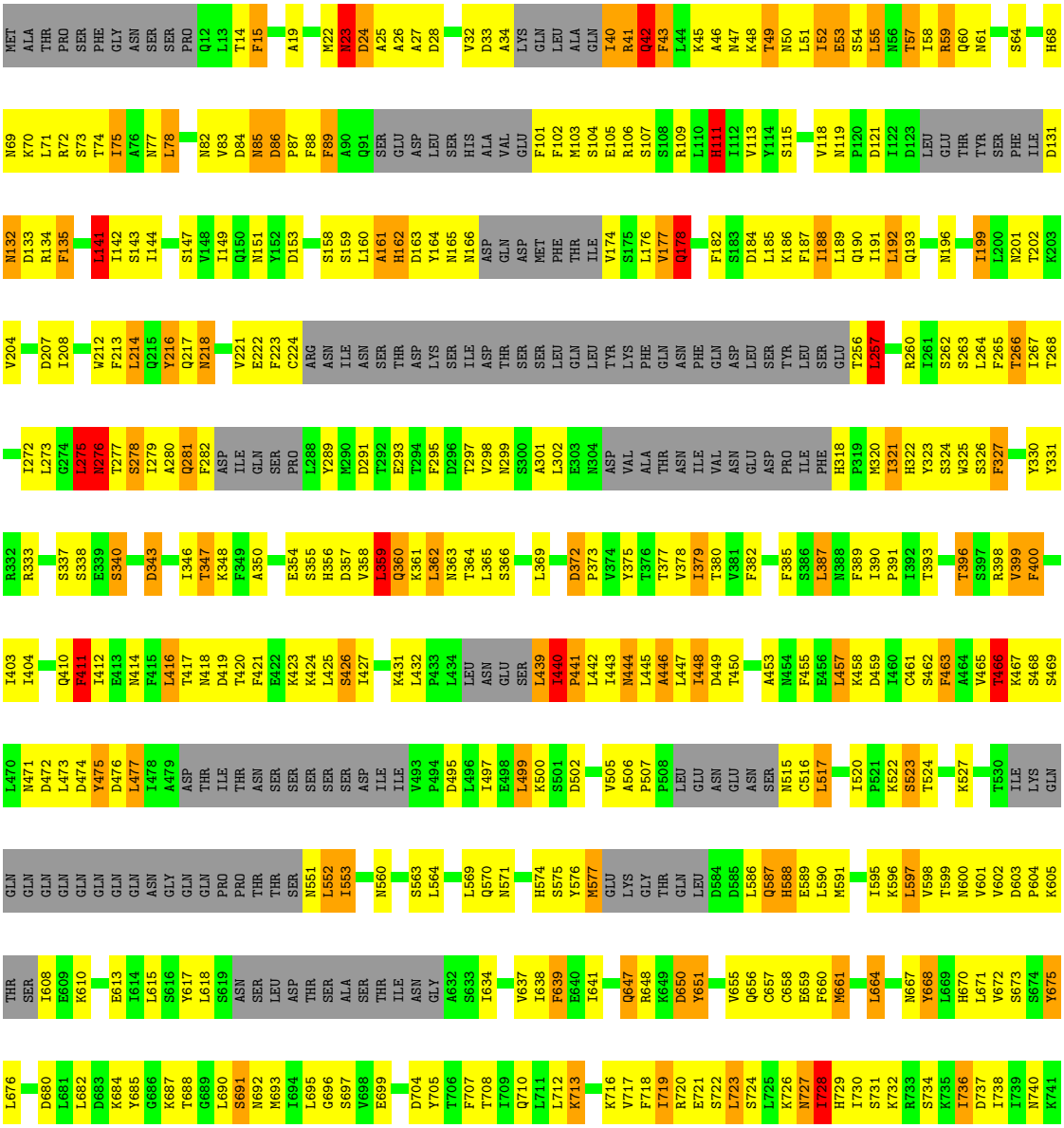


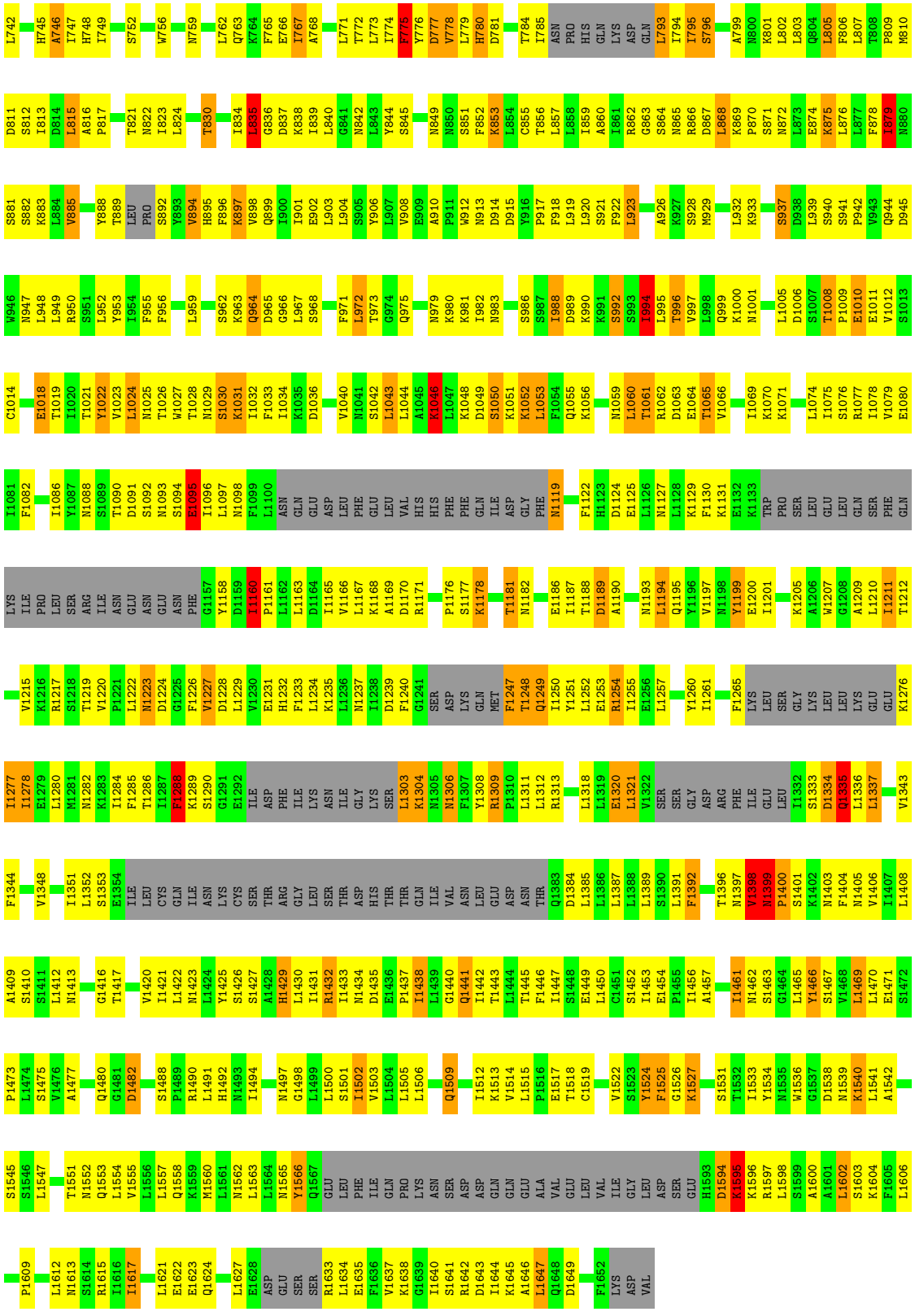


• Molecule 8: Nucleoporin NUP188

Chain P:

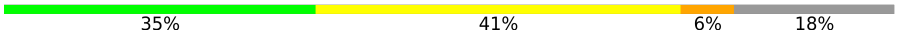


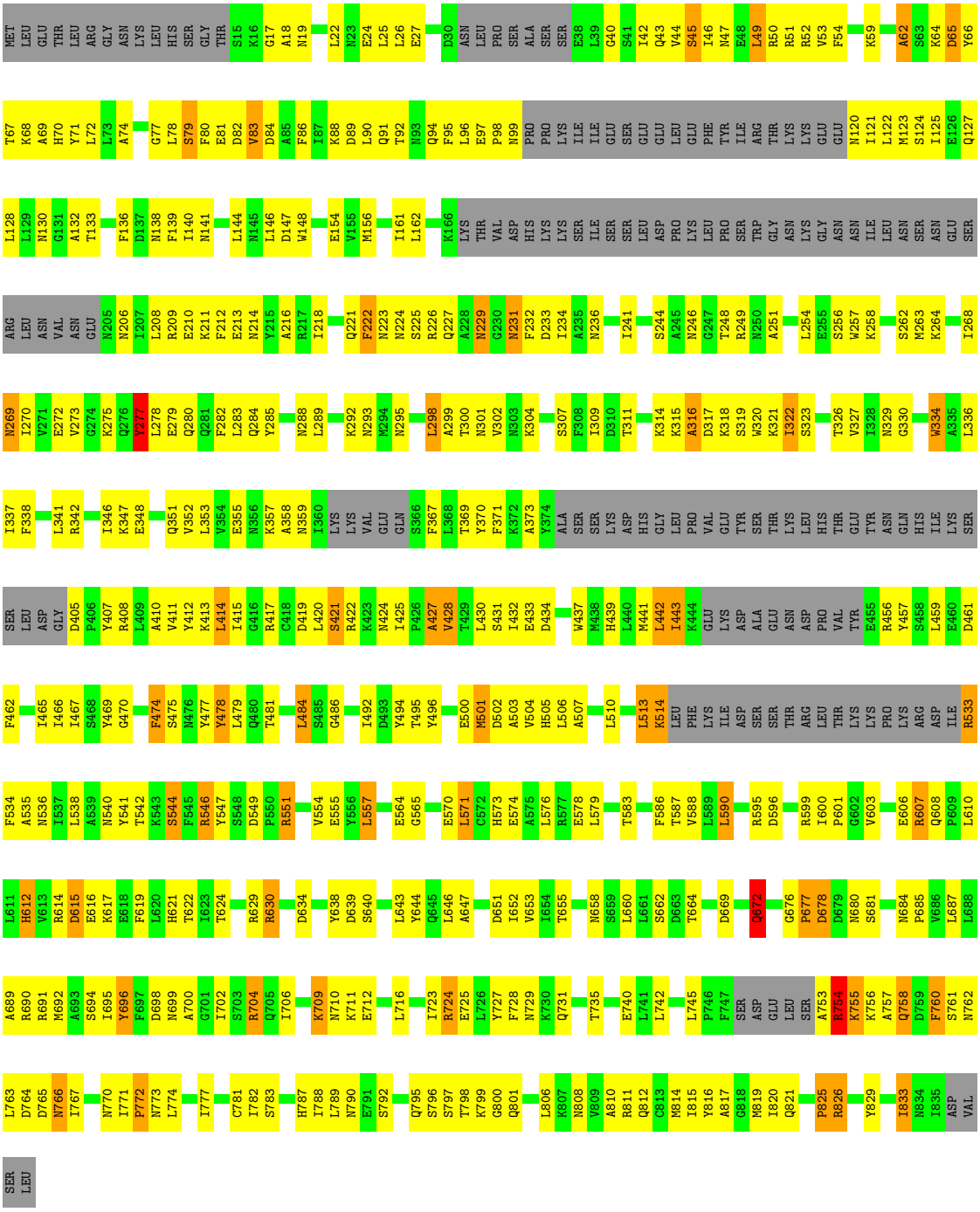





• Molecule 9: Nucleoporin NIC96

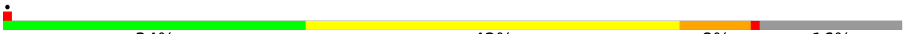
Chain Q:

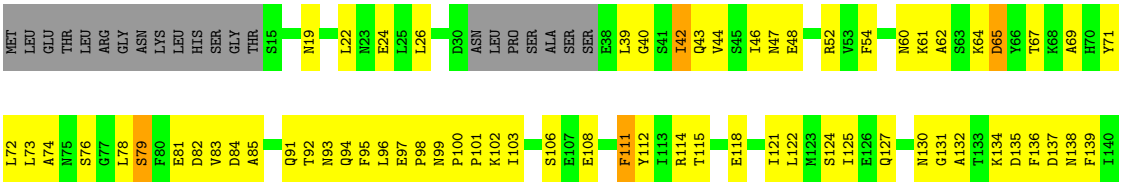


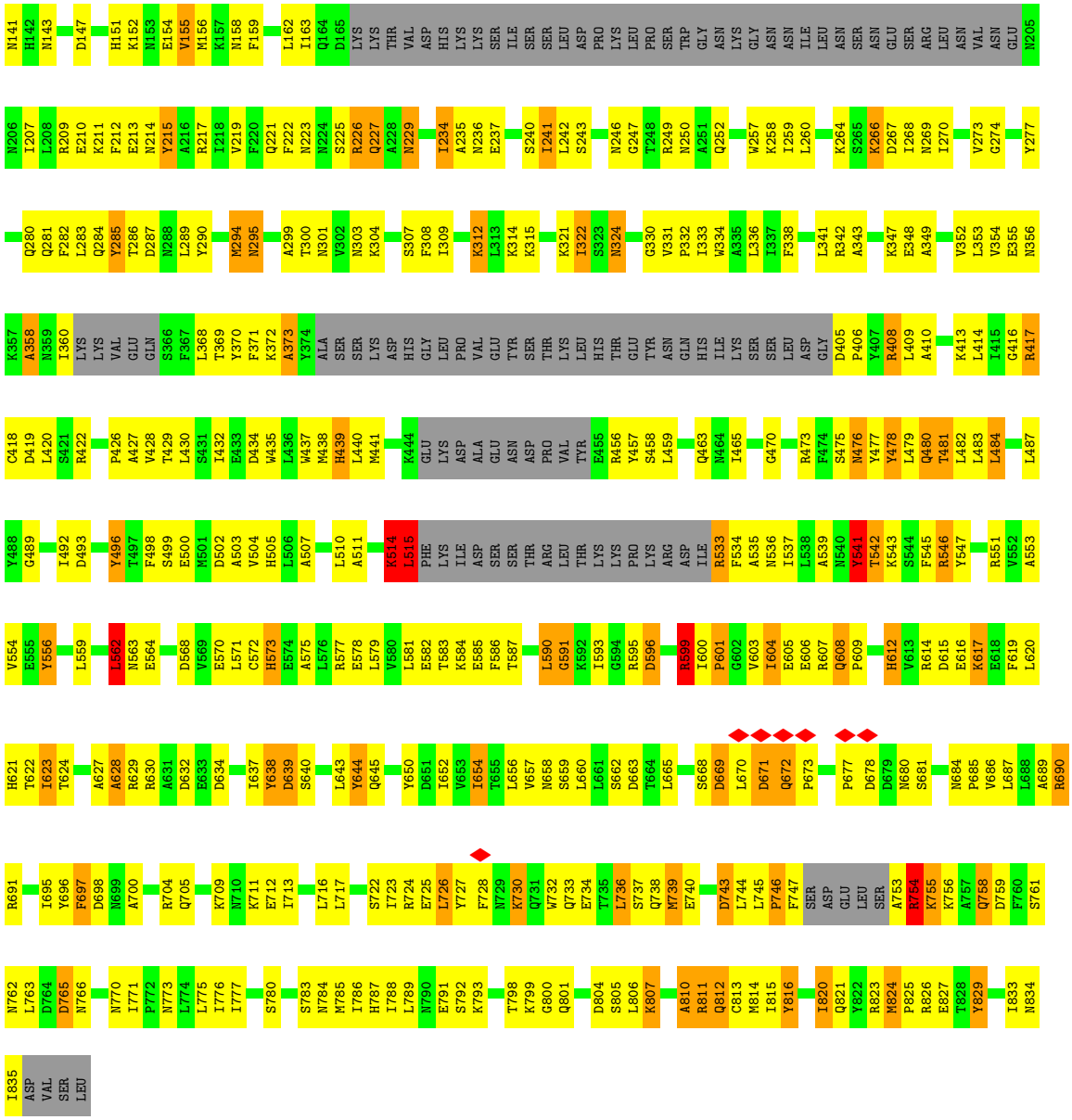


• Molecule 9: Nucleoporin NIC96

Chain R:

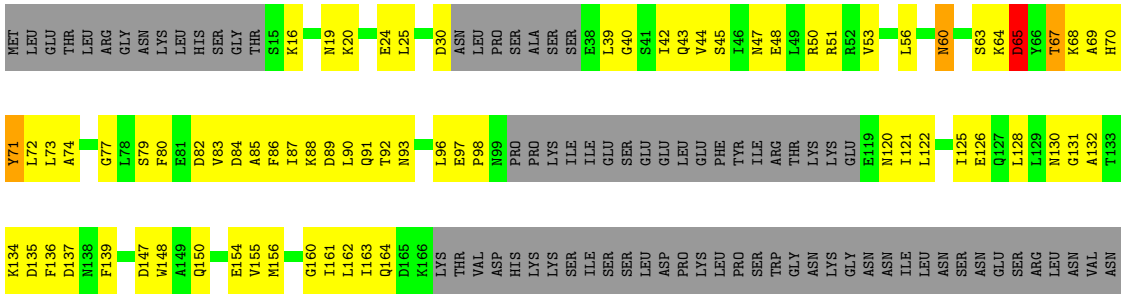


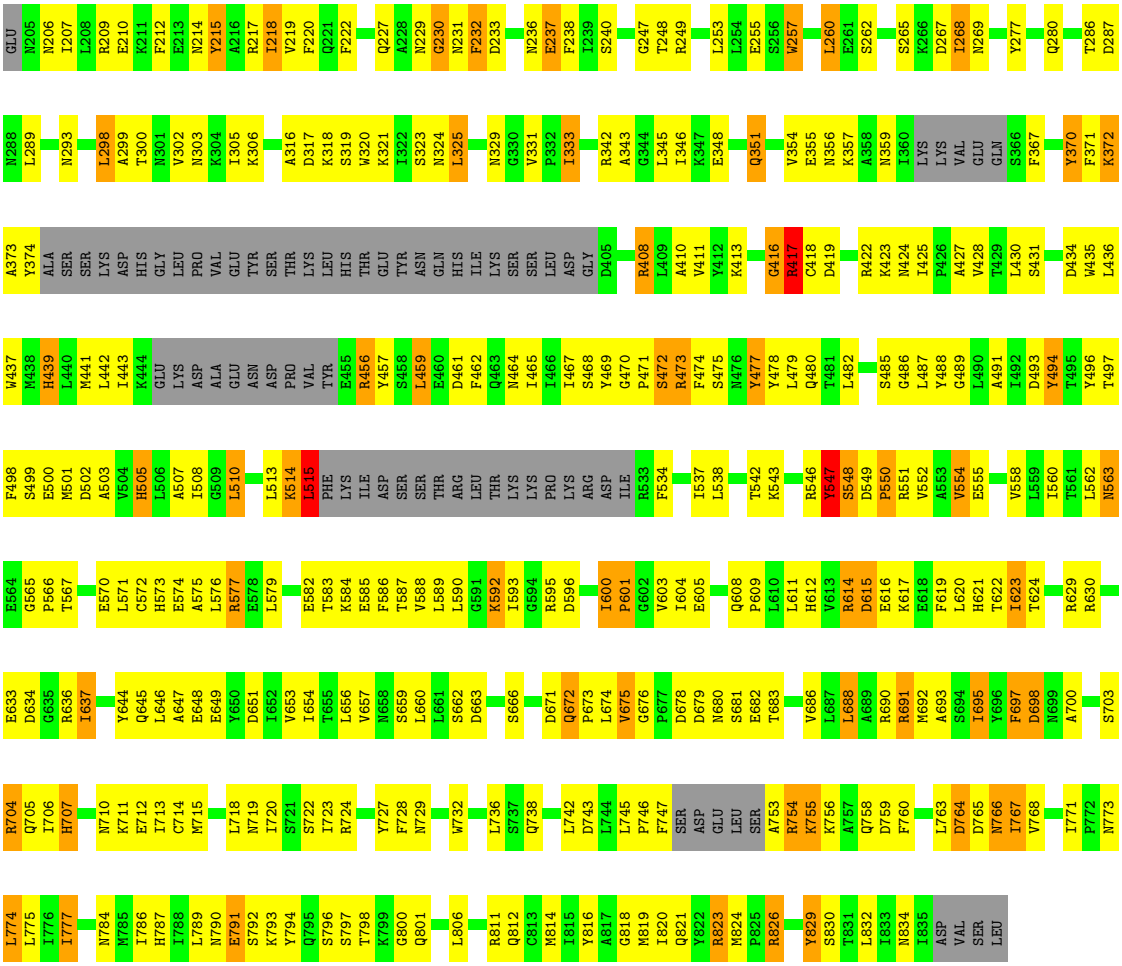





• Molecule 9: Nucleoporin NIC96

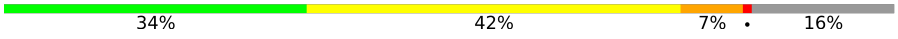
Chain S:

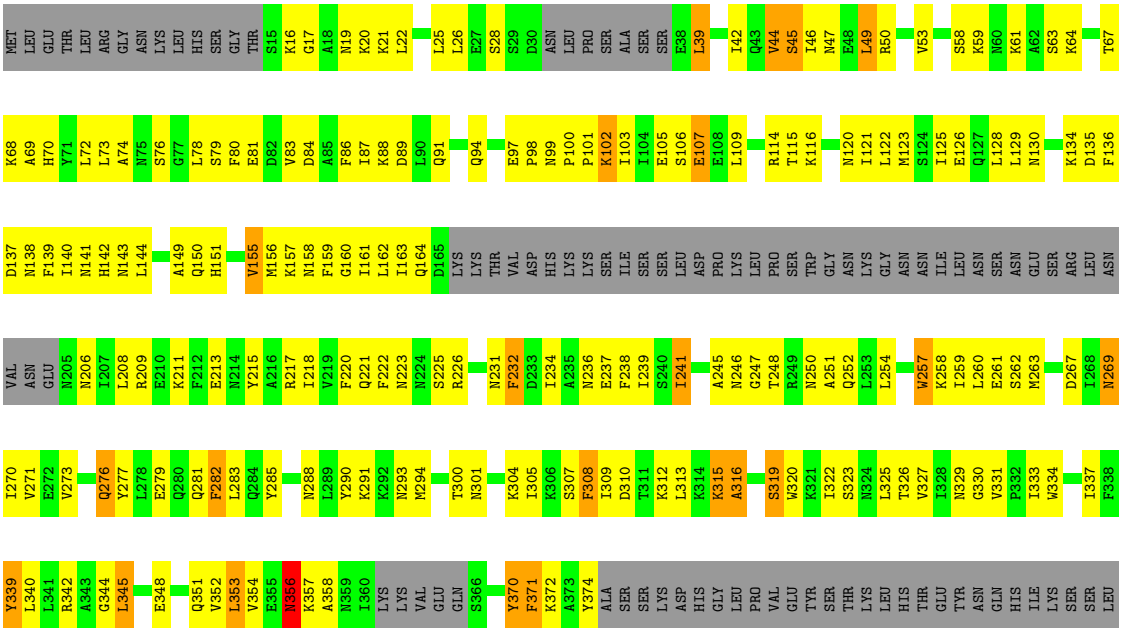


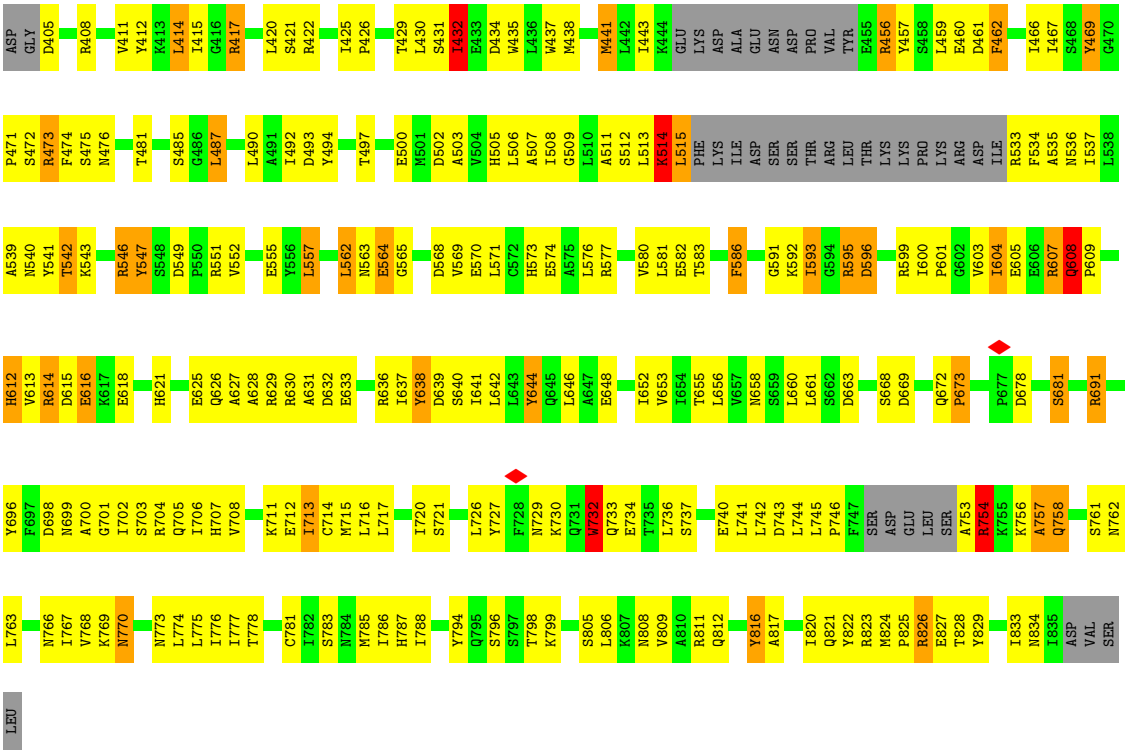


• Molecule 9: Nucleoporin NIC96

Chain T:

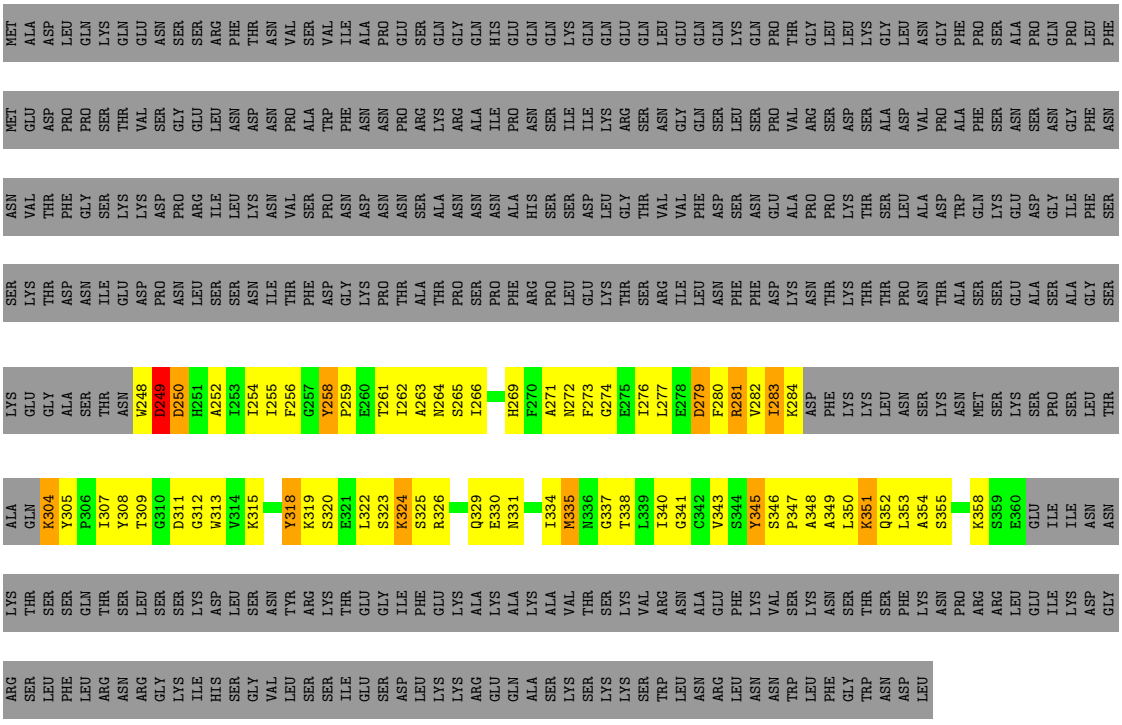




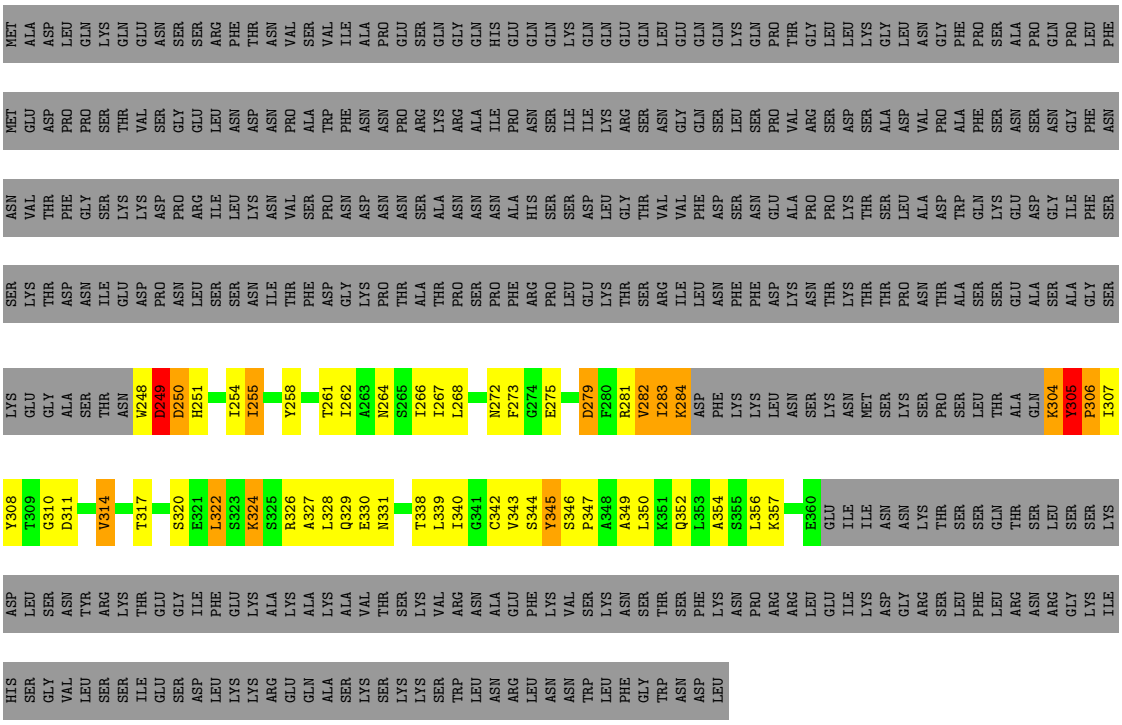
• Molecule 10: Nucleoporin NUP53

Chain U: 6% 12% 80%



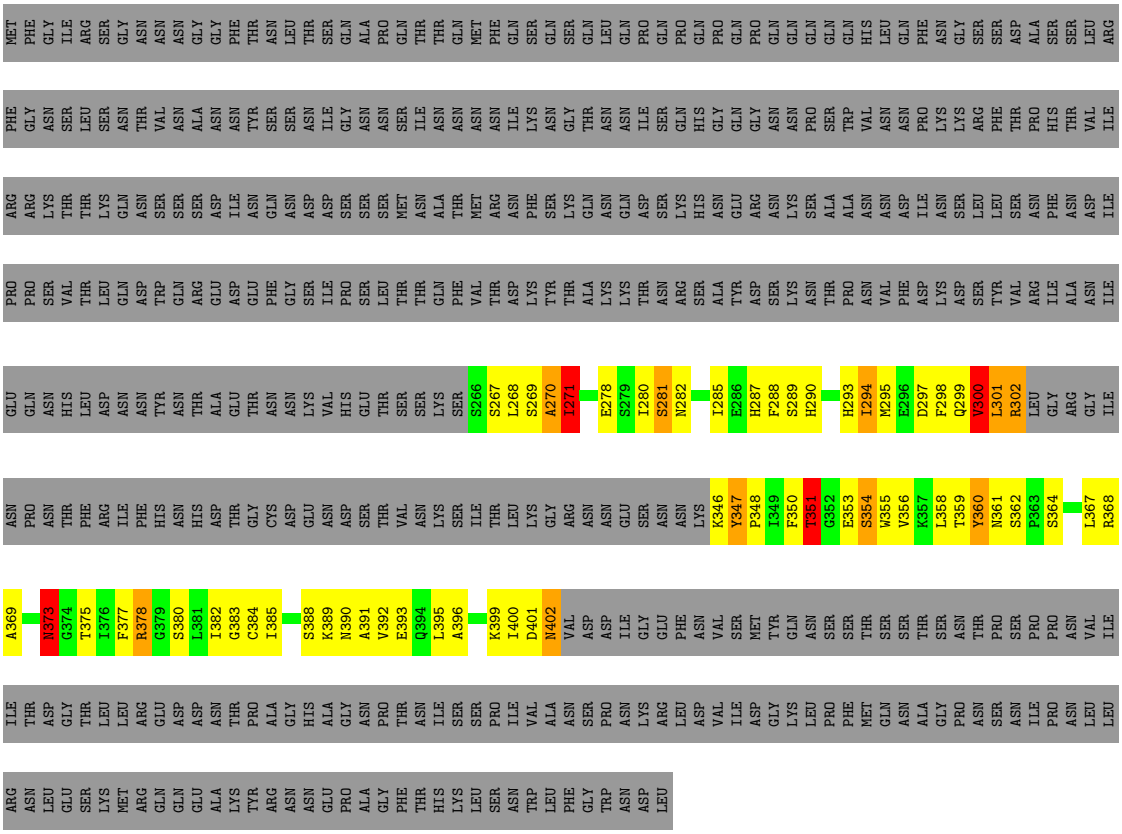
• Molecule 10: Nucleoporin NUP53

Chain W: 8% 8% 80%



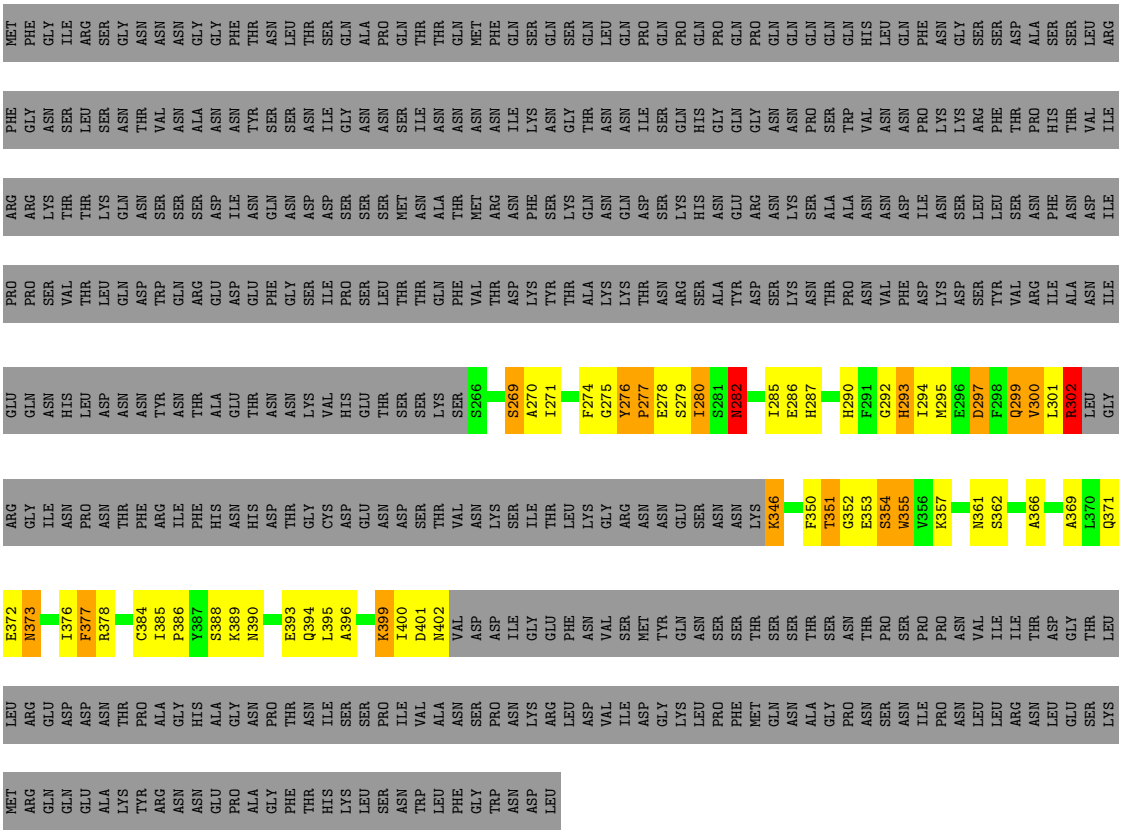
• Molecule 11: Nucleoporin ASM4

Chain V: 6% 9% 82%



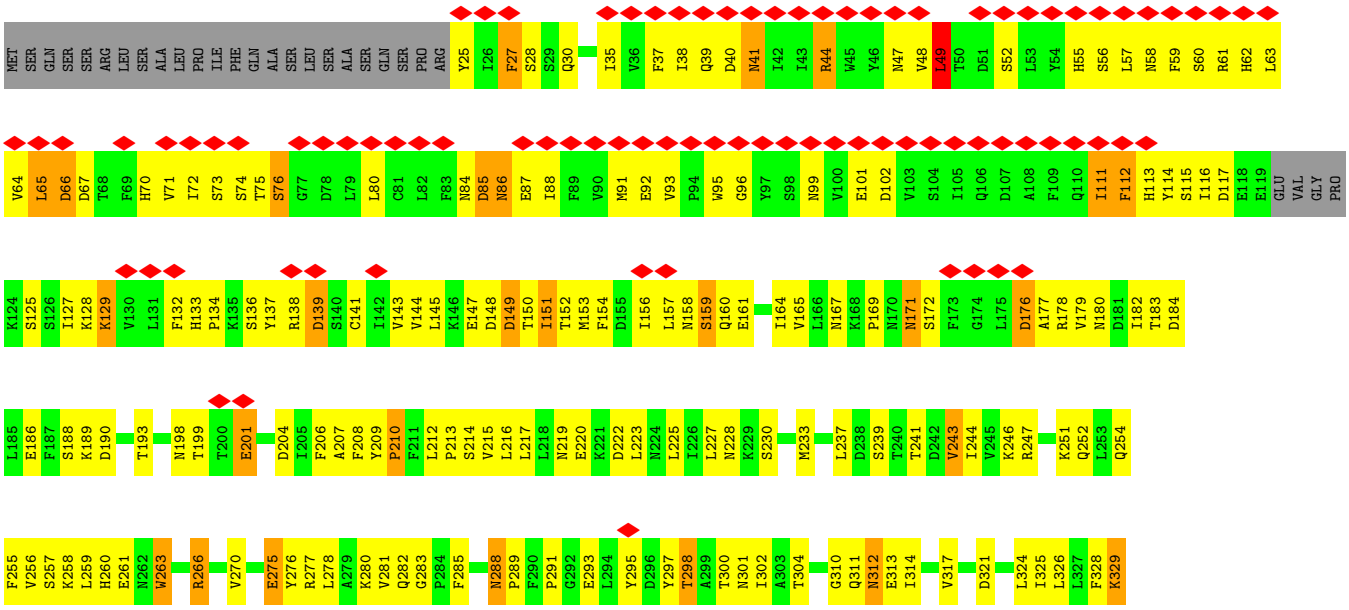
• Molecule 11: Nucleoporin ASM4

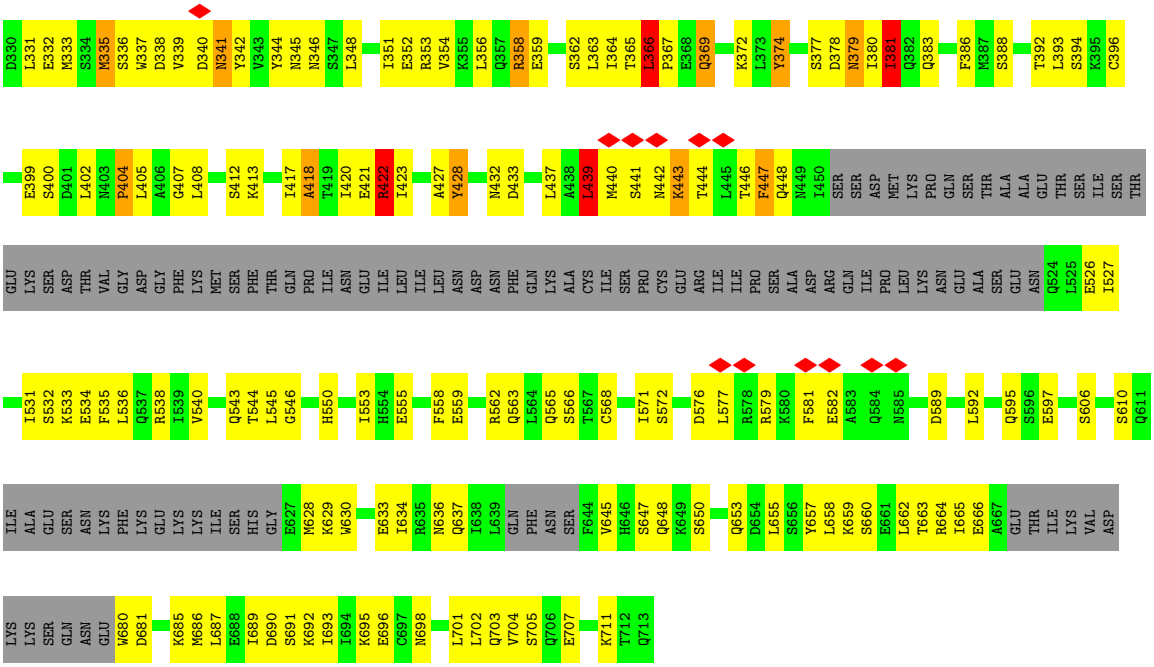
Chain X: 7% 7% • 82%



• Molecule 12: Nucleoporin NUP82

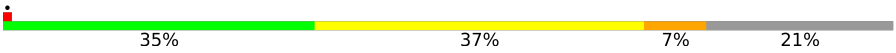
Chain u: 14% 35% 40% 5% • 19%

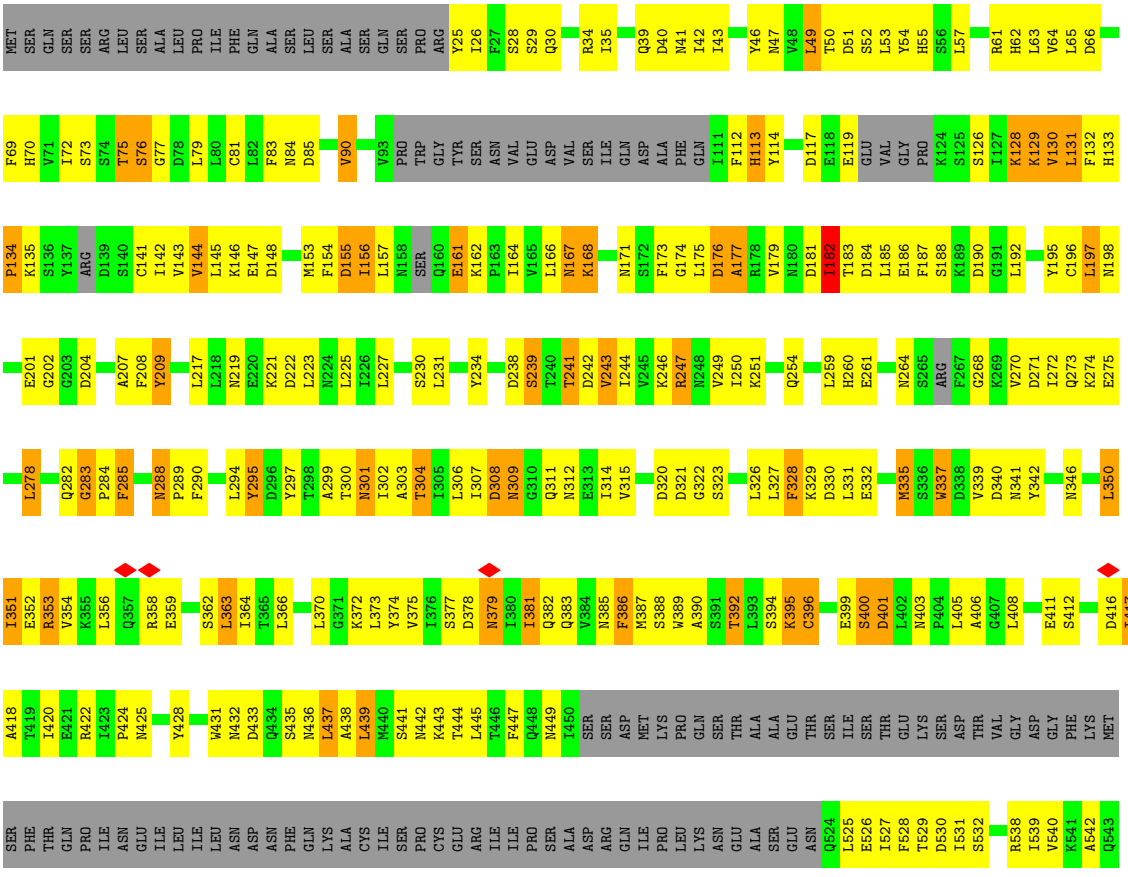


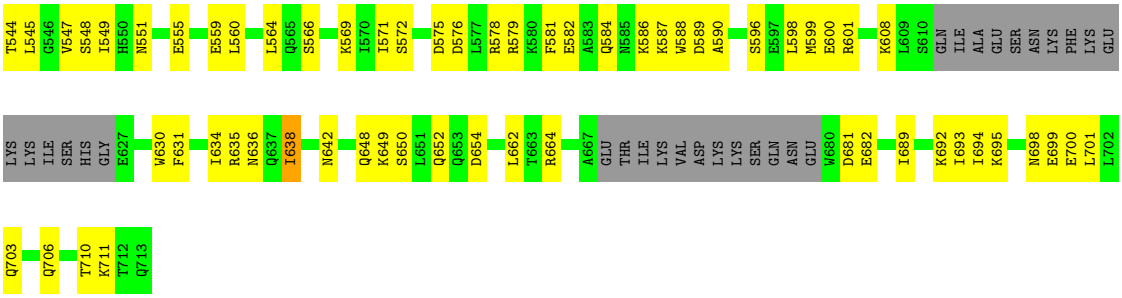


• Molecule 12: Nucleoporin NUP82

Chain v:

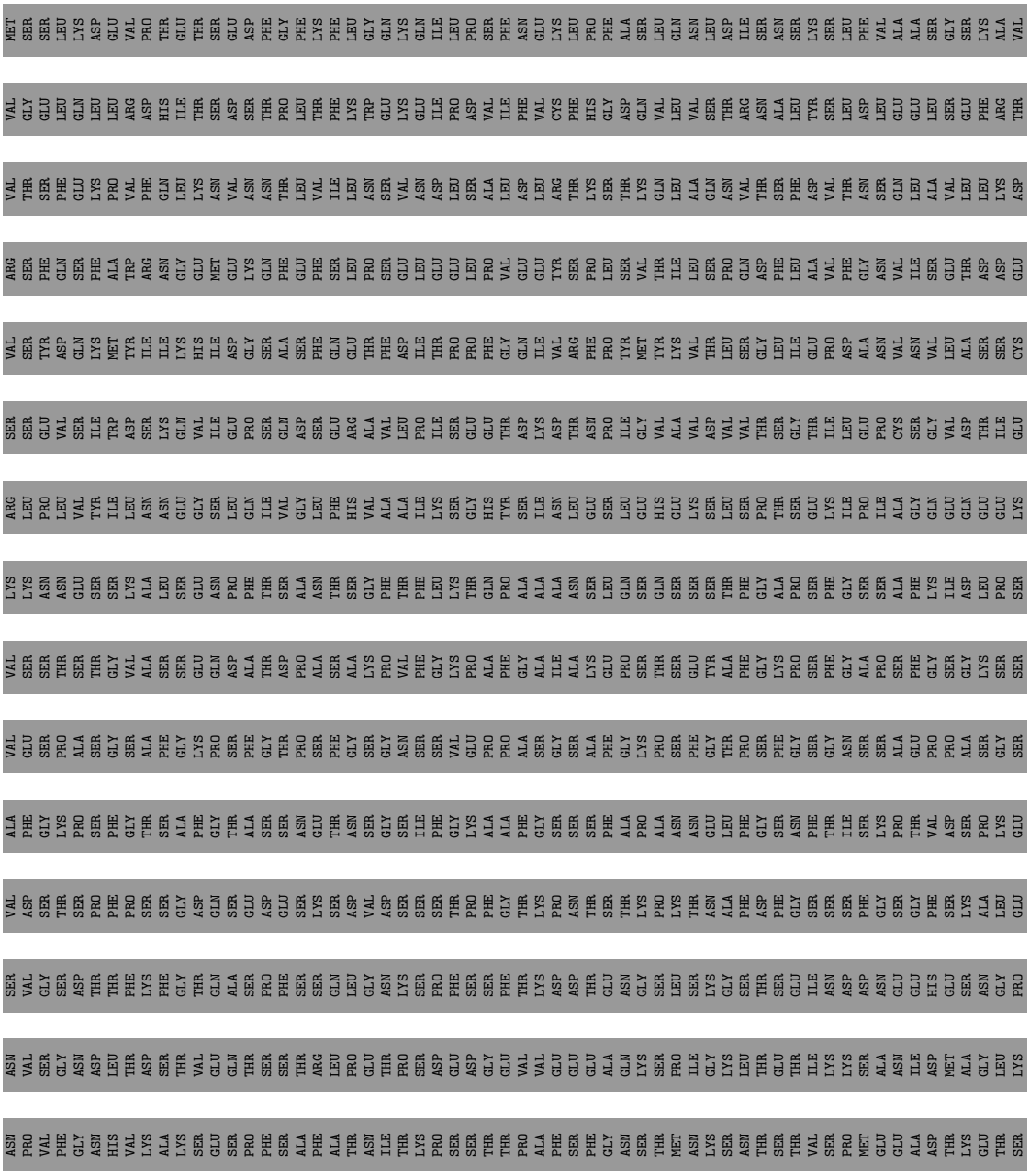


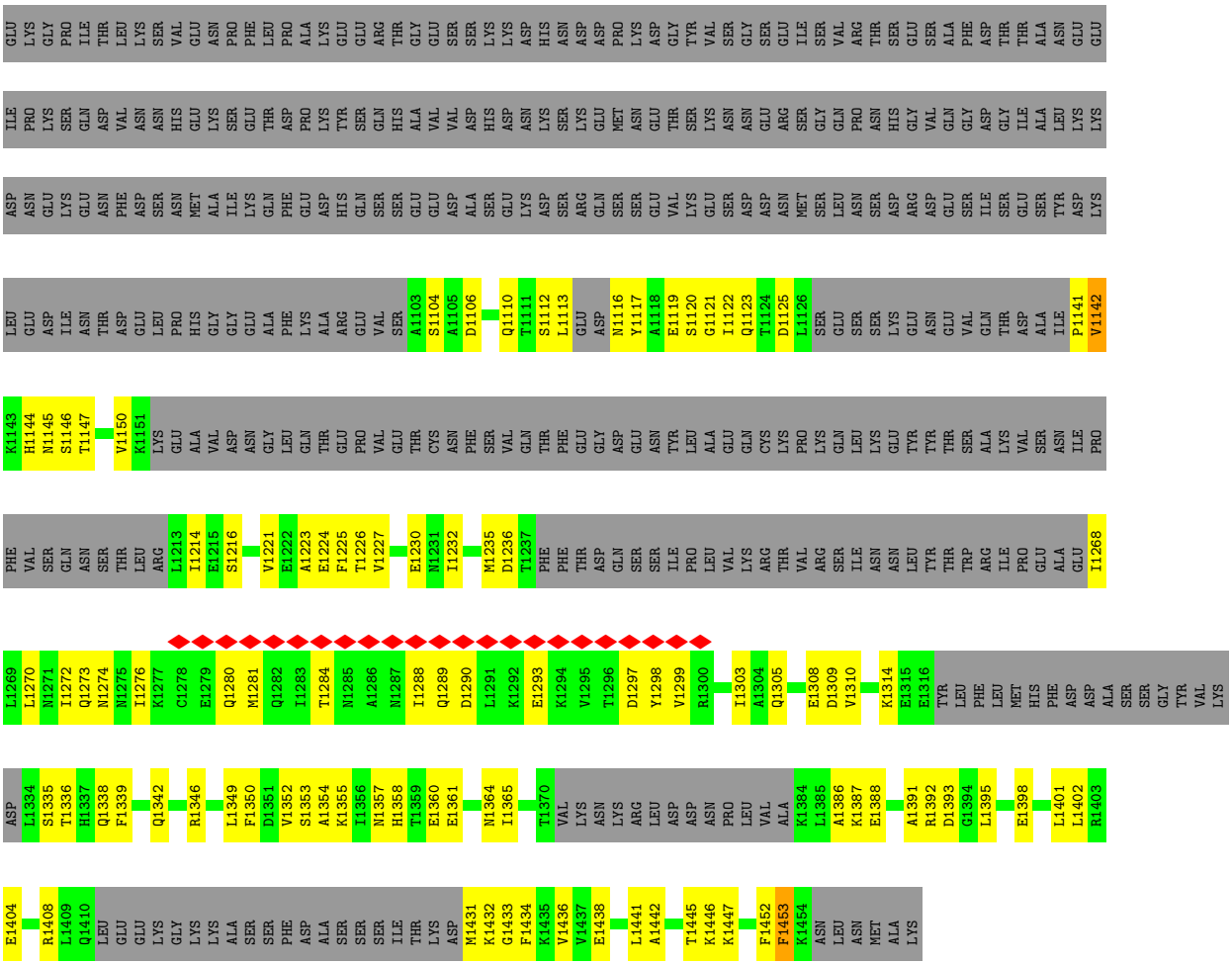






• Molecule 13: Nucleoporin NUP159

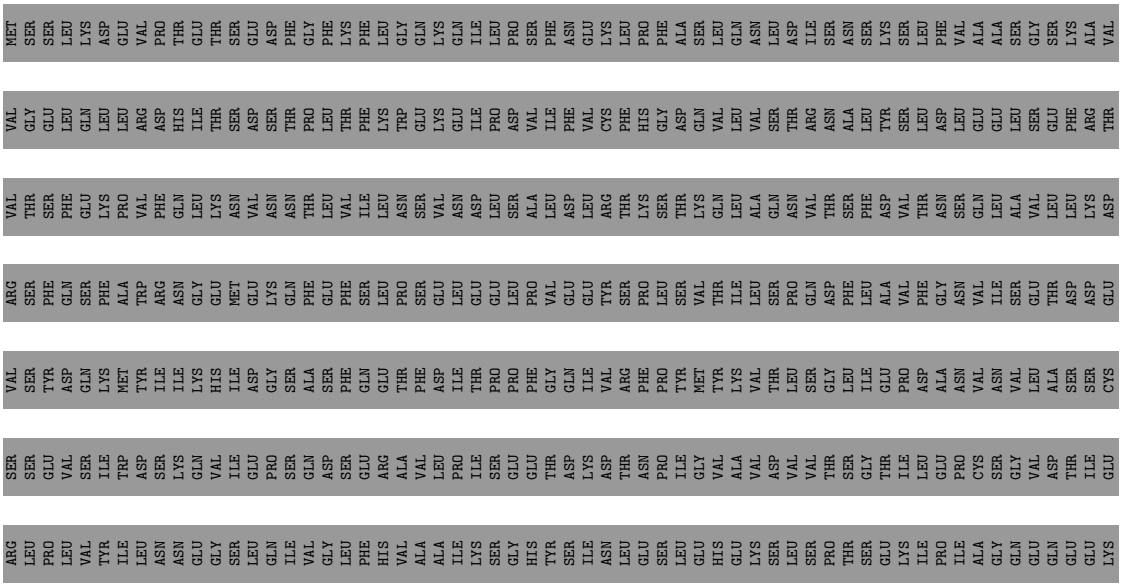
Chain w: 7% 7% 87%

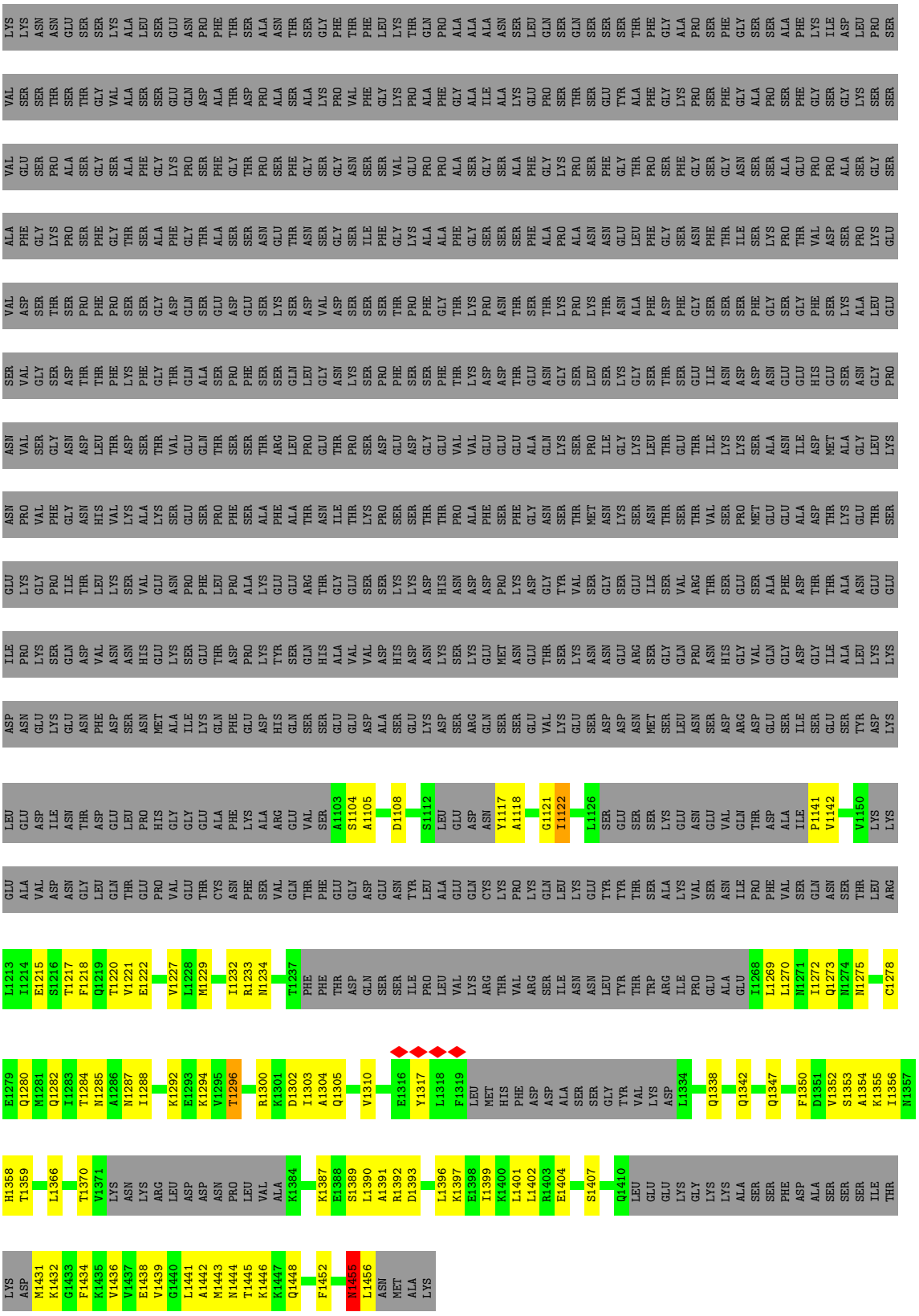




• Molecule 13: Nucleoporin NUP159

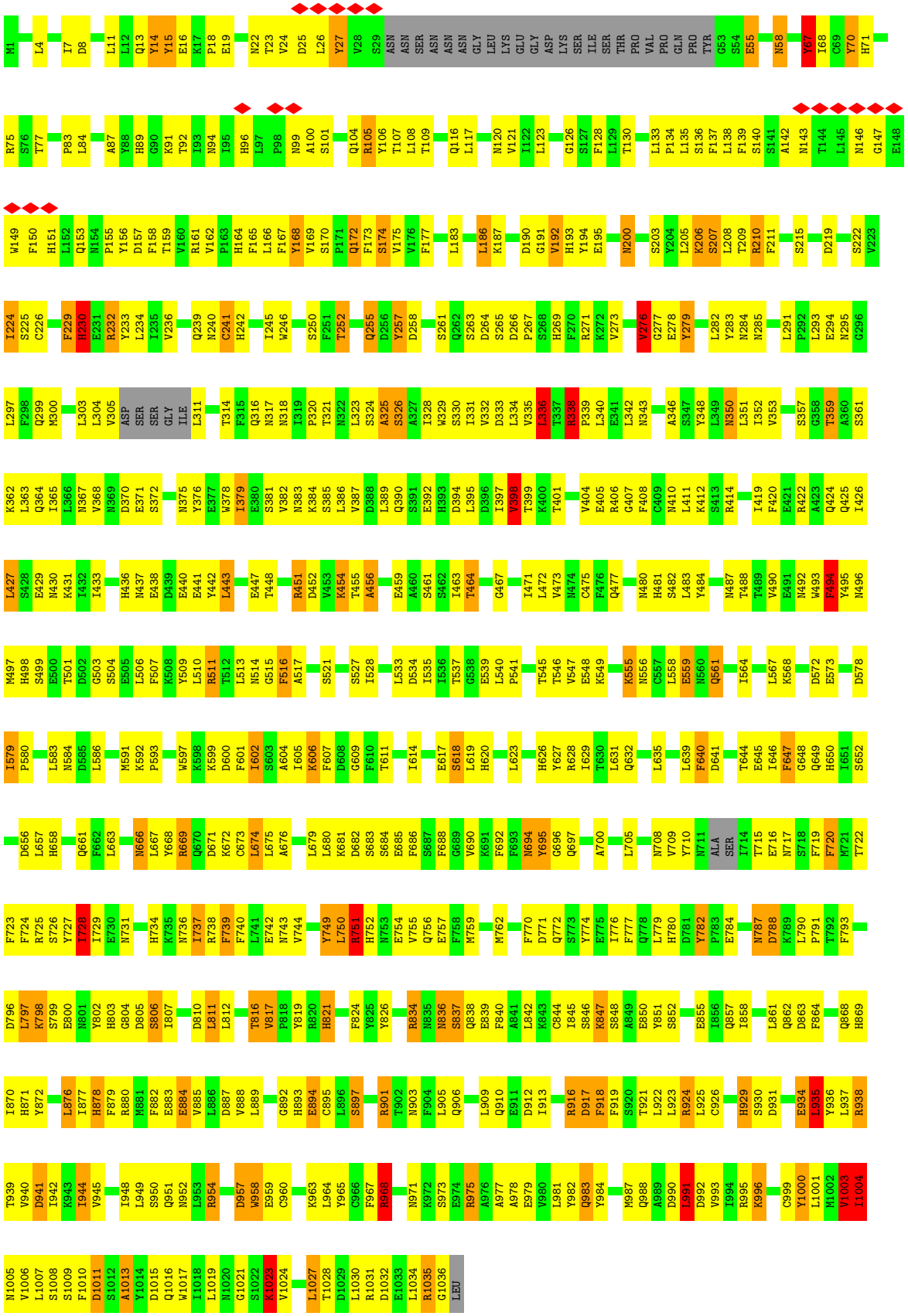
Chain x: 8% 6% 86%





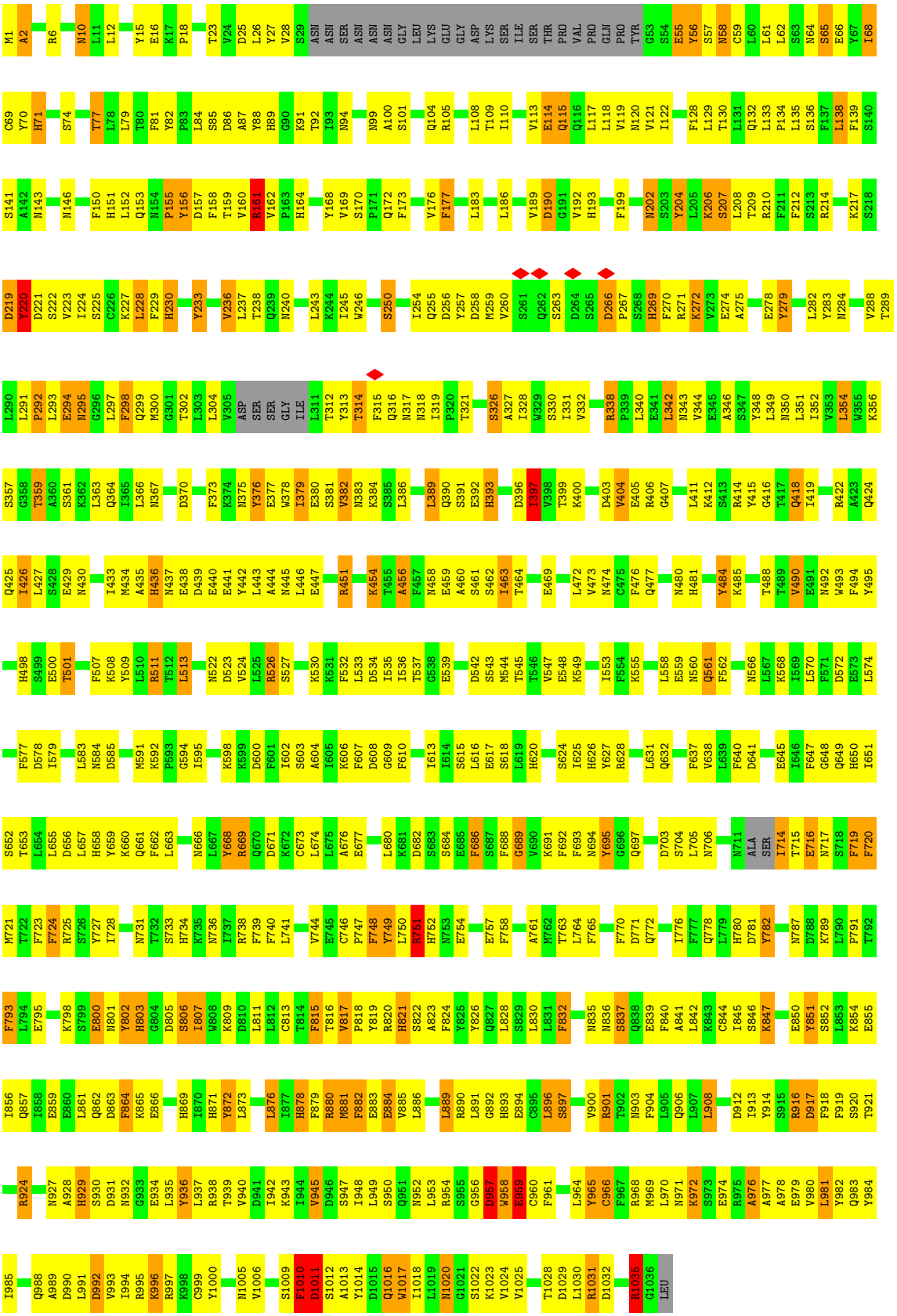
• Molecule 14: Nucleoporin NUP120

Chain h:



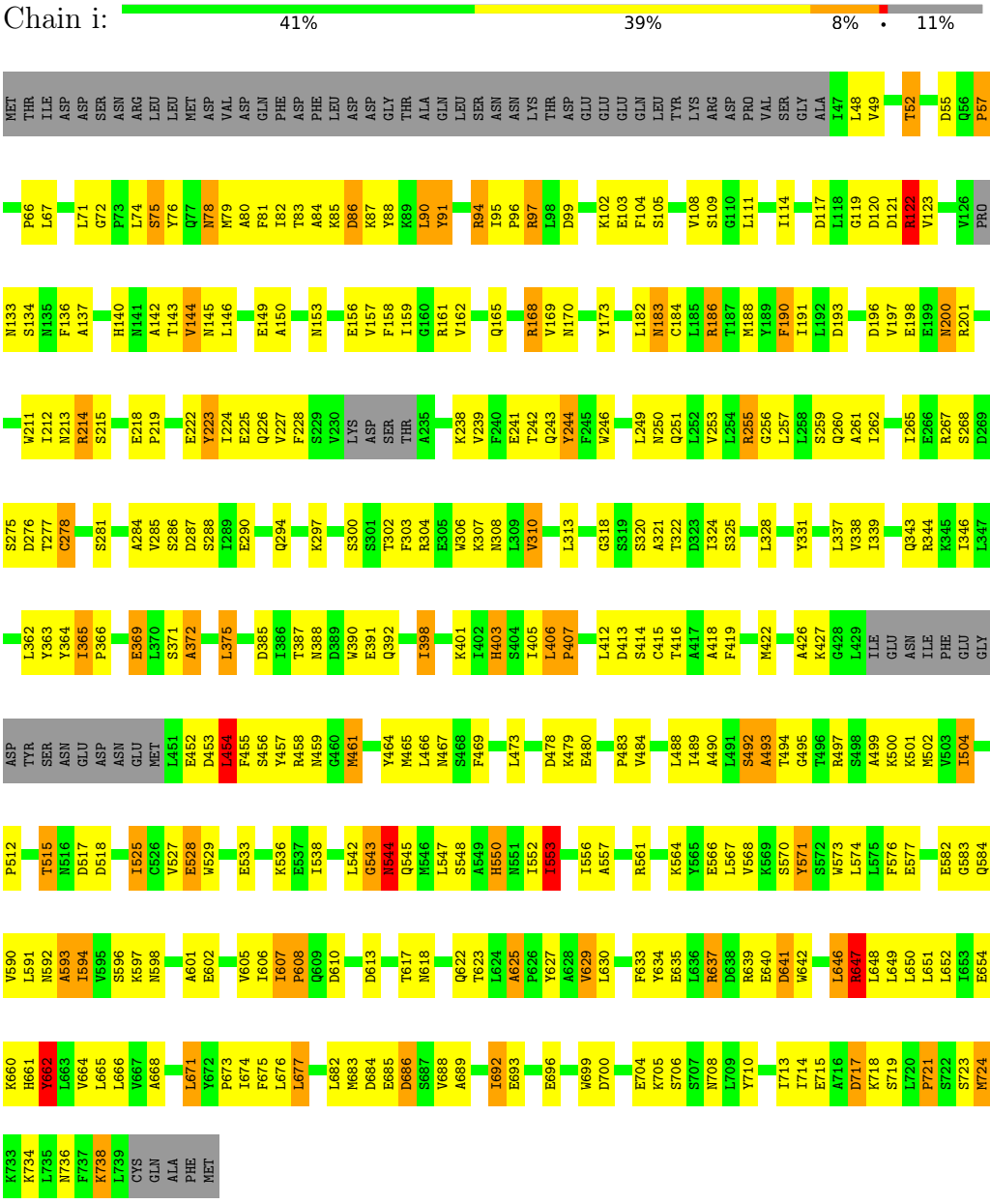
• Molecule 14: Nucleoporin NUP120

Chain a: 38% 47% 11%



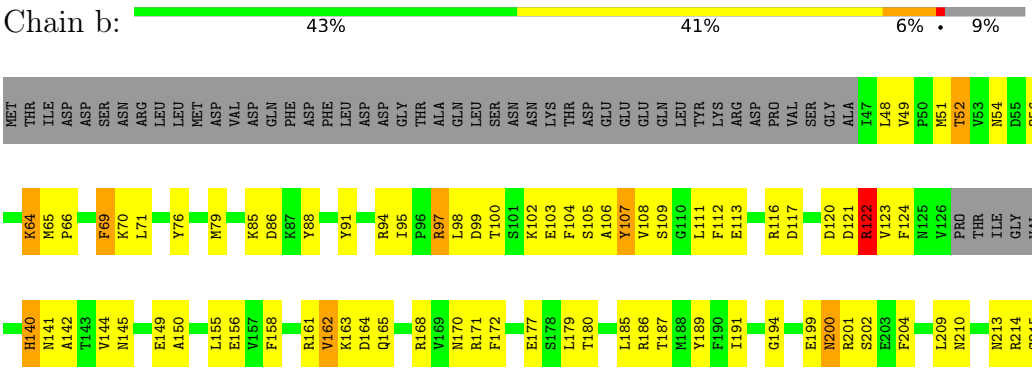
• Molecule 15: Nucleoporin NUP85

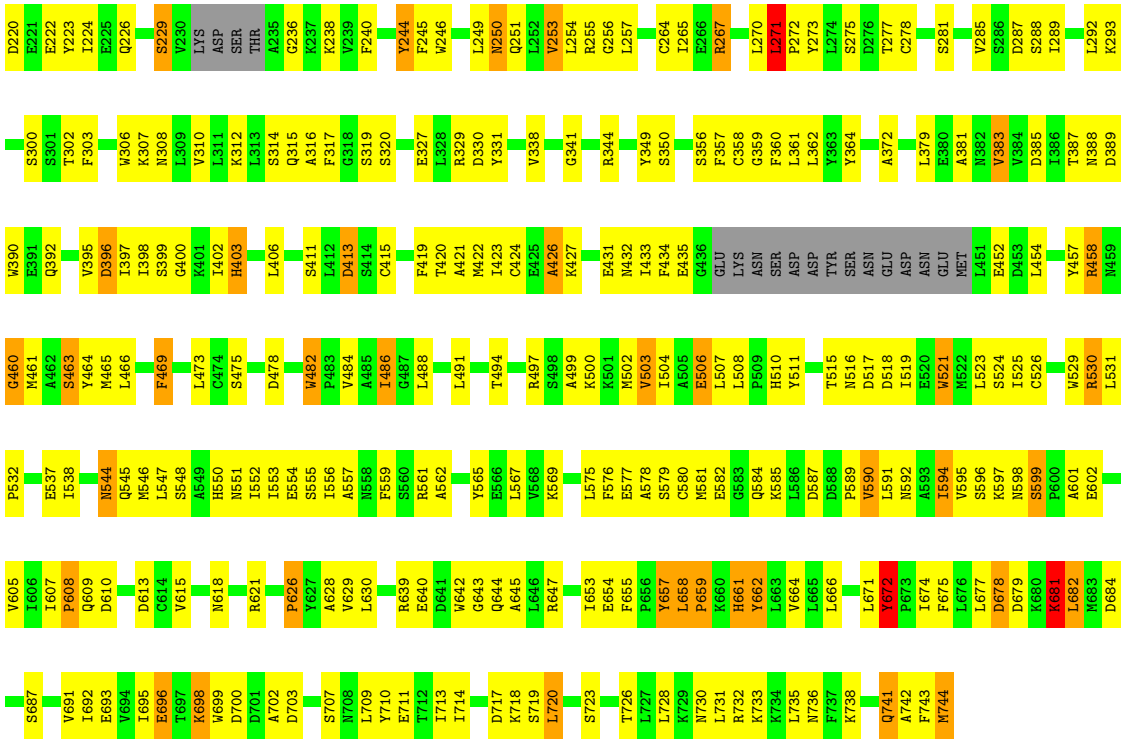
Chain i:




• Molecule 15: Nucleoporin NUP85

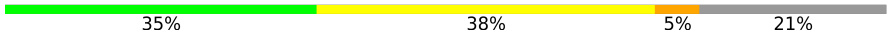
Chain b:

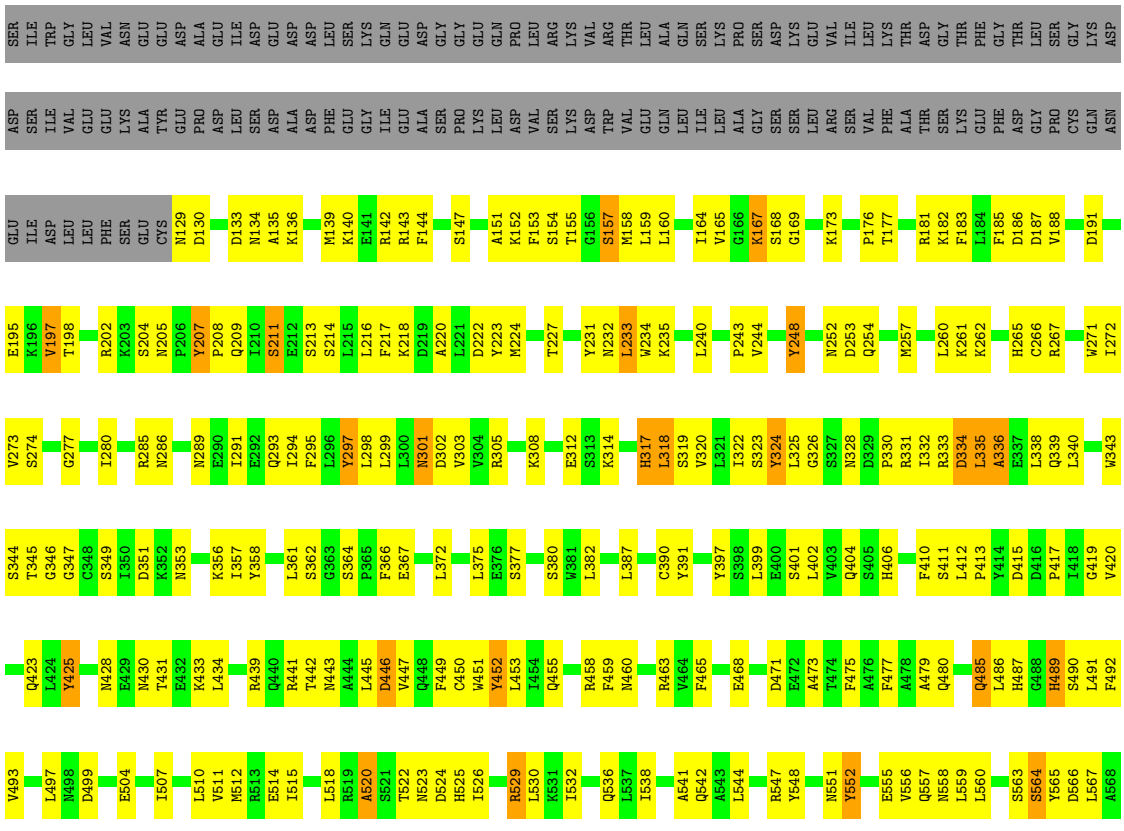


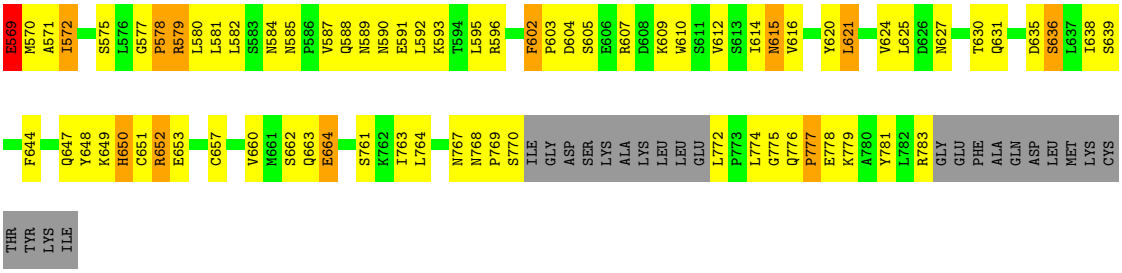


• Molecule 16: Nucleoporin 145c

Chain j:

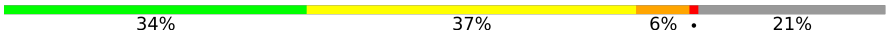


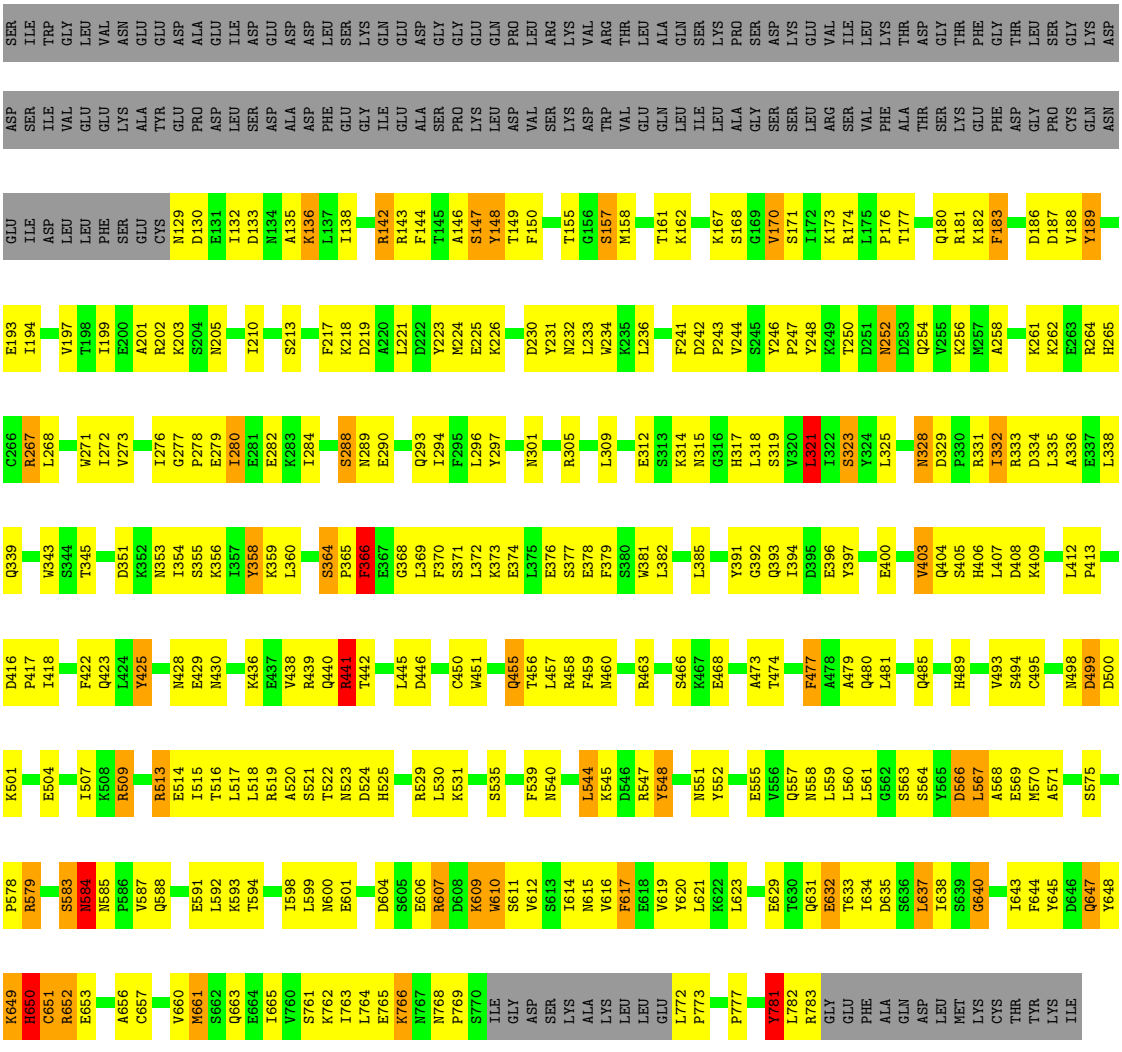





• Molecule 16: Nucleoporin 145c

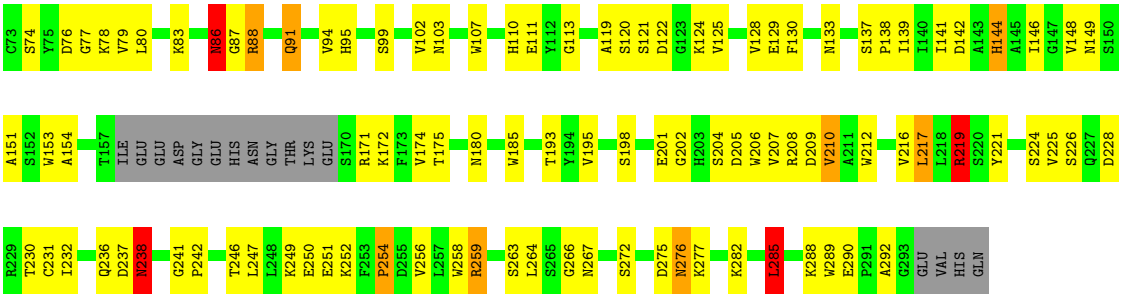
Chain c:



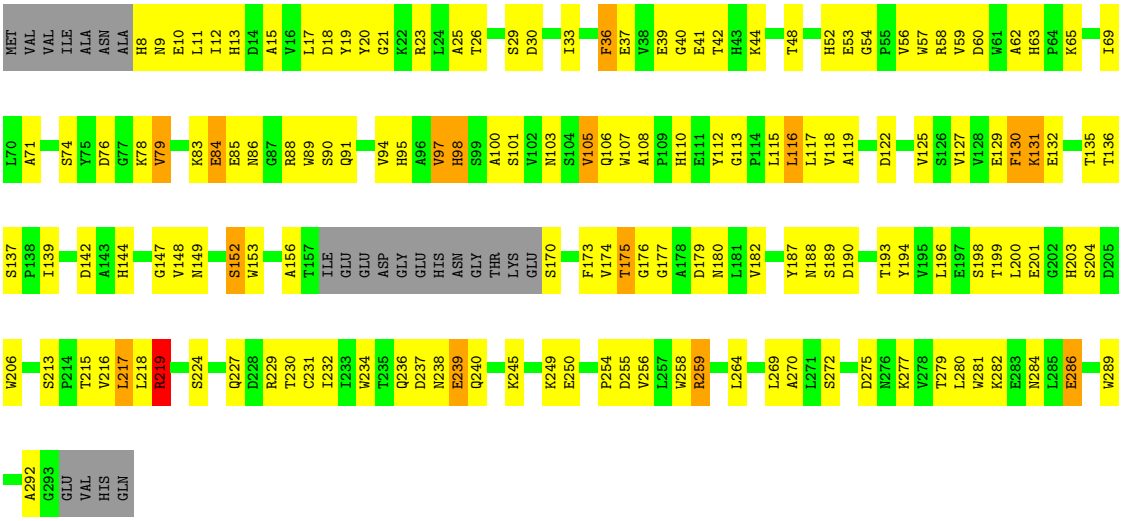
• Molecule 17: Protein transport protein SEC13

Chain k:



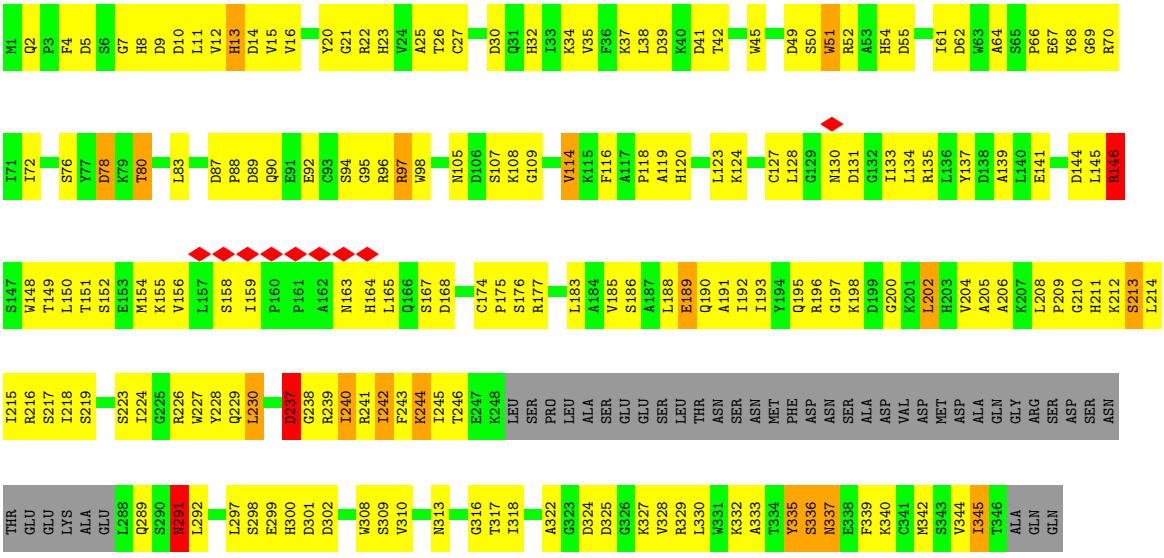
• Molecule 17: Protein transport protein SEC13

Chain d:



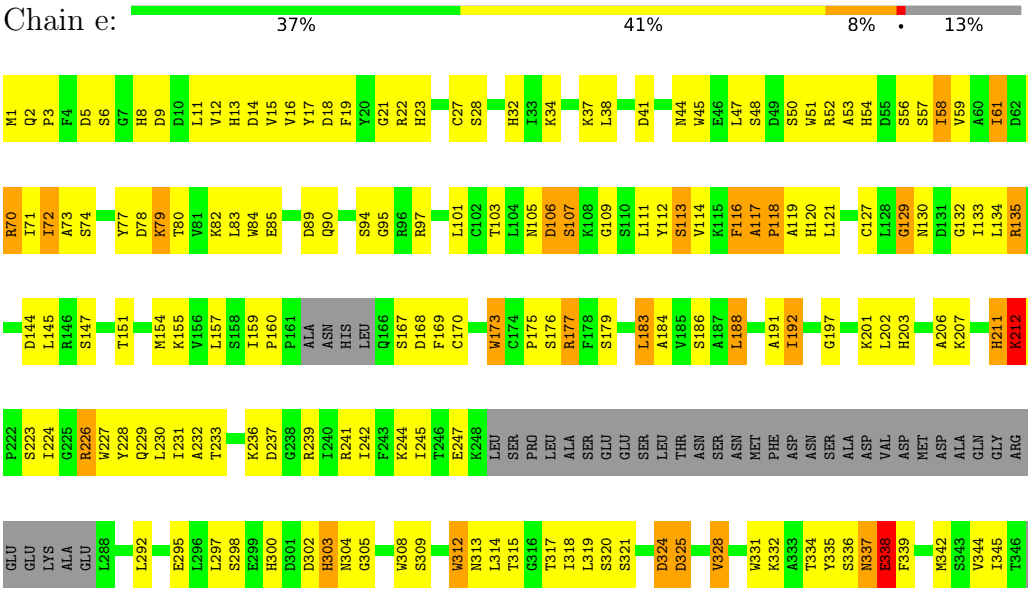
• Molecule 18: Nucleoporin SEH1

Chain l:



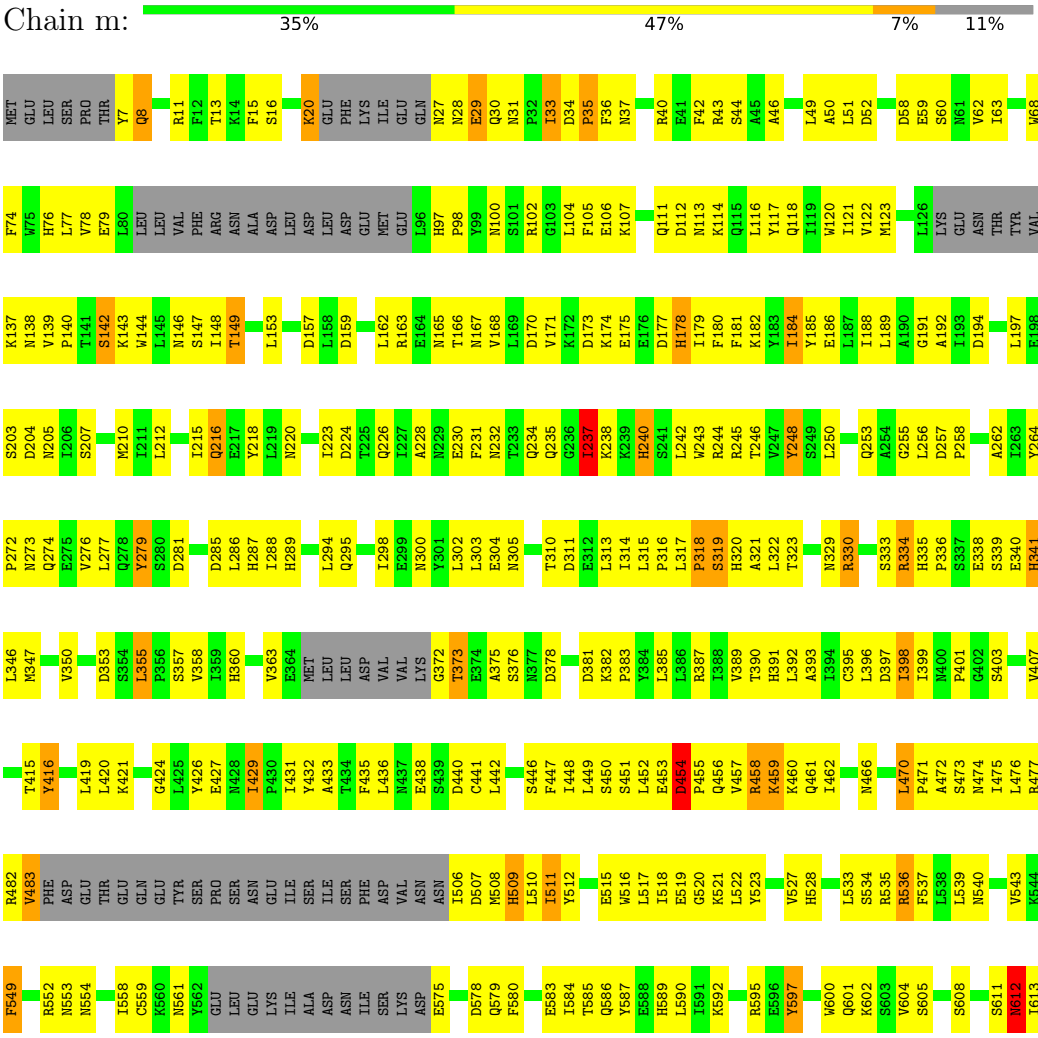
• Molecule 18: Nucleoporin SEH1

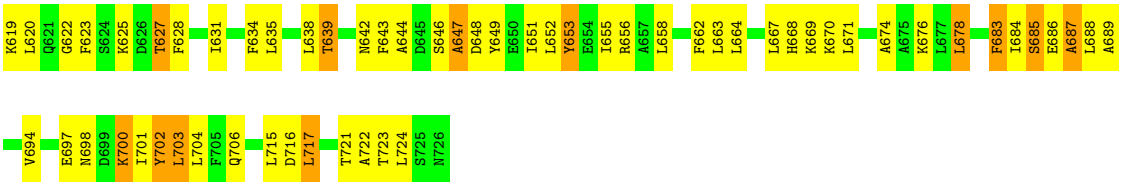
Chain e:




• Molecule 19: Nucleoporin NUP84

Chain m:

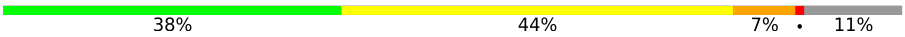


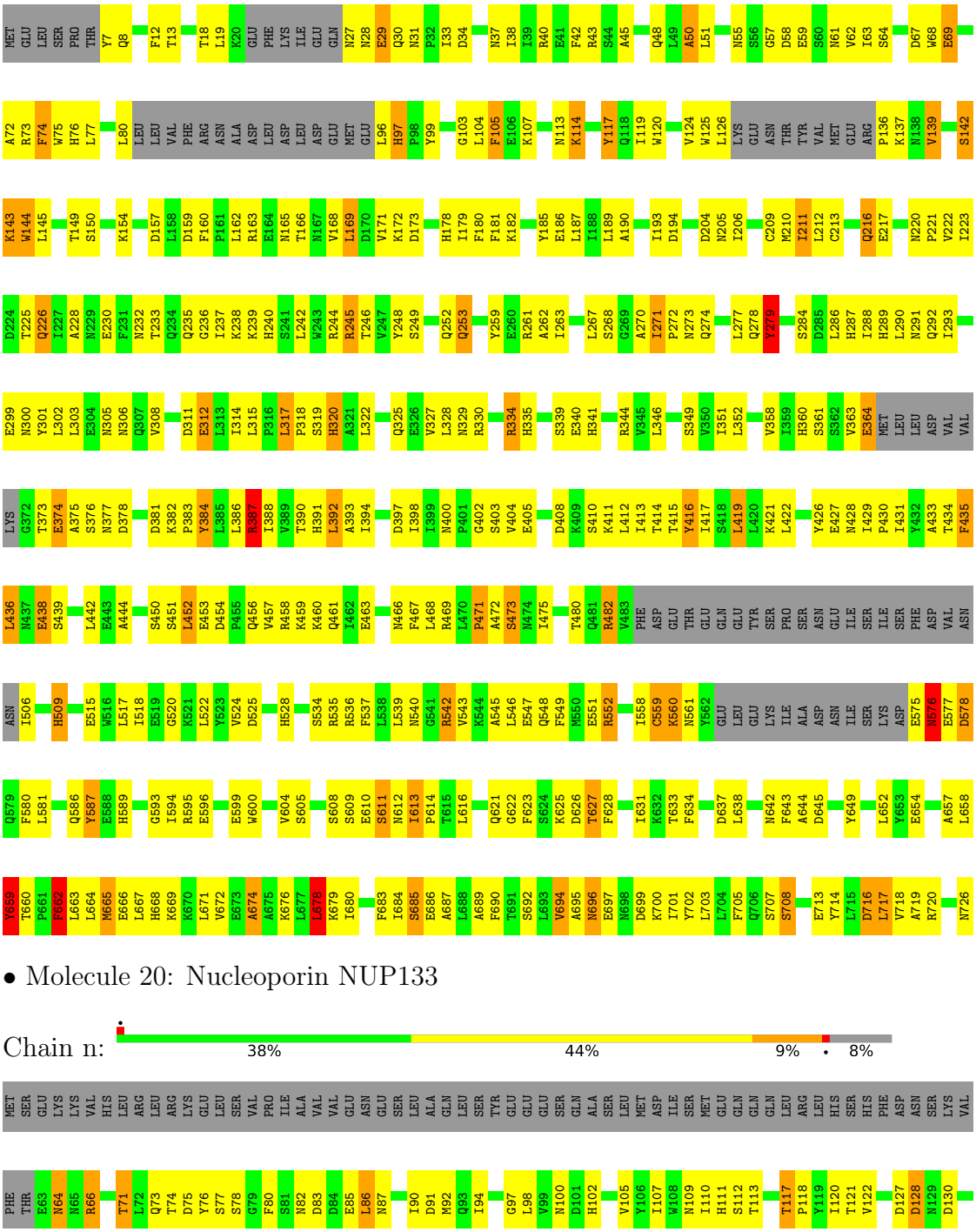




• Molecule 19: Nucleoporin NUP84

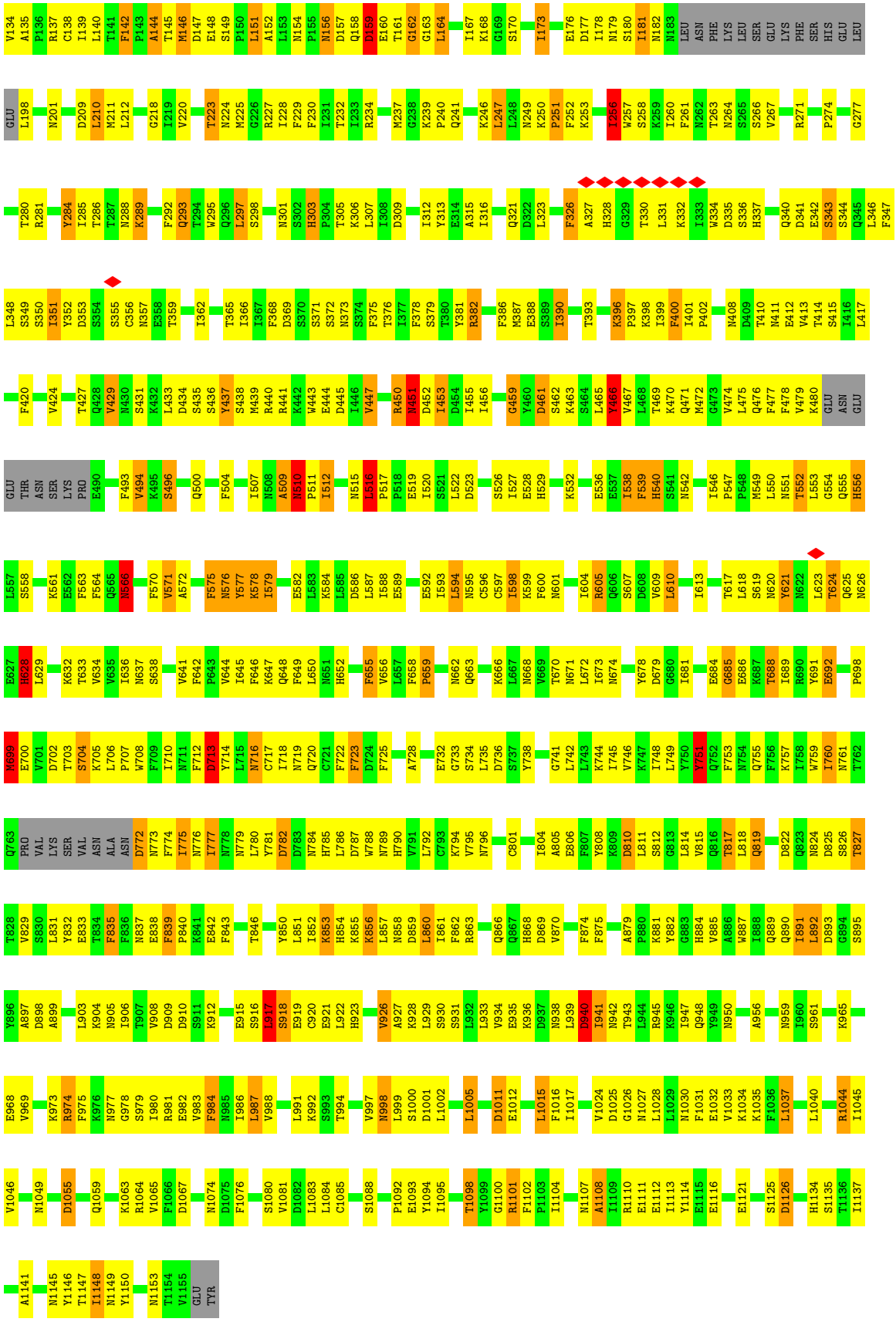
Chain f:



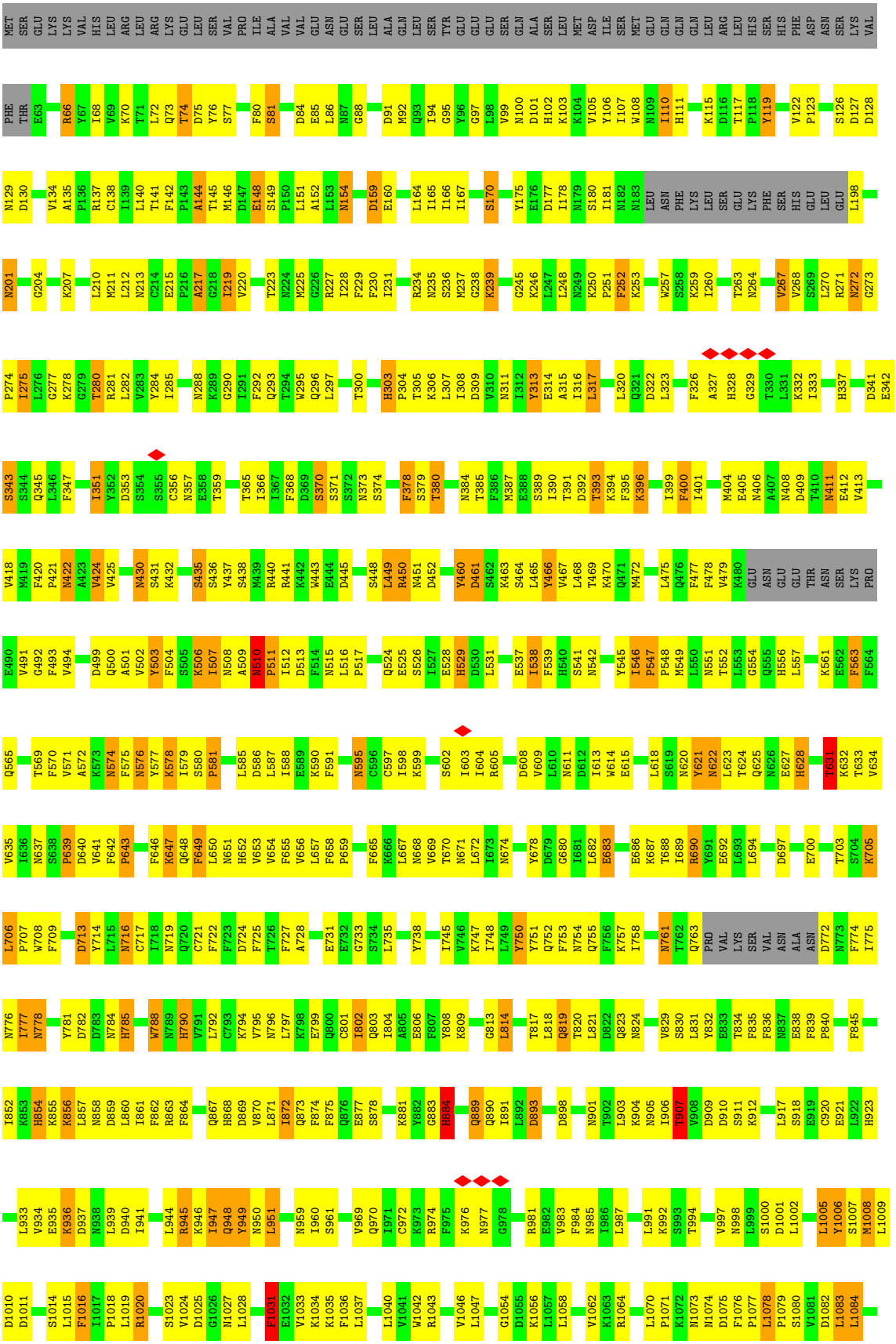
• Molecule 20: Nucleoporin NUP133

Chain n:



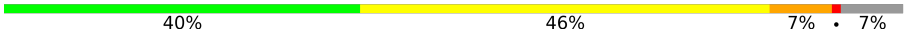
• Molecule 20: Nucleoporin NUP133

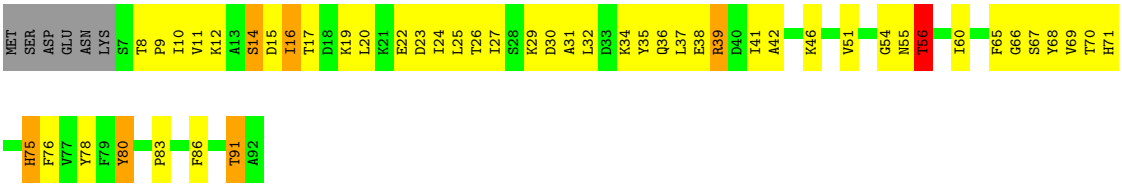
Chain g:



• Molecule 21: Dynein light chain 1, cytoplasmic

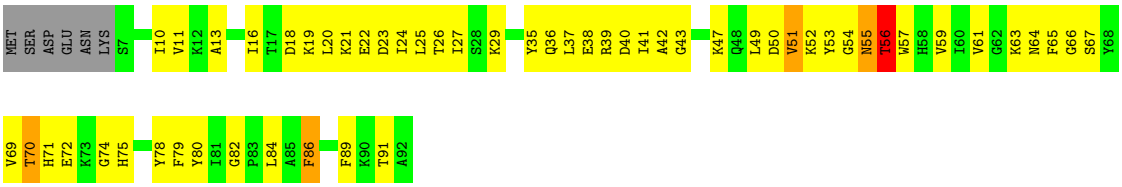
Chain o:



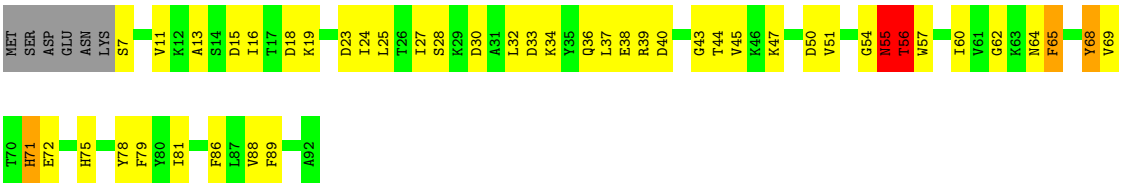

• Molecule 21: Dynein light chain 1, cytoplasmic

Chain p:



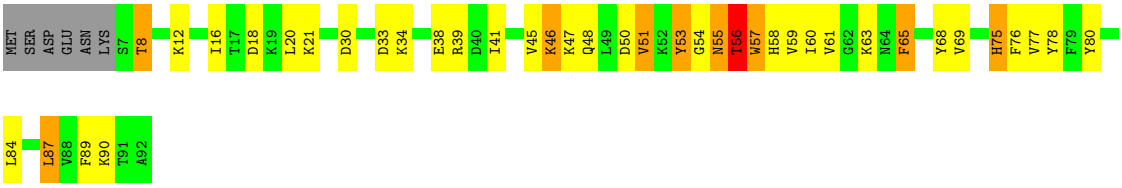

• Molecule 21: Dynein light chain 1, cytoplasmic

Chain q:



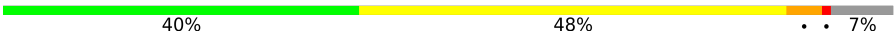

• Molecule 21: Dynein light chain 1, cytoplasmic

Chain r:



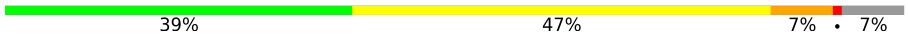

• Molecule 21: Dynein light chain 1, cytoplasmic

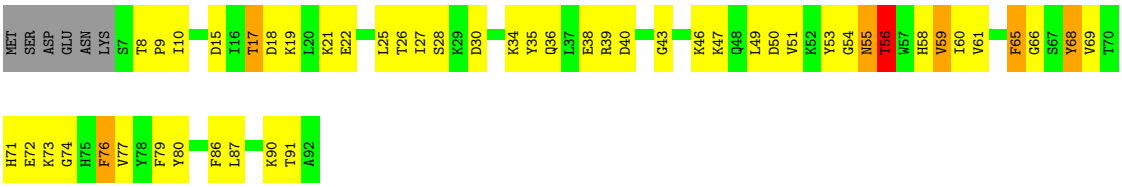
Chain s:



• Molecule 21: Dynein light chain 1, cytoplasmic

Chain t:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SUBTOMOGRAM AVERAGING | Depositor |
| Imposed symmetry | POINT, C8 | Depositor |
| Number of subtomograms used | 518 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY; e2spt_ctf.py was used to identify the precise z height of the particle in the tomogram. This precise height was then used for computing the CTF and performing the CTF correction. | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 4.5 | Depositor |
| Minimum defocus (nm) | 2500 | Depositor |
| Maximum defocus (nm) | 6000 | Depositor |
| Magnification | 42000 | Depositor |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 4082.771 | Depositor |
| Minimum map value | -3.928 | Depositor |
| Average map value | 1772.170 | Depositor |
| Map value standard deviation | 428.825 | Depositor |
| Recommended contour level | 1950 | Depositor |
| Map size (Å) | 2156.7998, 2156.7998, 2156.7998 | wwPDB |
| Map dimensions | 320, 320, 320 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 6.7399993, 6.7399993, 6.7399993 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | 0 | 2.25 | 302/8936 (3.4%) | 2.48 | 599/12074 (5.0%) |
| 1 | Y | 2.34 | 313/8944 (3.5%) | 2.51 | 641/12084 (5.3%) |
| 2 | 1 | 2.31 | 288/9089 (3.2%) | 2.54 | 632/12299 (5.1%) |
| 2 | Z | 2.24 | 289/9076 (3.2%) | 2.49 | 609/12281 (5.0%) |
| 4 | A | 2.17 | 42/1327 (3.2%) | 2.49 | 86/1788 (4.8%) |
| 4 | D | 2.20 | 38/1328 (2.9%) | 2.39 | 75/1791 (4.2%) |
| 4 | G | 2.22 | 41/1334 (3.1%) | 2.63 | 105/1799 (5.8%) |
| 4 | J | 2.21 | 43/1334 (3.2%) | 2.44 | 88/1799 (4.9%) |
| 4 | y | 2.35 | 40/941 (4.3%) | 2.65 | 88/1307 (6.7%) |
| 4 | z | 2.21 | 28/957 (2.9%) | 2.55 | 82/1328 (6.2%) |
| 5 | B | 2.44 | 63/1793 (3.5%) | 2.66 | 149/2411 (6.2%) |
| 5 | E | 2.11 | 47/1793 (2.6%) | 2.39 | 99/2411 (4.1%) |
| 5 | H | 2.37 | 60/1793 (3.3%) | 2.45 | 122/2411 (5.1%) |
| 5 | K | 2.29 | 70/1793 (3.9%) | 2.41 | 102/2411 (4.2%) |
| 6 | C | 2.21 | 45/1364 (3.3%) | 2.44 | 97/1837 (5.3%) |
| 6 | F | 2.27 | 47/1368 (3.4%) | 2.49 | 85/1842 (4.6%) |
| 6 | I | 2.36 | 58/1364 (4.3%) | 2.53 | 106/1837 (5.8%) |
| 6 | L | 2.25 | 39/1368 (2.9%) | 2.64 | 110/1842 (6.0%) |
| 7 | M | 2.24 | 400/12132 (3.3%) | 2.59 | 1018/16441 (6.2%) |
| 7 | O | 2.27 | 416/12125 (3.4%) | 2.58 | 964/16431 (5.9%) |
| 8 | N | 2.27 | 355/11158 (3.2%) | 2.57 | 857/15090 (5.7%) |
| 8 | P | 2.21 | 361/11158 (3.2%) | 2.49 | 804/15090 (5.3%) |
| 9 | Q | 2.27 | 192/5257 (3.7%) | 2.55 | 416/7126 (5.8%) |
| 9 | R | 2.29 | 207/5361 (3.9%) | 2.60 | 448/7273 (6.2%) |
| 9 | S | 2.24 | 183/5270 (3.5%) | 2.52 | 388/7144 (5.4%) |
| 9 | T | 2.32 | 195/5361 (3.6%) | 2.58 | 447/7273 (6.1%) |
| 10 | U | 2.42 | 33/761 (4.3%) | 2.82 | 67/1027 (6.5%) |
| 10 | W | 2.89 | 38/761 (5.0%) | 3.04 | 74/1027 (7.2%) |
| 11 | V | 2.48 | 32/756 (4.2%) | 2.98 | 82/1021 (8.0%) |
| 11 | X | 2.37 | 31/756 (4.1%) | 2.57 | 56/1021 (5.5%) |
| 12 | u | 2.32 | 175/4278 (4.1%) | 2.55 | 312/5833 (5.3%) |
| 12 | v | 2.32 | 156/4119 (3.8%) | 2.52 | 307/5612 (5.5%) |
| 13 | w | 2.39 | 43/1084 (4.0%) | 2.78 | 117/1485 (7.9%) |
| 13 | x | 2.42 | 40/1102 (3.6%) | 2.75 | 108/1510 (7.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 14 | a | 2.23 | 290/8464 (3.4%) | 2.41 | 503/11469 (4.4%) |
| 14 | h | 2.25 | 297/8464 (3.5%) | 2.42 | 537/11469 (4.7%) |
| 15 | b | 2.17 | 169/5533 (3.1%) | 2.37 | 322/7493 (4.3%) |
| 15 | i | 2.21 | 177/5434 (3.3%) | 2.37 | 316/7362 (4.3%) |
| 16 | c | 2.18 | 148/4600 (3.2%) | 2.42 | 269/6211 (4.3%) |
| 16 | j | 2.21 | 153/4600 (3.3%) | 2.38 | 243/6211 (3.9%) |
| 17 | d | 2.29 | 83/2220 (3.7%) | 2.32 | 114/3028 (3.8%) |
| 17 | k | 2.27 | 81/2220 (3.6%) | 2.31 | 109/3028 (3.6%) |
| 18 | e | 2.30 | 94/2466 (3.8%) | 2.36 | 130/3341 (3.9%) |
| 18 | l | 2.34 | 111/2499 (4.4%) | 2.35 | 146/3388 (4.3%) |
| 19 | f | 2.23 | 183/5359 (3.4%) | 2.37 | 300/7258 (4.1%) |
| 19 | m | 2.25 | 192/5359 (3.6%) | 2.44 | 361/7258 (5.0%) |
| 20 | g | 2.20 | 276/8806 (3.1%) | 2.40 | 554/11936 (4.6%) |
| 20 | n | 2.20 | 289/8806 (3.3%) | 2.39 | 532/11936 (4.5%) |
| 21 | o | 2.66 | 34/707 (4.8%) | 2.59 | 54/954 (5.7%) |
| 21 | p | 2.60 | 28/707 (4.0%) | 2.72 | 58/954 (6.1%) |
| 21 | q | 2.64 | 35/707 (5.0%) | 2.59 | 46/954 (4.8%) |
| 21 | r | 2.48 | 20/707 (2.8%) | 2.43 | 40/954 (4.2%) |
| 21 | s | 2.59 | 27/707 (3.8%) | 2.70 | 55/954 (5.8%) |
| 21 | t | 2.67 | 35/707 (5.0%) | 2.74 | 60/954 (6.3%) |
| All | All | 2.27 | 7432/216413 (3.4%) | 2.50 | 15089/293068 (5.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | 0 | 4 | 34 |
| 1 | Y | 6 | 30 |
| 2 | 1 | 12 | 30 |
| 2 | Z | 9 | 25 |
| 4 | A | 0 | 1 |
| 4 | D | 0 | 3 |
| 4 | G | 2 | 3 |
| 4 | J | 0 | 2 |
| 5 | B | 4 | 4 |
| 5 | E | 0 | 3 |
| 5 | H | 2 | 3 |
| 5 | K | 2 | 2 |
| 6 | C | 0 | 2 |
| 6 | F | 1 | 3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 6 | I | 1 | 5 |
| 6 | L | 2 | 5 |
| 7 | M | 5 | 44 |
| 7 | O | 6 | 49 |
| 8 | N | 14 | 44 |
| 8 | P | 6 | 41 |
| 9 | Q | 2 | 16 |
| 9 | R | 2 | 11 |
| 9 | S | 0 | 14 |
| 9 | T | 4 | 19 |
| 10 | U | 4 | 4 |
| 10 | W | 6 | 2 |
| 11 | V | 3 | 2 |
| 11 | X | 2 | 1 |
| 12 | u | 0 | 8 |
| 12 | v | 0 | 14 |
| 13 | x | 0 | 2 |
| 14 | a | 1 | 57 |
| 14 | h | 1 | 49 |
| 15 | b | 0 | 23 |
| 15 | i | 0 | 31 |
| 16 | c | 0 | 21 |
| 16 | j | 0 | 22 |
| 17 | d | 0 | 9 |
| 17 | k | 0 | 3 |
| 18 | e | 0 | 10 |
| 18 | l | 0 | 10 |
| 19 | f | 0 | 21 |
| 19 | m | 1 | 12 |
| 20 | g | 0 | 37 |
| 20 | n | 0 | 34 |
| 21 | o | 2 | 3 |
| 21 | p | 2 | 6 |
| 21 | q | 2 | 5 |
| 21 | r | 2 | 4 |
| 21 | s | 2 | 5 |
| 21 | t | 2 | 6 |
| All | All | 114 | 794 |

All (7432) bond length outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 791 | MET | C-O | 60.97 | 2.45 | 1.23 |
| 8 | N | 794 | ILE | CA-CB | -33.88 | 1.08 | 1.54 |
| 21 | p | 55 | ASN | N-CA | -30.14 | 1.07 | 1.46 |
| 2 | Z | 678 | LYS | N-CA | -28.38 | 1.13 | 1.46 |
| 21 | s | 55 | ASN | N-CA | -27.09 | 1.10 | 1.46 |
| 21 | q | 55 | ASN | N-CA | -26.93 | 1.11 | 1.46 |
| 1 | Y | 832 | VAL | CA-CB | -26.82 | 1.18 | 1.54 |
| 8 | P | 1094 | SER | N-CA | -26.74 | 1.14 | 1.46 |
| 8 | N | 1059 | ASN | N-CA | -26.36 | 1.13 | 1.46 |
| 10 | W | 305 | TYR | CA-CB | -25.61 | 1.12 | 1.53 |
| 5 | B | 323 | LEU | N-CA | -25.30 | 1.13 | 1.46 |
| 5 | B | 324 | TYR | CA-CB | -25.22 | 1.10 | 1.53 |
| 5 | H | 323 | LEU | N-CA | -25.07 | 1.13 | 1.46 |
| 9 | T | 514 | LYS | N-CA | -24.05 | 1.15 | 1.46 |
| 21 | o | 55 | ASN | N-CA | -23.84 | 1.15 | 1.46 |
| 7 | O | 1188 | THR | N-CA | -23.29 | 1.16 | 1.46 |
| 1 | Y | 1022 | ASP | CA-C | -23.13 | 1.21 | 1.52 |
| 10 | W | 284 | LYS | CA-CB | -22.87 | 1.07 | 1.53 |
| 9 | Q | 754 | ARG | CA-CB | -22.61 | 1.15 | 1.53 |
| 2 | Z | 456 | THR | N-CA | -22.42 | 1.18 | 1.46 |
| 21 | t | 55 | ASN | N-CA | -22.38 | 1.16 | 1.46 |
| 11 | V | 302 | ARG | CA-CB | -22.26 | 1.08 | 1.53 |
| 8 | P | 1095 | GLU | CA-CB | -21.74 | 1.16 | 1.53 |
| 7 | O | 1189 | MET | CA-CB | -21.48 | 1.17 | 1.53 |
| 6 | I | 370 | ASP | CA-CB | -21.43 | 1.17 | 1.53 |
| 1 | 0 | 832 | VAL | CA-CB | -21.37 | 1.25 | 1.54 |
| 21 | r | 55 | ASN | N-CA | -21.17 | 1.18 | 1.46 |
| 5 | H | 324 | TYR | CA-CB | -21.11 | 1.17 | 1.53 |
| 2 | 1 | 745 | ILE | CA-C | -20.69 | 1.26 | 1.52 |
| 5 | B | 318 | GLU | N-CA | -20.66 | 1.19 | 1.46 |
| 1 | 0 | 1022 | ASP | CA-CB | -20.48 | 1.18 | 1.53 |
| 2 | 1 | 744 | GLY | N-CA | -20.42 | 1.12 | 1.45 |
| 21 | t | 56 | THR | CA-C | -20.30 | 1.25 | 1.52 |
| 4 | G | 726 | VAL | N-CA | -20.22 | 1.21 | 1.46 |
| 8 | N | 257 | LEU | CA-CB | -19.90 | 1.19 | 1.53 |
| 8 | N | 552 | LEU | CA-CB | -19.90 | 1.19 | 1.53 |
| 2 | 1 | 309 | LEU | CA-CB | -19.87 | 1.13 | 1.53 |
| 7 | M | 1189 | MET | CA-CB | -19.84 | 1.20 | 1.53 |
| 7 | O | 1137 | ASN | N-CA | -19.66 | 1.08 | 1.46 |
| 7 | O | 1138 | PHE | CA-CB | -19.64 | 1.20 | 1.53 |
| 7 | O | 603 | GLU | CA-CB | -19.63 | 1.20 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 915 | LYS | N-CA | -19.52 | 1.21 | 1.46 |
| 2 | 1 | 1300 | SER | N-CA | -19.44 | 1.21 | 1.46 |
| 5 | K | 318 | GLU | N-CA | -19.34 | 1.21 | 1.46 |
| 2 | 1 | 922 | LYS | CA-CB | -19.33 | 1.20 | 1.53 |
| 2 | 1 | 916 | PHE | CA-CB | -19.10 | 1.15 | 1.53 |
| 2 | Z | 922 | LYS | CA-CB | -18.88 | 1.21 | 1.53 |
| 2 | 1 | 678 | LYS | CA-CB | -18.86 | 1.21 | 1.53 |
| 1 | 0 | 1258 | LEU | CA-CB | -18.65 | 1.22 | 1.53 |
| 19 | m | 373 | THR | CA-C | -18.53 | 1.27 | 1.52 |
| 2 | 1 | 915 | LYS | N-CA | -18.28 | 1.22 | 1.46 |
| 2 | Z | 679 | SER | CA-CB | -18.09 | 1.22 | 1.53 |
| 1 | 0 | 1257 | GLN | N-CA | -18.00 | 1.12 | 1.46 |
| 8 | N | 1095 | GLU | CA-C | -17.99 | 1.28 | 1.52 |
| 19 | m | 372 | GLY | N-CA | -17.86 | 1.17 | 1.45 |
| 5 | B | 319 | THR | CA-CB | -17.51 | 1.23 | 1.53 |
| 10 | W | 304 | LYS | N-CA | -17.42 | 1.13 | 1.46 |
| 10 | W | 283 | ILE | N-CA | -17.30 | 1.21 | 1.46 |
| 21 | t | 56 | THR | CA-CB | -16.91 | 1.24 | 1.53 |
| 2 | 1 | 921 | SER | N-CA | -16.68 | 1.14 | 1.46 |
| 21 | o | 56 | THR | CA-CB | -16.67 | 1.25 | 1.53 |
| 8 | N | 551 | ASN | CA-CB | -16.61 | 1.20 | 1.53 |
| 9 | T | 754 | ARG | CA-CB | -16.61 | 1.25 | 1.53 |
| 10 | U | 249 | ASP | CA-CB | -16.48 | 1.25 | 1.53 |
| 7 | M | 1273 | LYS | CA-CB | -16.44 | 1.25 | 1.53 |
| 10 | W | 249 | ASP | CA-CB | -16.43 | 1.25 | 1.53 |
| 8 | N | 1060 | LEU | CA-CB | -16.40 | 1.25 | 1.53 |
| 6 | F | 370 | ASP | CA-CB | -16.23 | 1.26 | 1.53 |
| 7 | M | 352 | ILE | CA-C | 16.13 | 1.64 | 1.52 |
| 21 | s | 56 | THR | CA-CB | -16.06 | 1.26 | 1.53 |
| 2 | 1 | 1301 | SER | CA-CB | -15.93 | 1.26 | 1.53 |
| 11 | V | 402 | ASN | CA-CB | -15.86 | 1.21 | 1.53 |
| 5 | K | 319 | THR | CA-CB | -15.80 | 1.26 | 1.53 |
| 21 | q | 56 | THR | CA-CB | -15.73 | 1.26 | 1.53 |
| 11 | X | 401 | ASP | N-CA | -15.58 | 1.26 | 1.46 |
| 10 | U | 284 | LYS | CA-CB | -15.58 | 1.22 | 1.53 |
| 8 | P | 257 | LEU | CA-CB | -15.51 | 1.27 | 1.53 |
| 2 | 1 | 679 | SER | CA-CB | -15.49 | 1.27 | 1.53 |
| 2 | Z | 921 | SER | N-CA | -15.37 | 1.17 | 1.46 |
| 7 | O | 602 | ASN | N-CA | -15.35 | 1.17 | 1.46 |
| 2 | Z | 457 | SER | CA-CB | -15.31 | 1.22 | 1.53 |
| 2 | 1 | 1039 | LEU | N-CA | -15.23 | 1.17 | 1.46 |
| 2 | 1 | 308 | ASN | N-CA | -15.15 | 1.25 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 1258 | LEU | CA-C | -15.01 | 1.32 | 1.52 |
| 8 | N | 576 | TYR | N-CA | -14.84 | 1.27 | 1.46 |
| 8 | N | 132 | ASN | CA-CB | -14.79 | 1.28 | 1.53 |
| 21 | p | 56 | THR | CA-CB | -14.79 | 1.28 | 1.53 |
| 9 | T | 753 | ALA | N-CA | -14.77 | 1.18 | 1.46 |
| 2 | Z | 916 | PHE | CA-CB | -14.71 | 1.24 | 1.53 |
| 8 | P | 577 | MET | CA-CB | -14.64 | 1.24 | 1.53 |
| 21 | p | 56 | THR | CA-C | -14.60 | 1.33 | 1.52 |
| 21 | r | 56 | THR | CA-C | -14.57 | 1.33 | 1.52 |
| 1 | 0 | 831 | LYS | CA-CB | -14.57 | 1.24 | 1.53 |
| 21 | o | 56 | THR | CA-C | -14.44 | 1.33 | 1.52 |
| 9 | R | 514 | LYS | N-CA | -14.00 | 1.28 | 1.46 |
| 6 | L | 370 | ASP | CA-CB | -13.98 | 1.29 | 1.53 |
| 2 | Z | 891 | ARG | CA-CB | -13.95 | 1.25 | 1.53 |
| 10 | W | 248 | TRP | N-CA | -13.87 | 1.19 | 1.46 |
| 11 | V | 301 | LEU | N-CA | -13.60 | 1.28 | 1.46 |
| 8 | N | 577 | MET | CA-CB | -13.55 | 1.26 | 1.53 |
| 7 | M | 1137 | ASN | N-CA | -13.54 | 1.20 | 1.46 |
| 4 | G | 727 | SER | CA-CB | -13.52 | 1.26 | 1.53 |
| 18 | l | 317 | THR | CA-C | -13.21 | 1.39 | 1.52 |
| 1 | Y | 831 | LYS | N-CA | -13.06 | 1.21 | 1.46 |
| 7 | M | 1188 | THR | N-CA | -12.83 | 1.29 | 1.46 |
| 11 | X | 402 | ASN | CA-CB | -12.69 | 1.28 | 1.53 |
| 21 | r | 56 | THR | CA-CB | -12.56 | 1.32 | 1.53 |
| 6 | I | 369 | LEU | CA-CB | -12.56 | 1.28 | 1.53 |
| 7 | M | 1342 | TYR | CA-CB | 12.50 | 1.65 | 1.53 |
| 8 | N | 131 | ASP | N-CA | -12.28 | 1.23 | 1.46 |
| 12 | u | 353 | ARG | CA-C | -12.27 | 1.38 | 1.52 |
| 8 | N | 1094 | SER | CA-CB | -12.26 | 1.34 | 1.52 |
| 10 | U | 248 | TRP | N-CA | -12.26 | 1.23 | 1.46 |
| 1 | Y | 1257 | GLN | N-CA | -12.26 | 1.23 | 1.46 |
| 5 | B | 324 | TYR | CA-C | 12.20 | 1.69 | 1.52 |
| 11 | V | 401 | ASP | N-CA | -12.13 | 1.30 | 1.46 |
| 1 | Y | 1258 | LEU | CA-CB | -11.98 | 1.33 | 1.53 |
| 8 | N | 808 | THR | CA-C | 11.78 | 1.62 | 1.52 |
| 7 | M | 1138 | PHE | CA-CB | -11.75 | 1.33 | 1.53 |
| 21 | s | 56 | THR | CA-C | -11.66 | 1.37 | 1.52 |
| 21 | q | 56 | THR | CA-C | -11.52 | 1.37 | 1.52 |
| 9 | R | 515 | LEU | CA-CB | -11.49 | 1.30 | 1.53 |
| 21 | r | 87 | LEU | N-CA | -11.40 | 1.32 | 1.46 |
| 16 | j | 564 | SER | CA-C | -11.27 | 1.43 | 1.52 |
| 9 | S | 267 | ASP | CA-C | -11.21 | 1.39 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | P | 576 | TYR | N-CA | -11.20 | 1.31 | 1.46 |
| 9 | T | 218 | ILE | CA-C | -11.20 | 1.38 | 1.52 |
| 1 | 0 | 1236 | LEU | N-CA | -11.12 | 1.32 | 1.46 |
| 2 | 1 | 282 | ASN | CA-CB | 11.09 | 1.61 | 1.53 |
| 14 | h | 104 | GLN | CA-C | -11.07 | 1.47 | 1.53 |
| 18 | e | 120 | HIS | ND1-CE1 | 11.00 | 1.43 | 1.32 |
| 11 | V | 361 | ASN | CA-C | -10.88 | 1.45 | 1.52 |
| 7 | O | 1526 | ILE | CA-CB | -10.84 | 1.41 | 1.54 |
| 9 | T | 345 | LEU | C-N | 10.81 | 1.47 | 1.34 |
| 20 | n | 297 | LEU | CA-C | -10.80 | 1.39 | 1.52 |
| 8 | N | 1095 | GLU | CA-CB | -10.78 | 1.35 | 1.53 |
| 16 | c | 777 | PRO | CA-C | -10.76 | 1.40 | 1.53 |
| 19 | m | 523 | TYR | N-CA | -10.71 | 1.36 | 1.46 |
| 20 | n | 471 | GLN | CA-CB | 10.70 | 1.61 | 1.53 |
| 18 | l | 152 | SER | CA-C | -10.68 | 1.40 | 1.52 |
| 9 | R | 301 | ASN | C-N | 10.56 | 1.45 | 1.34 |
| 8 | N | 132 | ASN | CA-C | -10.54 | 1.38 | 1.52 |
| 9 | T | 100 | PRO | CA-C | 10.54 | 1.61 | 1.52 |
| 1 | Y | 1440 | ASP | CA-C | -10.51 | 1.43 | 1.53 |
| 17 | k | 272 | SER | CA-C | -10.42 | 1.40 | 1.52 |
| 1 | Y | 1021 | TYR | CA-CB | -10.42 | 1.32 | 1.53 |
| 20 | n | 180 | SER | CA-CB | 10.35 | 1.66 | 1.52 |
| 12 | v | 46 | TYR | CA-C | -10.35 | 1.43 | 1.53 |
| 15 | b | 475 | SER | CA-C | -10.30 | 1.38 | 1.52 |
| 14 | a | 524 | VAL | CA-CB | -10.30 | 1.42 | 1.54 |
| 19 | m | 685 | SER | CA-C | -10.26 | 1.39 | 1.52 |
| 2 | 1 | 1301 | SER | CA-C | -10.22 | 1.39 | 1.52 |
| 2 | 1 | 678 | LYS | N-CA | 10.19 | 1.61 | 1.46 |
| 8 | N | 597 | LEU | C-N | 10.18 | 1.46 | 1.34 |
| 20 | g | 347 | PHE | CA-CB | 10.16 | 1.67 | 1.52 |
| 8 | N | 552 | LEU | CA-C | -10.12 | 1.39 | 1.52 |
| 9 | Q | 753 | ALA | CA-CB | -10.10 | 1.19 | 1.52 |
| 4 | J | 692 | LYS | C-N | 10.09 | 1.44 | 1.34 |
| 14 | h | 162 | VAL | CA-C | -10.09 | 1.44 | 1.53 |
| 8 | P | 449 | ASP | CA-C | -10.07 | 1.44 | 1.52 |
| 2 | 1 | 745 | ILE | CA-CB | -10.07 | 1.40 | 1.54 |
| 7 | O | 603 | GLU | CA-C | -10.07 | 1.39 | 1.52 |
| 2 | Z | 136 | THR | C-O | -10.02 | 1.16 | 1.25 |
| 2 | Z | 1283 | PHE | N-CA | -9.99 | 1.37 | 1.46 |
| 14 | a | 79 | LEU | CA-C | -9.98 | 1.43 | 1.53 |
| 7 | M | 916 | ILE | CA-C | 9.96 | 1.65 | 1.52 |
| 6 | L | 369 | LEU | N-CA | -9.96 | 1.27 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 680 | PHE | CA-C | -9.95 | 1.43 | 1.53 |
| 9 | R | 299 | ALA | CA-C | -9.94 | 1.39 | 1.52 |
| 5 | B | 316 | VAL | CA-C | 9.90 | 1.64 | 1.52 |
| 8 | P | 1046 | LYS | CA-C | -9.88 | 1.39 | 1.52 |
| 10 | U | 283 | ILE | N-CA | -9.85 | 1.34 | 1.46 |
| 16 | j | 441 | ARG | CA-C | -9.84 | 1.48 | 1.53 |
| 14 | a | 830 | LEU | N-CA | -9.83 | 1.34 | 1.46 |
| 1 | 0 | 394 | GLU | C-N | 9.81 | 1.56 | 1.33 |
| 2 | 1 | 679 | SER | CA-C | -9.79 | 1.39 | 1.52 |
| 18 | l | 240 | ILE | N-CA | -9.77 | 1.34 | 1.46 |
| 8 | P | 1440 | GLY | CA-C | -9.76 | 1.41 | 1.52 |
| 9 | T | 595 | ARG | CA-C | -9.74 | 1.42 | 1.53 |
| 4 | J | 766 | ILE | C-N | 9.72 | 1.45 | 1.33 |
| 2 | 1 | 309 | LEU | CA-C | 9.71 | 1.73 | 1.52 |
| 9 | T | 515 | LEU | CA-CB | -9.71 | 1.34 | 1.53 |
| 14 | h | 669 | ARG | CD-NE | 9.66 | 1.59 | 1.46 |
| 10 | W | 320 | SER | CA-C | -9.65 | 1.40 | 1.52 |
| 19 | m | 554 | ASN | C-N | 9.65 | 1.44 | 1.34 |
| 1 | 0 | 713 | ILE | CA-CB | -9.64 | 1.42 | 1.53 |
| 7 | O | 980 | ASP | N-CA | -9.64 | 1.34 | 1.46 |
| 1 | 0 | 1009 | HIS | ND1-CE1 | 9.63 | 1.42 | 1.32 |
| 8 | N | 996 | THR | C-N | 9.59 | 1.42 | 1.33 |
| 1 | 0 | 393 | ILE | C-N | -9.59 | 1.13 | 1.33 |
| 7 | O | 1199 | ASP | N-CA | -9.58 | 1.38 | 1.46 |
| 14 | h | 282 | LEU | CA-C | -9.57 | 1.41 | 1.52 |
| 16 | j | 425 | TYR | CA-C | -9.55 | 1.39 | 1.52 |
| 9 | T | 515 | LEU | CA-C | -9.52 | 1.32 | 1.52 |
| 9 | Q | 275 | LYS | CA-C | -9.52 | 1.43 | 1.52 |
| 2 | 1 | 1385 | ASP | C-N | 9.50 | 1.45 | 1.33 |
| 6 | C | 308 | ILE | CA-C | 9.50 | 1.62 | 1.52 |
| 14 | a | 343 | ASN | N-CA | -9.50 | 1.38 | 1.47 |
| 19 | f | 58 | ASP | CA-CB | 9.47 | 1.68 | 1.53 |
| 9 | T | 323 | SER | CA-C | -9.46 | 1.40 | 1.52 |
| 5 | B | 309 | ARG | NE-CZ | 9.45 | 1.43 | 1.33 |
| 9 | Q | 226 | ARG | NE-CZ | 9.44 | 1.43 | 1.33 |
| 7 | M | 1407 | ILE | CA-C | 9.40 | 1.64 | 1.52 |
| 7 | O | 560 | GLN | C-N | 9.38 | 1.45 | 1.33 |
| 8 | P | 204 | VAL | CA-CB | -9.35 | 1.47 | 1.54 |
| 8 | P | 218 | ASN | CA-C | 9.35 | 1.61 | 1.52 |
| 1 | Y | 666 | PRO | CA-C | -9.35 | 1.43 | 1.52 |
| 15 | i | 66 | PRO | N-CD | 9.33 | 1.60 | 1.47 |
| 8 | N | 928 | SER | N-CA | -9.32 | 1.39 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 582 | THR | C-N | 9.31 | 1.44 | 1.33 |
| 14 | h | 383 | ASN | N-CA | -9.31 | 1.35 | 1.46 |
| 20 | g | 166 | ILE | CA-CB | 9.30 | 1.64 | 1.54 |
| 21 | o | 83 | PRO | CA-C | 9.28 | 1.61 | 1.52 |
| 14 | h | 27 | TYR | CA-C | -9.28 | 1.41 | 1.52 |
| 8 | N | 603 | ASP | CA-C | 9.27 | 1.64 | 1.52 |
| 14 | a | 143 | ASN | CA-C | -9.26 | 1.41 | 1.52 |
| 9 | R | 240 | SER | C-N | 9.22 | 1.43 | 1.34 |
| 1 | Y | 1414 | SER | CA-C | -9.22 | 1.40 | 1.52 |
| 12 | u | 428 | TYR | CA-CB | 9.20 | 1.64 | 1.53 |
| 8 | P | 465 | VAL | CA-C | -9.18 | 1.41 | 1.52 |
| 9 | S | 122 | LEU | CA-C | -9.18 | 1.41 | 1.52 |
| 7 | M | 1251 | ARG | CD-NE | 9.15 | 1.59 | 1.46 |
| 6 | L | 311 | ASP | CA-CB | 9.15 | 1.67 | 1.53 |
| 20 | g | 554 | GLY | CA-C | -9.14 | 1.39 | 1.51 |
| 8 | P | 1337 | LEU | C-N | 9.14 | 1.46 | 1.33 |
| 1 | Y | 253 | GLU | CA-C | -9.14 | 1.41 | 1.52 |
| 8 | P | 1408 | LEU | CA-C | -9.14 | 1.41 | 1.52 |
| 14 | h | 506 | LEU | CA-C | -9.13 | 1.41 | 1.52 |
| 8 | P | 1320 | GLU | CA-C | -9.12 | 1.40 | 1.52 |
| 8 | N | 1122 | PHE | CA-C | -9.08 | 1.41 | 1.53 |
| 8 | N | 761 | PHE | N-CA | -9.07 | 1.35 | 1.46 |
| 9 | Q | 709 | LYS | CA-C | -9.05 | 1.40 | 1.52 |
| 20 | n | 757 | LYS | C-N | 9.05 | 1.44 | 1.33 |
| 16 | j | 280 | ILE | CA-C | -9.04 | 1.41 | 1.52 |
| 6 | F | 369 | LEU | N-CA | -9.03 | 1.29 | 1.46 |
| 2 | Z | 1277 | ARG | NE-CZ | 9.03 | 1.43 | 1.33 |
| 7 | O | 750 | TRP | CA-C | 9.02 | 1.63 | 1.52 |
| 15 | b | 678 | ASP | C-N | 9.01 | 1.40 | 1.33 |
| 1 | 0 | 915 | GLU | N-CA | -9.01 | 1.38 | 1.46 |
| 9 | S | 48 | GLU | C-N | 9.00 | 1.45 | 1.33 |
| 2 | Z | 711 | GLY | CA-C | -8.99 | 1.41 | 1.52 |
| 9 | S | 549 | ASP | CA-CB | 8.98 | 1.61 | 1.53 |
| 14 | a | 58 | ASN | CA-C | -8.94 | 1.41 | 1.52 |
| 6 | F | 292 | HIS | ND1-CE1 | 8.93 | 1.41 | 1.32 |
| 7 | O | 950 | GLU | CA-C | -8.92 | 1.42 | 1.52 |
| 7 | O | 159 | LYS | C-N | 8.92 | 1.46 | 1.33 |
| 7 | O | 465 | GLU | CA-C | -8.91 | 1.41 | 1.52 |
| 2 | 1 | 932 | ILE | N-CA | -8.91 | 1.38 | 1.46 |
| 9 | S | 707 | HIS | ND1-CE1 | 8.91 | 1.41 | 1.32 |
| 20 | n | 755 | GLN | CA-C | -8.91 | 1.41 | 1.52 |
| 12 | u | 289 | PRO | CA-C | -8.89 | 1.43 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 18 | e | 95 | GLY | C-N | 8.88 | 1.46 | 1.33 |
| 1 | Y | 592 | TYR | CA-C | -8.87 | 1.42 | 1.52 |
| 20 | n | 1024 | VAL | N-CA | -8.85 | 1.34 | 1.46 |
| 20 | n | 922 | LEU | CA-C | -8.84 | 1.41 | 1.52 |
| 2 | 1 | 1302 | ALA | CA-C | -8.83 | 1.41 | 1.52 |
| 7 | O | 779 | PRO | CA-C | -8.83 | 1.39 | 1.52 |
| 1 | 0 | 181 | ARG | CA-C | -8.82 | 1.42 | 1.52 |
| 20 | n | 335 | ASP | CA-C | -8.82 | 1.42 | 1.52 |
| 9 | T | 39 | LEU | CA-C | -8.82 | 1.41 | 1.52 |
| 16 | j | 590 | ASN | CA-CB | 8.82 | 1.68 | 1.53 |
| 14 | h | 156 | TYR | CA-C | -8.81 | 1.41 | 1.52 |
| 12 | v | 81 | CYS | CA-C | -8.80 | 1.42 | 1.52 |
| 7 | O | 16 | GLU | CA-C | -8.79 | 1.41 | 1.52 |
| 18 | e | 337 | ASN | CA-CB | 8.79 | 1.68 | 1.53 |
| 8 | N | 615 | LEU | CA-C | 8.79 | 1.64 | 1.52 |
| 13 | x | 1233 | ARG | CA-C | -8.78 | 1.41 | 1.52 |
| 7 | M | 1197 | PHE | CA-C | -8.77 | 1.41 | 1.52 |
| 9 | R | 590 | LEU | CA-C | -8.76 | 1.42 | 1.52 |
| 14 | h | 404 | VAL | N-CA | -8.75 | 1.35 | 1.46 |
| 19 | m | 78 | VAL | N-CA | -8.75 | 1.36 | 1.46 |
| 2 | Z | 422 | LEU | CA-C | -8.73 | 1.42 | 1.52 |
| 6 | I | 339 | LEU | C-N | 8.73 | 1.43 | 1.34 |
| 7 | M | 1138 | PHE | CA-C | -8.73 | 1.41 | 1.52 |
| 12 | v | 326 | LEU | CA-C | -8.72 | 1.41 | 1.52 |
| 7 | O | 237 | PHE | N-CA | -8.72 | 1.36 | 1.46 |
| 15 | b | 364 | TYR | C-N | 8.69 | 1.43 | 1.33 |
| 1 | 0 | 713 | ILE | CA-C | -8.69 | 1.43 | 1.53 |
| 15 | i | 364 | TYR | C-N | 8.68 | 1.39 | 1.33 |
| 17 | k | 264 | LEU | C-N | 8.68 | 1.45 | 1.33 |
| 1 | 0 | 419 | LYS | C-N | 8.67 | 1.45 | 1.33 |
| 20 | n | 281 | ARG | NE-CZ | 8.66 | 1.42 | 1.33 |
| 8 | P | 1337 | LEU | CA-CB | 8.66 | 1.66 | 1.53 |
| 8 | P | 576 | TYR | CA-CB | -8.66 | 1.38 | 1.53 |
| 12 | v | 354 | VAL | N-CA | -8.65 | 1.35 | 1.46 |
| 12 | u | 144 | VAL | N-CA | -8.65 | 1.35 | 1.46 |
| 19 | m | 517 | LEU | N-CA | -8.64 | 1.36 | 1.46 |
| 2 | Z | 486 | GLN | N-CA | -8.64 | 1.36 | 1.46 |
| 19 | m | 305 | ASN | N-CA | -8.63 | 1.34 | 1.46 |
| 7 | O | 35 | LEU | CA-C | -8.63 | 1.42 | 1.52 |
| 6 | I | 402 | ASP | CA-CB | 8.63 | 1.66 | 1.53 |
| 17 | k | 210 | VAL | CA-C | -8.61 | 1.41 | 1.52 |
| 2 | 1 | 819 | ILE | C-N | 8.61 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 11 | X | 271 | ILE | C-N | 8.60 | 1.41 | 1.33 |
| 21 | q | 68 | TYR | CA-C | -8.60 | 1.43 | 1.52 |
| 2 | 1 | 1118 | LEU | CA-CB | 8.60 | 1.63 | 1.52 |
| 20 | n | 785 | HIS | N-CA | -8.60 | 1.36 | 1.46 |
| 8 | N | 136 | ASN | CA-CB | 8.59 | 1.62 | 1.53 |
| 19 | f | 145 | LEU | CA-C | -8.59 | 1.44 | 1.52 |
| 9 | Q | 731 | GLN | CA-CB | 8.58 | 1.66 | 1.53 |
| 19 | m | 516 | TRP | NE1-CE2 | -8.57 | 1.28 | 1.37 |
| 9 | T | 754 | ARG | CA-C | -8.57 | 1.41 | 1.52 |
| 2 | Z | 1249 | PRO | CA-C | -8.57 | 1.43 | 1.53 |
| 7 | M | 1502 | THR | CA-C | -8.56 | 1.42 | 1.52 |
| 20 | g | 115 | LYS | CA-C | -8.56 | 1.42 | 1.52 |
| 8 | N | 755 | ASN | CA-CB | 8.56 | 1.65 | 1.53 |
| 20 | n | 929 | LEU | CA-CB | 8.56 | 1.67 | 1.53 |
| 9 | R | 287 | ASP | CA-C | -8.56 | 1.40 | 1.52 |
| 1 | 0 | 943 | ASP | CA-CB | 8.55 | 1.65 | 1.53 |
| 18 | e | 80 | THR | CA-C | -8.55 | 1.42 | 1.52 |
| 20 | g | 280 | THR | CA-C | -8.55 | 1.44 | 1.53 |
| 4 | z | 818 | ILE | CA-C | -8.54 | 1.42 | 1.52 |
| 16 | j | 154 | SER | N-CA | -8.54 | 1.35 | 1.46 |
| 14 | a | 651 | ILE | CA-C | -8.54 | 1.42 | 1.52 |
| 16 | j | 635 | ASP | N-CA | -8.53 | 1.36 | 1.46 |
| 9 | Q | 723 | ILE | CA-CB | 8.53 | 1.64 | 1.54 |
| 9 | S | 90 | LEU | CA-C | -8.52 | 1.42 | 1.52 |
| 14 | h | 957 | ASP | CA-C | -8.52 | 1.42 | 1.52 |
| 7 | M | 1435 | LYS | C-O | -8.52 | 1.13 | 1.24 |
| 13 | x | 1288 | ILE | N-CA | -8.52 | 1.36 | 1.46 |
| 16 | j | 453 | LEU | C-N | 8.51 | 1.44 | 1.33 |
| 20 | n | 572 | ALA | N-CA | -8.51 | 1.36 | 1.46 |
| 8 | N | 1541 | LEU | N-CA | -8.51 | 1.35 | 1.46 |
| 14 | a | 332 | VAL | C-N | 8.51 | 1.44 | 1.33 |
| 2 | Z | 231 | TYR | CA-CB | 8.50 | 1.63 | 1.52 |
| 7 | O | 244 | LEU | CA-C | -8.49 | 1.40 | 1.52 |
| 9 | T | 130 | ASN | CA-C | -8.49 | 1.41 | 1.52 |
| 14 | a | 893 | HIS | ND1-CE1 | 8.49 | 1.41 | 1.32 |
| 20 | g | 449 | LEU | CA-C | -8.48 | 1.42 | 1.52 |
| 19 | m | 31 | ASN | CA-CB | 8.47 | 1.63 | 1.53 |
| 1 | Y | 297 | HIS | ND1-CE1 | 8.47 | 1.41 | 1.32 |
| 6 | I | 323 | SER | N-CA | -8.47 | 1.36 | 1.46 |
| 7 | O | 1588 | VAL | CA-CB | -8.47 | 1.44 | 1.54 |
| 12 | v | 186 | GLU | CA-C | -8.46 | 1.42 | 1.53 |
| 17 | k | 138 | PRO | CA-C | -8.46 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1344 | PHE | CA-CB | 8.46 | 1.67 | 1.53 |
| 2 | 1 | 614 | TYR | CA-C | -8.45 | 1.42 | 1.52 |
| 16 | c | 458 | ARG | NE-CZ | 8.45 | 1.42 | 1.33 |
| 9 | S | 443 | ILE | CA-C | -8.45 | 1.43 | 1.52 |
| 2 | Z | 1161 | HIS | CB-CG | -8.45 | 1.38 | 1.50 |
| 8 | N | 568 | ILE | N-CA | -8.44 | 1.35 | 1.46 |
| 1 | 0 | 589 | HIS | CA-C | -8.44 | 1.40 | 1.52 |
| 9 | T | 757 | ALA | N-CA | -8.42 | 1.35 | 1.46 |
| 1 | Y | 167 | SER | N-CA | -8.42 | 1.36 | 1.46 |
| 9 | T | 615 | ASP | CA-CB | 8.42 | 1.63 | 1.52 |
| 7 | O | 1288 | ASN | CA-C | -8.42 | 1.43 | 1.53 |
| 18 | l | 32 | HIS | ND1-CE1 | 8.41 | 1.41 | 1.32 |
| 2 | Z | 1322 | TYR | CA-C | -8.41 | 1.42 | 1.52 |
| 5 | H | 391 | GLU | C-N | 8.40 | 1.44 | 1.33 |
| 14 | a | 626 | HIS | ND1-CE1 | 8.40 | 1.41 | 1.32 |
| 21 | o | 71 | HIS | CE1-NE2 | -8.39 | 1.24 | 1.32 |
| 1 | Y | 1022 | ASP | CA-CB | -8.39 | 1.39 | 1.53 |
| 2 | 1 | 248 | ASN | CA-C | -8.39 | 1.42 | 1.52 |
| 20 | n | 261 | PHE | CA-CB | 8.38 | 1.65 | 1.53 |
| 20 | n | 532 | LYS | N-CA | -8.38 | 1.36 | 1.46 |
| 18 | l | 238 | GLY | C-N | 8.38 | 1.44 | 1.33 |
| 8 | N | 1028 | THR | CA-C | -8.38 | 1.41 | 1.52 |
| 1 | Y | 192 | LEU | CA-C | -8.38 | 1.42 | 1.52 |
| 19 | m | 363 | VAL | CA-C | -8.38 | 1.42 | 1.52 |
| 12 | u | 183 | THR | CA-C | -8.38 | 1.42 | 1.52 |
| 7 | M | 1336 | ILE | CA-CB | -8.37 | 1.49 | 1.54 |
| 9 | S | 649 | GLU | N-CA | 8.36 | 1.56 | 1.46 |
| 14 | a | 157 | ASP | CA-C | -8.37 | 1.41 | 1.53 |
| 12 | v | 157 | LEU | CA-C | -8.36 | 1.41 | 1.52 |
| 20 | n | 735 | LEU | CA-C | -8.36 | 1.45 | 1.52 |
| 12 | u | 364 | ILE | N-CA | -8.35 | 1.36 | 1.46 |
| 1 | 0 | 658 | ILE | CA-CB | 8.35 | 1.64 | 1.54 |
| 1 | Y | 124 | ARG | NE-CZ | 8.35 | 1.42 | 1.33 |
| 12 | v | 153 | MET | N-CA | -8.34 | 1.35 | 1.46 |
| 6 | F | 293 | HIS | ND1-CE1 | 8.34 | 1.40 | 1.32 |
| 6 | F | 452 | ASP | CA-C | -8.34 | 1.42 | 1.52 |
| 20 | n | 328 | HIS | ND1-CE1 | 8.34 | 1.40 | 1.32 |
| 2 | Z | 380 | ASP | CA-CB | 8.33 | 1.66 | 1.53 |
| 14 | h | 821 | HIS | CA-C | -8.33 | 1.41 | 1.52 |
| 9 | R | 833 | ILE | CA-C | 8.33 | 1.63 | 1.52 |
| 12 | v | 184 | ASP | CA-C | -8.33 | 1.42 | 1.52 |
| 15 | b | 213 | ASN | C-N | 8.33 | 1.44 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 234 | ILE | CA-C | -8.32 | 1.42 | 1.52 |
| 19 | f | 415 | THR | CA-C | 8.32 | 1.64 | 1.52 |
| 9 | R | 112 | TYR | C-N | 8.32 | 1.42 | 1.33 |
| 2 | Z | 667 | ALA | CA-CB | 8.31 | 1.65 | 1.54 |
| 7 | O | 1439 | GLU | N-CA | -8.31 | 1.36 | 1.46 |
| 8 | P | 1255 | ILE | CA-C | -8.31 | 1.42 | 1.52 |
| 7 | O | 210 | LYS | C-N | 8.31 | 1.45 | 1.33 |
| 7 | M | 1274 | ASP | CA-C | -8.30 | 1.44 | 1.52 |
| 7 | O | 820 | GLN | CA-CB | 8.30 | 1.65 | 1.53 |
| 21 | o | 68 | TYR | CA-CB | 8.30 | 1.63 | 1.53 |
| 7 | O | 736 | PHE | C-N | 8.30 | 1.41 | 1.33 |
| 1 | Y | 851 | GLU | CA-C | -8.29 | 1.42 | 1.52 |
| 20 | n | 959 | ASN | CA-CB | 8.28 | 1.66 | 1.53 |
| 20 | n | 1141 | ALA | CA-C | -8.28 | 1.41 | 1.52 |
| 8 | P | 1423 | ASN | CA-CB | 8.27 | 1.63 | 1.53 |
| 10 | U | 272 | ASN | CA-CB | 8.27 | 1.66 | 1.54 |
| 1 | Y | 146 | THR | CA-C | -8.26 | 1.43 | 1.52 |
| 1 | Y | 421 | VAL | N-CA | -8.25 | 1.36 | 1.46 |
| 7 | M | 310 | MET | N-CA | -8.25 | 1.36 | 1.46 |
| 9 | S | 79 | SER | CA-C | -8.25 | 1.43 | 1.53 |
| 7 | M | 869 | VAL | CA-CB | -8.25 | 1.45 | 1.54 |
| 8 | N | 272 | ILE | CA-CB | -8.25 | 1.44 | 1.54 |
| 19 | f | 124 | VAL | N-CA | 8.24 | 1.56 | 1.46 |
| 2 | 1 | 240 | ARG | CA-CB | 8.23 | 1.63 | 1.53 |
| 19 | m | 678 | LEU | CA-C | -8.23 | 1.41 | 1.52 |
| 1 | Y | 783 | ASP | CA-C | -8.22 | 1.42 | 1.52 |
| 7 | O | 825 | ILE | CA-CB | -8.22 | 1.50 | 1.54 |
| 12 | u | 159 | SER | C-N | 8.22 | 1.45 | 1.33 |
| 2 | 1 | 749 | ARG | NE-CZ | 8.21 | 1.42 | 1.33 |
| 20 | n | 267 | VAL | CA-C | -8.21 | 1.43 | 1.53 |
| 7 | M | 1423 | SER | CA-CB | 8.21 | 1.66 | 1.53 |
| 11 | X | 396 | ALA | N-CA | -8.20 | 1.36 | 1.46 |
| 8 | P | 47 | ASN | N-CA | -8.20 | 1.34 | 1.45 |
| 9 | Q | 607 | ARG | CA-C | -8.20 | 1.41 | 1.52 |
| 17 | k | 250 | GLU | CA-CB | 8.20 | 1.64 | 1.53 |
| 1 | Y | 432 | ASN | CA-C | -8.19 | 1.43 | 1.52 |
| 7 | M | 510 | PHE | CA-CB | 8.19 | 1.66 | 1.53 |
| 1 | 0 | 1307 | LEU | N-CA | -8.18 | 1.36 | 1.46 |
| 9 | T | 99 | ASN | N-CA | -8.18 | 1.40 | 1.46 |
| 6 | I | 378 | HIS | ND1-CE1 | 8.18 | 1.40 | 1.32 |
| 16 | c | 199 | ILE | CA-C | -8.18 | 1.43 | 1.52 |
| 15 | b | 433 | ILE | CA-C | -8.18 | 1.43 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | N | 1227 | VAL | N-CA | -8.17 | 1.37 | 1.46 |
| 14 | h | 135 | LEU | C-N | 8.17 | 1.45 | 1.33 |
| 15 | b | 422 | MET | CA-CB | 8.17 | 1.66 | 1.53 |
| 8 | P | 1217 | ARG | C-N | 8.17 | 1.44 | 1.33 |
| 9 | Q | 412 | TYR | CA-C | -8.17 | 1.41 | 1.52 |
| 14 | a | 803 | HIS | ND1-CE1 | 8.16 | 1.40 | 1.32 |
| 5 | K | 298 | SER | C-N | 8.16 | 1.45 | 1.33 |
| 14 | a | 393 | HIS | ND1-CE1 | 8.16 | 1.40 | 1.32 |
| 5 | E | 352 | ILE | CA-C | -8.15 | 1.42 | 1.52 |
| 16 | c | 314 | LYS | N-CA | -8.15 | 1.35 | 1.46 |
| 8 | P | 1334 | ASP | CA-C | -8.14 | 1.42 | 1.52 |
| 14 | h | 492 | ASN | CA-C | -8.14 | 1.42 | 1.52 |
| 5 | K | 352 | ILE | N-CA | -8.13 | 1.36 | 1.46 |
| 18 | e | 107 | SER | N-CA | -8.13 | 1.35 | 1.46 |
| 2 | 1 | 1390 | LEU | C-N | 8.13 | 1.44 | 1.33 |
| 12 | v | 65 | LEU | C-N | 8.13 | 1.43 | 1.33 |
| 7 | O | 155 | LEU | C-N | 8.12 | 1.44 | 1.34 |
| 7 | O | 1071 | ALA | CA-C | 8.13 | 1.62 | 1.52 |
| 9 | T | 577 | ARG | CD-NE | 8.12 | 1.57 | 1.46 |
| 14 | a | 436 | HIS | CA-C | -8.12 | 1.42 | 1.52 |
| 20 | g | 270 | LEU | CA-C | -8.11 | 1.42 | 1.52 |
| 8 | N | 717 | VAL | C-N | 8.11 | 1.43 | 1.33 |
| 20 | n | 704 | SER | C-N | 8.11 | 1.45 | 1.33 |
| 20 | n | 352 | TYR | C-N | 8.10 | 1.44 | 1.33 |
| 5 | K | 444 | LEU | N-CA | -8.10 | 1.35 | 1.46 |
| 2 | 1 | 588 | ASN | CA-C | -8.10 | 1.42 | 1.52 |
| 16 | j | 397 | TYR | C-N | 8.10 | 1.44 | 1.33 |
| 5 | K | 341 | LYS | CA-C | -8.09 | 1.42 | 1.52 |
| 6 | L | 396 | THR | N-CA | -8.09 | 1.36 | 1.46 |
| 8 | N | 1192 | LEU | N-CA | -8.08 | 1.36 | 1.46 |
| 12 | v | 588 | TRP | N-CA | -8.08 | 1.36 | 1.46 |
| 21 | p | 22 | GLU | CA-C | -8.08 | 1.42 | 1.52 |
| 8 | N | 184 | ASP | CA-CB | 8.07 | 1.66 | 1.53 |
| 15 | i | 67 | LEU | CA-C | -8.07 | 1.41 | 1.52 |
| 2 | 1 | 363 | VAL | CA-C | -8.06 | 1.42 | 1.52 |
| 15 | i | 211 | TRP | C-N | 8.06 | 1.41 | 1.33 |
| 1 | 0 | 1089 | LEU | N-CA | -8.06 | 1.36 | 1.46 |
| 9 | R | 659 | SER | CA-C | -8.06 | 1.42 | 1.52 |
| 21 | o | 55 | ASN | CA-CB | 8.06 | 1.67 | 1.53 |
| 19 | m | 613 | ILE | N-CA | -8.06 | 1.37 | 1.46 |
| 8 | N | 256 | THR | N-CA | -8.06 | 1.30 | 1.46 |
| 2 | 1 | 561 | LEU | CA-C | -8.06 | 1.42 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1156 | TYR | C-N | 8.06 | 1.44 | 1.33 |
| 18 | l | 300 | HIS | ND1-CE1 | 8.05 | 1.40 | 1.32 |
| 14 | h | 406 | ARG | CD-NE | 8.05 | 1.57 | 1.46 |
| 19 | f | 157 | ASP | CA-C | -8.05 | 1.42 | 1.52 |
| 8 | P | 1457 | ALA | CA-C | -8.04 | 1.42 | 1.52 |
| 2 | 1 | 252 | LYS | CA-C | -8.04 | 1.42 | 1.52 |
| 5 | H | 377 | ASN | CA-C | -8.04 | 1.42 | 1.52 |
| 9 | S | 413 | LYS | CA-CB | 8.03 | 1.65 | 1.54 |
| 15 | b | 530 | ARG | CZ-NH1 | 8.03 | 1.44 | 1.32 |
| 2 | Z | 147 | PRO | C-N | 8.03 | 1.44 | 1.33 |
| 21 | t | 58 | HIS | ND1-CE1 | 8.02 | 1.40 | 1.32 |
| 19 | f | 450 | SER | CA-CB | 8.02 | 1.63 | 1.53 |
| 1 | 0 | 421 | VAL | CA-C | -8.02 | 1.42 | 1.52 |
| 14 | h | 750 | LEU | CA-C | 8.02 | 1.63 | 1.52 |
| 9 | S | 163 | ILE | C-N | 8.02 | 1.44 | 1.33 |
| 14 | h | 496 | ASN | CA-C | -8.02 | 1.42 | 1.53 |
| 1 | 0 | 510 | GLN | CA-CB | 8.02 | 1.64 | 1.53 |
| 7 | M | 1187 | ASN | CA-C | -8.02 | 1.42 | 1.52 |
| 8 | P | 1477 | ALA | CA-C | -8.02 | 1.42 | 1.52 |
| 1 | Y | 1413 | VAL | CA-CB | -8.02 | 1.45 | 1.54 |
| 8 | N | 793 | LEU | CA-CB | -8.02 | 1.37 | 1.53 |
| 19 | m | 456 | GLN | CA-C | -8.02 | 1.42 | 1.53 |
| 9 | Q | 417 | ARG | CD-NE | 8.01 | 1.57 | 1.46 |
| 2 | Z | 132 | LEU | CA-C | -8.01 | 1.42 | 1.52 |
| 12 | v | 350 | LEU | C-N | 8.01 | 1.44 | 1.33 |
| 8 | N | 1094 | SER | N-CA | -8.00 | 1.35 | 1.46 |
| 7 | O | 1023 | LEU | C-N | 8.00 | 1.44 | 1.34 |
| 21 | t | 18 | ASP | N-CA | -8.00 | 1.36 | 1.46 |
| 15 | b | 452 | GLU | CA-C | 7.99 | 1.63 | 1.52 |
| 2 | Z | 1124 | ASP | CA-C | -7.99 | 1.42 | 1.52 |
| 2 | 1 | 143 | VAL | N-CA | -7.99 | 1.36 | 1.46 |
| 20 | n | 604 | ILE | CA-CB | 7.98 | 1.63 | 1.54 |
| 6 | F | 283 | TYR | CA-C | -7.98 | 1.45 | 1.53 |
| 1 | Y | 1177 | ILE | CA-CB | -7.98 | 1.45 | 1.54 |
| 18 | l | 54 | HIS | ND1-CE1 | 7.98 | 1.40 | 1.32 |
| 14 | h | 513 | LEU | C-N | 7.97 | 1.45 | 1.33 |
| 15 | i | 564 | LYS | C-N | 7.97 | 1.43 | 1.33 |
| 5 | H | 326 | LYS | N-CA | -7.97 | 1.36 | 1.46 |
| 21 | q | 75 | HIS | C-N | 7.97 | 1.44 | 1.33 |
| 1 | Y | 516 | LEU | CA-CB | 7.97 | 1.63 | 1.53 |
| 14 | a | 1023 | LYS | C-N | 7.97 | 1.42 | 1.33 |
| 14 | h | 626 | HIS | ND1-CE1 | 7.97 | 1.40 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 1668 | LYS | C-N | 7.97 | 1.44 | 1.33 |
| 9 | S | 681 | SER | CA-CB | 7.97 | 1.65 | 1.53 |
| 18 | e | 12 | VAL | N-CA | -7.96 | 1.36 | 1.46 |
| 8 | N | 185 | LEU | CA-CB | 7.96 | 1.65 | 1.53 |
| 9 | R | 603 | VAL | N-CA | -7.96 | 1.36 | 1.46 |
| 14 | h | 336 | LEU | C-N | 7.96 | 1.43 | 1.33 |
| 5 | B | 304 | THR | CA-C | -7.96 | 1.43 | 1.52 |
| 9 | S | 693 | ALA | N-CA | -7.95 | 1.40 | 1.47 |
| 14 | a | 275 | ALA | CA-C | -7.94 | 1.42 | 1.52 |
| 5 | H | 522 | TYR | CA-C | -7.94 | 1.42 | 1.52 |
| 6 | I | 461 | HIS | CG-ND1 | 7.94 | 1.47 | 1.38 |
| 15 | b | 257 | LEU | N-CA | -7.94 | 1.36 | 1.46 |
| 9 | R | 259 | ILE | CA-C | -7.94 | 1.43 | 1.52 |
| 7 | M | 4 | SER | CA-C | -7.93 | 1.42 | 1.52 |
| 12 | v | 630 | TRP | N-CA | -7.93 | 1.36 | 1.46 |
| 15 | i | 721 | PRO | CA-C | -7.93 | 1.41 | 1.52 |
| 7 | M | 888 | PRO | CA-CB | 7.93 | 1.65 | 1.54 |
| 12 | v | 385 | ASN | N-CA | -7.93 | 1.36 | 1.46 |
| 1 | 0 | 1463 | ARG | CD-NE | 7.92 | 1.57 | 1.46 |
| 8 | N | 51 | LEU | C-N | 7.92 | 1.42 | 1.33 |
| 7 | O | 1153 | TYR | CA-CB | 7.92 | 1.65 | 1.53 |
| 5 | B | 390 | HIS | ND1-CE1 | 7.92 | 1.40 | 1.32 |
| 7 | M | 614 | THR | CA-C | -7.92 | 1.42 | 1.52 |
| 19 | m | 520 | GLY | CA-C | -7.91 | 1.43 | 1.52 |
| 2 | Z | 1282 | VAL | C-N | 7.91 | 1.42 | 1.33 |
| 14 | a | 879 | PHE | N-CA | 7.91 | 1.56 | 1.46 |
| 1 | 0 | 912 | VAL | CA-C | -7.90 | 1.45 | 1.52 |
| 7 | O | 106 | TYR | CA-C | -7.90 | 1.42 | 1.52 |
| 19 | f | 233 | THR | CA-CB | 7.90 | 1.65 | 1.53 |
| 1 | 0 | 616 | ASN | CA-CB | 7.89 | 1.64 | 1.53 |
| 9 | T | 137 | ASP | CA-C | -7.89 | 1.42 | 1.52 |
| 9 | S | 784 | ASN | C-N | 7.89 | 1.44 | 1.34 |
| 15 | i | 427 | LYS | CA-C | -7.89 | 1.42 | 1.52 |
| 14 | a | 880 | ARG | NE-CZ | 7.88 | 1.41 | 1.33 |
| 20 | g | 579 | ILE | CA-C | -7.88 | 1.42 | 1.52 |
| 2 | 1 | 1365 | GLN | N-CA | -7.87 | 1.35 | 1.45 |
| 7 | O | 152 | HIS | ND1-CE1 | 7.87 | 1.40 | 1.32 |
| 5 | H | 420 | ALA | C-N | 7.87 | 1.44 | 1.33 |
| 7 | M | 1156 | TYR | CA-C | 7.87 | 1.62 | 1.52 |
| 4 | y | 692 | LYS | CA-C | -7.87 | 1.42 | 1.52 |
| 2 | 1 | 503 | SER | N-CA | 7.86 | 1.53 | 1.46 |
| 19 | m | 545 | ALA | N-CA | -7.86 | 1.37 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 14 | a | 676 | ALA | N-CA | -7.86 | 1.37 | 1.46 |
| 8 | N | 754 | TYR | N-CA | -7.86 | 1.36 | 1.46 |
| 1 | 0 | 975 | ILE | CA-C | -7.86 | 1.44 | 1.52 |
| 7 | M | 1515 | LEU | CA-C | -7.85 | 1.42 | 1.52 |
| 9 | Q | 330 | GLY | C-N | 7.85 | 1.42 | 1.33 |
| 18 | l | 299 | GLU | CA-C | -7.84 | 1.43 | 1.52 |
| 1 | 0 | 153 | VAL | CA-C | -7.84 | 1.42 | 1.52 |
| 16 | c | 637 | LEU | CA-C | -7.84 | 1.44 | 1.52 |
| 1 | Y | 173 | MET | CA-C | -7.83 | 1.42 | 1.52 |
| 16 | c | 180 | GLN | N-CA | -7.83 | 1.36 | 1.46 |
| 5 | H | 442 | THR | CA-C | -7.83 | 1.42 | 1.52 |
| 2 | Z | 431 | ARG | NE-CZ | 7.83 | 1.41 | 1.33 |
| 18 | e | 321 | SER | CA-CB | 7.83 | 1.63 | 1.52 |
| 1 | 0 | 1331 | ARG | CA-C | -7.83 | 1.42 | 1.53 |
| 1 | Y | 1373 | LYS | C-N | 7.82 | 1.42 | 1.34 |
| 18 | l | 242 | ILE | CA-C | -7.82 | 1.44 | 1.52 |
| 7 | M | 148 | PHE | CA-CB | 7.82 | 1.65 | 1.53 |
| 17 | d | 122 | ASP | CA-C | 7.82 | 1.63 | 1.52 |
| 1 | 0 | 1482 | ASP | CA-C | -7.81 | 1.44 | 1.52 |
| 7 | M | 1003 | LEU | CA-C | -7.81 | 1.42 | 1.52 |
| 19 | m | 528 | HIS | CA-C | -7.81 | 1.42 | 1.52 |
| 18 | e | 202 | LEU | N-CA | -7.81 | 1.36 | 1.45 |
| 5 | E | 540 | LYS | CA-C | -7.81 | 1.43 | 1.52 |
| 7 | M | 119 | PHE | C-N | 7.81 | 1.43 | 1.33 |
| 14 | h | 1004 | ILE | C-N | 7.80 | 1.46 | 1.33 |
| 17 | d | 188 | ASN | CA-C | -7.80 | 1.43 | 1.52 |
| 20 | n | 1126 | ASP | C-N | 7.80 | 1.44 | 1.33 |
| 5 | E | 530 | ASP | CA-CB | 7.80 | 1.65 | 1.53 |
| 12 | u | 219 | ASN | CA-C | -7.80 | 1.43 | 1.52 |
| 2 | 1 | 927 | HIS | ND1-CE1 | 7.79 | 1.40 | 1.32 |
| 1 | 0 | 181 | ARG | NE-CZ | 7.79 | 1.41 | 1.33 |
| 7 | O | 133 | GLU | C-N | 7.79 | 1.44 | 1.33 |
| 1 | Y | 181 | ARG | NE-CZ | 7.78 | 1.41 | 1.33 |
| 7 | M | 178 | ASN | CA-CB | 7.78 | 1.65 | 1.53 |
| 7 | O | 1346 | ASN | CA-CB | 7.78 | 1.63 | 1.53 |
| 1 | 0 | 1456 | TYR | CA-C | -7.77 | 1.42 | 1.52 |
| 14 | h | 397 | ILE | N-CA | -7.77 | 1.37 | 1.46 |
| 6 | I | 346 | ASP | CA-CB | 7.77 | 1.65 | 1.53 |
| 14 | a | 527 | SER | C-N | 7.77 | 1.43 | 1.33 |
| 8 | P | 1531 | SER | C-N | 7.77 | 1.44 | 1.34 |
| 14 | h | 138 | LEU | CA-CB | 7.76 | 1.65 | 1.54 |
| 18 | l | 219 | SER | CA-C | -7.76 | 1.43 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 16 | j | 441 | ARG | NE-CZ | 7.76 | 1.41 | 1.33 |
| 9 | S | 218 | ILE | C-N | 7.76 | 1.43 | 1.33 |
| 1 | Y | 158 | ASP | CA-CB | 7.76 | 1.65 | 1.53 |
| 8 | P | 697 | SER | CA-CB | 7.76 | 1.65 | 1.53 |
| 10 | U | 259 | PRO | CA-C | -7.76 | 1.45 | 1.53 |
| 14 | h | 1019 | LEU | CA-C | 7.75 | 1.63 | 1.52 |
| 14 | a | 447 | GLU | C-N | 7.75 | 1.44 | 1.34 |
| 7 | O | 348 | LEU | CA-C | -7.75 | 1.42 | 1.52 |
| 14 | h | 710 | TYR | CA-CB | 7.75 | 1.66 | 1.53 |
| 7 | O | 1414 | SER | CA-CB | 7.75 | 1.65 | 1.53 |
| 2 | 1 | 1079 | PHE | C-N | 7.75 | 1.43 | 1.33 |
| 16 | c | 264 | ARG | CD-NE | 7.74 | 1.57 | 1.46 |
| 18 | e | 244 | LYS | CA-C | -7.74 | 1.43 | 1.52 |
| 5 | B | 518 | ARG | C-N | 7.74 | 1.44 | 1.33 |
| 5 | K | 346 | GLN | CA-CB | 7.74 | 1.64 | 1.53 |
| 8 | P | 956 | PHE | CA-CB | 7.74 | 1.66 | 1.53 |
| 2 | Z | 615 | ARG | CA-C | -7.74 | 1.42 | 1.52 |
| 9 | Q | 799 | LYS | CA-C | -7.73 | 1.42 | 1.52 |
| 1 | 0 | 589 | HIS | CA-CB | 7.73 | 1.67 | 1.53 |
| 2 | 1 | 1089 | GLU | CA-C | -7.73 | 1.43 | 1.52 |
| 7 | O | 741 | GLY | C-N | 7.73 | 1.44 | 1.33 |
| 14 | a | 752 | HIS | ND1-CE1 | 7.73 | 1.40 | 1.32 |
| 6 | C | 461 | HIS | ND1-CE1 | 7.73 | 1.40 | 1.32 |
| 9 | Q | 144 | LEU | N-CA | -7.72 | 1.38 | 1.46 |
| 12 | u | 133 | HIS | CA-C | -7.72 | 1.44 | 1.52 |
| 5 | E | 365 | GLN | CA-C | -7.71 | 1.42 | 1.52 |
| 12 | u | 73 | SER | N-CA | -7.71 | 1.36 | 1.46 |
| 19 | f | 268 | SER | CA-C | -7.71 | 1.46 | 1.53 |
| 20 | n | 919 | GLU | C-N | 7.71 | 1.44 | 1.33 |
| 12 | u | 417 | ILE | N-CA | -7.71 | 1.38 | 1.46 |
| 4 | J | 763 | SER | CA-C | -7.70 | 1.42 | 1.52 |
| 9 | Q | 352 | VAL | C-N | 7.70 | 1.44 | 1.33 |
| 15 | b | 561 | ARG | NE-CZ | 7.70 | 1.41 | 1.33 |
| 2 | Z | 792 | SER | C-N | 7.70 | 1.43 | 1.33 |
| 14 | h | 944 | ILE | CA-C | -7.70 | 1.43 | 1.52 |
| 1 | 0 | 1362 | ASN | CA-C | 7.70 | 1.59 | 1.52 |
| 2 | Z | 656 | HIS | N-CA | 7.69 | 1.54 | 1.46 |
| 17 | d | 229 | ARG | CA-C | -7.69 | 1.43 | 1.53 |
| 2 | Z | 341 | THR | N-CA | -7.69 | 1.36 | 1.46 |
| 12 | u | 377 | SER | CA-C | -7.69 | 1.43 | 1.52 |
| 19 | m | 346 | LEU | CA-C | -7.68 | 1.42 | 1.52 |
| 7 | M | 239 | HIS | CB-CG | 7.68 | 1.60 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | R | 115 | THR | N-CA | -7.68 | 1.36 | 1.46 |
| 20 | n | 824 | ASN | N-CA | 7.68 | 1.56 | 1.46 |
| 1 | 0 | 266 | GLN | C-N | 7.68 | 1.43 | 1.33 |
| 7 | O | 1649 | LYS | CA-C | -7.68 | 1.42 | 1.52 |
| 14 | h | 938 | ARG | CA-CB | 7.68 | 1.65 | 1.53 |
| 15 | i | 80 | ALA | CA-C | -7.68 | 1.43 | 1.52 |
| 8 | P | 720 | ARG | CD-NE | 7.67 | 1.56 | 1.46 |
| 16 | c | 557 | GLN | CA-C | -7.67 | 1.42 | 1.52 |
| 7 | M | 264 | LYS | C-N | 7.67 | 1.45 | 1.33 |
| 19 | m | 268 | SER | CA-C | -7.67 | 1.43 | 1.53 |
| 9 | S | 121 | ILE | CA-C | -7.67 | 1.43 | 1.52 |
| 9 | R | 273 | VAL | N-CA | -7.67 | 1.36 | 1.46 |
| 15 | i | 49 | VAL | N-CA | 7.67 | 1.51 | 1.45 |
| 2 | Z | 845 | PHE | CA-C | -7.66 | 1.42 | 1.52 |
| 9 | R | 503 | ALA | C-N | 7.66 | 1.43 | 1.33 |
| 20 | g | 110 | ILE | N-CA | -7.66 | 1.37 | 1.46 |
| 8 | N | 906 | TYR | CA-CB | 7.65 | 1.65 | 1.53 |
| 9 | R | 771 | ILE | CA-CB | -7.65 | 1.48 | 1.53 |
| 9 | T | 262 | SER | CA-C | -7.65 | 1.42 | 1.52 |
| 12 | u | 328 | PHE | CA-C | -7.65 | 1.43 | 1.52 |
| 1 | 0 | 444 | VAL | CA-CB | -7.65 | 1.45 | 1.53 |
| 6 | I | 452 | ASP | CA-CB | 7.65 | 1.65 | 1.53 |
| 16 | j | 260 | LEU | CA-C | 7.65 | 1.63 | 1.52 |
| 18 | l | 333 | ALA | CA-C | -7.65 | 1.42 | 1.52 |
| 2 | 1 | 592 | SER | CA-C | -7.64 | 1.45 | 1.53 |
| 21 | r | 47 | LYS | C-O | -7.64 | 1.15 | 1.24 |
| 14 | a | 850 | GLU | CA-C | -7.64 | 1.42 | 1.52 |
| 12 | v | 528 | PHE | CA-C | -7.64 | 1.43 | 1.52 |
| 1 | 0 | 644 | SER | N-CA | -7.64 | 1.35 | 1.46 |
| 13 | x | 1284 | THR | C-N | 7.64 | 1.44 | 1.33 |
| 7 | O | 1373 | ASP | CA-CB | 7.63 | 1.63 | 1.53 |
| 9 | R | 207 | ILE | C-N | 7.63 | 1.43 | 1.33 |
| 2 | Z | 751 | GLN | CA-C | -7.63 | 1.44 | 1.52 |
| 4 | y | 745 | TYR | CA-C | -7.63 | 1.42 | 1.52 |
| 16 | j | 301 | ASN | CA-C | -7.63 | 1.42 | 1.52 |
| 16 | j | 487 | HIS | ND1-CE1 | 7.63 | 1.40 | 1.32 |
| 1 | Y | 1401 | THR | CA-C | -7.63 | 1.42 | 1.52 |
| 15 | i | 197 | VAL | CA-C | -7.63 | 1.43 | 1.52 |
| 6 | F | 352 | VAL | CA-CB | 7.63 | 1.63 | 1.54 |
| 8 | N | 1282 | ASN | N-CA | -7.63 | 1.36 | 1.46 |
| 16 | j | 391 | TYR | CA-C | -7.63 | 1.42 | 1.52 |
| 16 | c | 201 | ALA | N-CA | -7.63 | 1.36 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | g | 714 | TYR | C-N | 7.62 | 1.44 | 1.33 |
| 9 | Q | 767 | ILE | CA-CB | 7.62 | 1.63 | 1.54 |
| 7 | O | 771 | ARG | N-CA | -7.62 | 1.36 | 1.46 |
| 2 | 1 | 450 | SER | C-N | 7.62 | 1.44 | 1.33 |
| 14 | a | 392 | GLU | CA-C | -7.62 | 1.43 | 1.52 |
| 7 | M | 62 | SER | C-N | 7.61 | 1.43 | 1.33 |
| 12 | u | 237 | LEU | N-CA | 7.61 | 1.55 | 1.46 |
| 16 | j | 322 | ILE | CA-C | -7.61 | 1.42 | 1.52 |
| 19 | m | 262 | ALA | C-N | 7.61 | 1.43 | 1.33 |
| 19 | f | 261 | ARG | CD-NE | 7.61 | 1.56 | 1.46 |
| 20 | g | 1084 | LEU | CA-C | -7.61 | 1.42 | 1.52 |
| 8 | N | 356 | HIS | ND1-CE1 | 7.60 | 1.40 | 1.32 |
| 9 | S | 92 | THR | CA-C | -7.60 | 1.43 | 1.52 |
| 1 | Y | 580 | VAL | CA-C | 7.60 | 1.58 | 1.52 |
| 1 | 0 | 522 | ALA | N-CA | -7.60 | 1.36 | 1.46 |
| 14 | h | 649 | GLN | CA-C | -7.60 | 1.43 | 1.52 |
| 14 | h | 230 | HIS | C-N | 7.60 | 1.43 | 1.33 |
| 15 | i | 499 | ALA | C-N | 7.60 | 1.44 | 1.34 |
| 17 | k | 185 | TRP | CA-CB | 7.59 | 1.66 | 1.53 |
| 1 | 0 | 831 | LYS | N-CA | 7.59 | 1.60 | 1.46 |
| 19 | f | 391 | HIS | ND1-CE1 | 7.59 | 1.40 | 1.32 |
| 19 | m | 330 | ARG | C-N | 7.59 | 1.42 | 1.34 |
| 15 | b | 358 | CYS | CA-C | -7.59 | 1.42 | 1.52 |
| 8 | P | 852 | PHE | CA-C | -7.58 | 1.43 | 1.52 |
| 17 | k | 59 | VAL | CA-C | -7.58 | 1.43 | 1.52 |
| 2 | Z | 1124 | ASP | C-N | 7.57 | 1.43 | 1.33 |
| 16 | c | 647 | GLN | CA-CB | 7.57 | 1.65 | 1.53 |
| 18 | e | 206 | ALA | CA-C | -7.57 | 1.43 | 1.52 |
| 9 | T | 727 | TYR | CA-C | -7.57 | 1.42 | 1.52 |
| 7 | M | 840 | ILE | C-N | 7.57 | 1.44 | 1.34 |
| 12 | v | 692 | LYS | C-N | 7.57 | 1.43 | 1.33 |
| 14 | h | 438 | GLU | CA-C | -7.57 | 1.43 | 1.52 |
| 19 | f | 637 | ASP | CA-C | -7.57 | 1.43 | 1.52 |
| 7 | O | 613 | LEU | CA-C | -7.56 | 1.43 | 1.52 |
| 16 | c | 371 | SER | N-CA | -7.56 | 1.36 | 1.46 |
| 20 | g | 1076 | PHE | C-N | 7.56 | 1.42 | 1.33 |
| 21 | r | 58 | HIS | ND1-CE1 | 7.56 | 1.40 | 1.32 |
| 8 | P | 862 | ARG | NE-CZ | 7.55 | 1.41 | 1.33 |
| 1 | 0 | 665 | ASN | CA-C | -7.55 | 1.42 | 1.52 |
| 6 | L | 372 | PHE | CA-C | -7.55 | 1.43 | 1.52 |
| 9 | S | 220 | PHE | C-N | 7.55 | 1.43 | 1.33 |
| 9 | S | 710 | ASN | C-N | 7.55 | 1.46 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 1261 | ARG | CZ-NH1 | 7.55 | 1.43 | 1.32 |
| 2 | 1 | 589 | VAL | CA-CB | 7.55 | 1.64 | 1.54 |
| 8 | N | 303 | GLU | CA-C | -7.55 | 1.42 | 1.52 |
| 4 | z | 756 | ASN | CA-CB | 7.55 | 1.65 | 1.53 |
| 15 | b | 733 | LYS | CA-C | -7.55 | 1.43 | 1.52 |
| 7 | O | 935 | GLN | C-N | 7.54 | 1.43 | 1.33 |
| 17 | d | 144 | HIS | CE1-NE2 | 7.54 | 1.40 | 1.32 |
| 20 | n | 292 | PHE | CA-CB | 7.54 | 1.63 | 1.53 |
| 5 | B | 439 | GLN | CA-CB | 7.54 | 1.65 | 1.53 |
| 2 | Z | 672 | VAL | N-CA | 7.54 | 1.55 | 1.46 |
| 9 | Q | 122 | LEU | C-N | 7.54 | 1.43 | 1.33 |
| 4 | J | 690 | GLN | CA-C | -7.53 | 1.42 | 1.52 |
| 7 | M | 1559 | LEU | CA-C | -7.53 | 1.42 | 1.52 |
| 9 | T | 53 | VAL | CA-C | 7.53 | 1.61 | 1.53 |
| 7 | M | 890 | VAL | C-N | 7.53 | 1.44 | 1.33 |
| 21 | r | 58 | HIS | N-CA | -7.53 | 1.36 | 1.46 |
| 2 | 1 | 1271 | ARG | NE-CZ | 7.53 | 1.41 | 1.33 |
| 9 | T | 456 | ARG | CA-C | -7.53 | 1.43 | 1.52 |
| 16 | j | 271 | TRP | C-N | 7.53 | 1.43 | 1.33 |
| 20 | g | 88 | GLY | CA-C | -7.53 | 1.42 | 1.52 |
| 7 | M | 896 | THR | N-CA | -7.52 | 1.36 | 1.46 |
| 2 | Z | 230 | ILE | C-N | 7.52 | 1.44 | 1.33 |
| 14 | a | 789 | LYS | C-N | 7.52 | 1.41 | 1.33 |
| 7 | O | 22 | PHE | C-N | 7.51 | 1.44 | 1.33 |
| 7 | M | 1246 | MET | CA-CB | 7.51 | 1.65 | 1.53 |
| 7 | M | 222 | GLU | CA-C | -7.51 | 1.42 | 1.52 |
| 1 | Y | 637 | LEU | CA-C | -7.51 | 1.43 | 1.53 |
| 12 | v | 596 | SER | C-N | 7.50 | 1.44 | 1.33 |
| 7 | M | 1247 | ARG | CD-NE | 7.50 | 1.56 | 1.46 |
| 9 | R | 132 | ALA | CA-C | -7.50 | 1.43 | 1.52 |
| 15 | i | 543 | GLY | CA-C | -7.50 | 1.41 | 1.51 |
| 21 | s | 89 | PHE | CA-C | -7.50 | 1.43 | 1.52 |
| 14 | a | 293 | LEU | C-N | 7.50 | 1.42 | 1.33 |
| 17 | d | 130 | PHE | CA-CB | 7.50 | 1.62 | 1.53 |
| 1 | Y | 1345 | GLN | C-N | 7.49 | 1.44 | 1.33 |
| 19 | m | 373 | THR | CA-CB | -7.49 | 1.40 | 1.53 |
| 16 | c | 278 | PRO | C-N | 7.49 | 1.44 | 1.34 |
| 9 | Q | 326 | THR | CA-C | -7.49 | 1.43 | 1.52 |
| 8 | N | 1423 | ASN | CA-CB | 7.49 | 1.65 | 1.53 |
| 8 | P | 865 | ASN | CA-C | -7.49 | 1.43 | 1.52 |
| 8 | N | 945 | ASP | CA-C | -7.48 | 1.43 | 1.52 |
| 19 | m | 586 | GLN | CA-C | -7.48 | 1.42 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | f | 621 | GLN | N-CA | -7.48 | 1.37 | 1.46 |
| 2 | 1 | 769 | HIS | ND1-CE1 | 7.48 | 1.40 | 1.32 |
| 7 | O | 523 | ARG | NE-CZ | 7.48 | 1.41 | 1.33 |
| 20 | g | 1031 | PHE | CA-C | -7.48 | 1.42 | 1.52 |
| 7 | M | 1484 | ARG | CA-C | -7.48 | 1.43 | 1.52 |
| 18 | e | 244 | LYS | C-N | 7.48 | 1.40 | 1.33 |
| 7 | O | 29 | LEU | C-N | -7.47 | 1.23 | 1.34 |
| 14 | a | 259 | MET | CA-CB | 7.47 | 1.62 | 1.52 |
| 1 | Y | 181 | ARG | CD-NE | 7.47 | 1.56 | 1.46 |
| 1 | 0 | 1209 | LYS | C-O | -7.47 | 1.15 | 1.23 |
| 1 | Y | 1475 | LYS | C-N | 7.47 | 1.43 | 1.33 |
| 16 | j | 579 | ARG | CA-CB | 7.47 | 1.63 | 1.53 |
| 8 | N | 1181 | THR | CA-C | -7.47 | 1.43 | 1.52 |
| 1 | Y | 1050 | ALA | C-N | 7.47 | 1.43 | 1.33 |
| 9 | R | 43 | GLN | N-CA | -7.46 | 1.37 | 1.46 |
| 1 | Y | 1009 | HIS | ND1-CE1 | 7.46 | 1.40 | 1.32 |
| 16 | j | 336 | ALA | N-CA | -7.46 | 1.37 | 1.46 |
| 1 | 0 | 769 | ARG | CD-NE | 7.46 | 1.56 | 1.46 |
| 1 | 0 | 648 | GLU | C-N | 7.46 | 1.42 | 1.33 |
| 2 | Z | 242 | HIS | ND1-CE1 | 7.46 | 1.40 | 1.32 |
| 19 | f | 404 | VAL | CA-C | -7.46 | 1.43 | 1.52 |
| 9 | S | 502 | ASP | CA-C | -7.45 | 1.42 | 1.52 |
| 1 | 0 | 429 | GLU | N-CA | -7.45 | 1.36 | 1.46 |
| 14 | h | 91 | LYS | CA-C | 7.45 | 1.61 | 1.52 |
| 1 | 0 | 643 | THR | C-N | 7.45 | 1.45 | 1.33 |
| 7 | M | 553 | ILE | N-CA | -7.45 | 1.37 | 1.46 |
| 8 | P | 724 | SER | C-N | 7.45 | 1.43 | 1.33 |
| 4 | y | 691 | ASN | CA-C | -7.45 | 1.43 | 1.52 |
| 17 | d | 105 | VAL | CA-C | -7.44 | 1.43 | 1.52 |
| 1 | Y | 1481 | ASN | CA-C | -7.44 | 1.44 | 1.53 |
| 2 | Z | 1015 | VAL | CA-CB | 7.44 | 1.62 | 1.54 |
| 20 | n | 281 | ARG | CD-NE | 7.44 | 1.56 | 1.46 |
| 14 | h | 837 | SER | C-N | 7.44 | 1.44 | 1.33 |
| 6 | C | 406 | PHE | CA-C | -7.43 | 1.46 | 1.53 |
| 14 | a | 250 | SER | N-CA | -7.43 | 1.36 | 1.46 |
| 16 | c | 329 | ASP | CA-C | -7.43 | 1.44 | 1.52 |
| 14 | h | 800 | GLU | CA-C | -7.43 | 1.43 | 1.52 |
| 21 | t | 90 | LYS | CA-C | 7.43 | 1.61 | 1.52 |
| 16 | c | 242 | ASP | CA-CB | 7.43 | 1.63 | 1.53 |
| 20 | g | 859 | ASP | C-N | 7.43 | 1.43 | 1.33 |
| 8 | P | 713 | LYS | C-N | 7.42 | 1.43 | 1.34 |
| 17 | k | 172 | LYS | C-N | 7.42 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | n | 139 | ILE | N-CA | -7.42 | 1.37 | 1.46 |
| 8 | P | 439 | LEU | C-N | 7.42 | 1.41 | 1.33 |
| 9 | T | 705 | GLN | CA-CB | 7.42 | 1.64 | 1.53 |
| 14 | h | 607 | PHE | CA-CB | 7.42 | 1.66 | 1.53 |
| 20 | n | 181 | ILE | CA-C | -7.42 | 1.43 | 1.52 |
| 7 | O | 911 | SER | N-CA | -7.42 | 1.37 | 1.46 |
| 19 | m | 519 | GLU | C-N | 7.42 | 1.43 | 1.33 |
| 21 | t | 15 | ASP | N-CA | -7.42 | 1.37 | 1.46 |
| 20 | g | 468 | LEU | CA-C | -7.42 | 1.43 | 1.52 |
| 2 | 1 | 1160 | ILE | CA-C | -7.42 | 1.42 | 1.52 |
| 1 | Y | 1027 | HIS | ND1-CE1 | 7.42 | 1.40 | 1.32 |
| 14 | a | 598 | LYS | N-CA | -7.41 | 1.37 | 1.46 |
| 8 | N | 773 | LEU | CA-CB | 7.41 | 1.63 | 1.53 |
| 8 | N | 1644 | ILE | C-N | 7.41 | 1.44 | 1.33 |
| 20 | g | 911 | SER | CA-CB | 7.41 | 1.62 | 1.52 |
| 18 | l | 188 | LEU | CA-C | -7.41 | 1.44 | 1.53 |
| 20 | n | 936 | LYS | CA-C | -7.41 | 1.43 | 1.52 |
| 7 | O | 1405 | PHE | CA-CB | 7.41 | 1.63 | 1.53 |
| 20 | n | 1107 | ASN | C-N | 7.41 | 1.44 | 1.33 |
| 21 | t | 55 | ASN | CA-CB | 7.41 | 1.65 | 1.53 |
| 20 | g | 507 | ILE | C-N | 7.41 | 1.42 | 1.33 |
| 7 | O | 791 | PHE | C-N | 7.40 | 1.43 | 1.33 |
| 20 | n | 315 | ALA | C-N | 7.40 | 1.43 | 1.33 |
| 20 | n | 1146 | TYR | N-CA | -7.40 | 1.36 | 1.46 |
| 7 | M | 1570 | VAL | CA-CB | 7.40 | 1.64 | 1.54 |
| 19 | f | 312 | GLU | C-N | 7.40 | 1.43 | 1.33 |
| 7 | M | 31 | ASP | CA-CB | 7.39 | 1.65 | 1.53 |
| 9 | T | 822 | TYR | CA-C | -7.39 | 1.43 | 1.52 |
| 14 | h | 303 | LEU | CA-C | -7.39 | 1.43 | 1.52 |
| 20 | n | 411 | ASN | CA-CB | 7.39 | 1.63 | 1.53 |
| 16 | c | 600 | ASN | N-CA | -7.39 | 1.36 | 1.46 |
| 12 | u | 111 | ILE | CA-C | -7.39 | 1.43 | 1.52 |
| 4 | A | 675 | GLN | C-N | 7.39 | 1.42 | 1.33 |
| 7 | O | 1499 | LEU | C-N | 7.39 | 1.44 | 1.33 |
| 12 | u | 439 | LEU | N-CA | -7.39 | 1.36 | 1.46 |
| 19 | m | 321 | ALA | CA-C | -7.39 | 1.42 | 1.52 |
| 9 | S | 64 | LYS | N-CA | -7.39 | 1.37 | 1.46 |
| 17 | d | 26 | THR | CA-C | -7.39 | 1.43 | 1.52 |
| 16 | j | 487 | HIS | CB-CG | 7.38 | 1.60 | 1.50 |
| 20 | g | 341 | ASP | N-CA | -7.38 | 1.37 | 1.46 |
| 9 | Q | 53 | VAL | N-CA | 7.38 | 1.55 | 1.46 |
| 7 | O | 1010 | LEU | N-CA | -7.38 | 1.37 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | P | 190 | GLN | C-O | -7.38 | 1.15 | 1.24 |
| 1 | Y | 1435 | GLU | CA-C | -7.38 | 1.43 | 1.52 |
| 4 | G | 644 | TRP | NE1-CE2 | 7.38 | 1.45 | 1.37 |
| 13 | x | 1220 | THR | CA-C | -7.38 | 1.43 | 1.52 |
| 16 | j | 431 | THR | N-CA | -7.38 | 1.37 | 1.46 |
| 18 | l | 244 | LYS | C-N | 7.38 | 1.42 | 1.33 |
| 5 | E | 469 | ARG | CA-C | 7.38 | 1.62 | 1.52 |
| 1 | 0 | 606 | GLN | CA-C | -7.37 | 1.44 | 1.53 |
| 1 | 0 | 1386 | PRO | CA-C | 7.37 | 1.61 | 1.52 |
| 8 | P | 47 | ASN | CA-CB | 7.37 | 1.65 | 1.54 |
| 8 | P | 427 | ILE | CA-CB | 7.37 | 1.64 | 1.54 |
| 16 | c | 226 | LYS | C-N | 7.37 | 1.44 | 1.33 |
| 1 | Y | 171 | THR | CA-C | -7.37 | 1.43 | 1.52 |
| 8 | N | 17 | HIS | ND1-CE1 | 7.37 | 1.40 | 1.32 |
| 20 | n | 982 | GLU | CA-C | -7.37 | 1.44 | 1.52 |
| 21 | t | 60 | ILE | C-N | 7.37 | 1.43 | 1.33 |
| 21 | t | 65 | PHE | N-CA | -7.37 | 1.36 | 1.46 |
| 1 | Y | 426 | VAL | N-CA | -7.37 | 1.37 | 1.46 |
| 12 | u | 56 | SER | CA-C | -7.37 | 1.43 | 1.52 |
| 19 | f | 625 | LYS | CA-CB | 7.36 | 1.64 | 1.53 |
| 9 | S | 538 | LEU | CA-C | 7.36 | 1.62 | 1.52 |
| 2 | Z | 348 | ASP | CA-CB | 7.36 | 1.63 | 1.53 |
| 5 | B | 537 | TYR | CA-CB | 7.36 | 1.64 | 1.53 |
| 4 | D | 797 | LEU | C-N | 7.36 | 1.43 | 1.33 |
| 1 | Y | 1453 | HIS | ND1-CE1 | 7.36 | 1.40 | 1.32 |
| 15 | b | 281 | SER | CA-CB | 7.36 | 1.64 | 1.54 |
| 9 | S | 547 | TYR | N-CA | -7.35 | 1.38 | 1.46 |
| 1 | Y | 772 | GLY | N-CA | -7.35 | 1.36 | 1.45 |
| 8 | N | 727 | ASN | N-CA | -7.34 | 1.37 | 1.46 |
| 7 | O | 1411 | HIS | ND1-CE1 | 7.34 | 1.39 | 1.32 |
| 16 | j | 159 | LEU | CA-C | -7.34 | 1.44 | 1.52 |
| 1 | 0 | 238 | MET | CA-C | -7.34 | 1.44 | 1.53 |
| 5 | H | 460 | TRP | CA-CB | 7.34 | 1.65 | 1.53 |
| 5 | K | 329 | HIS | CA-C | -7.34 | 1.43 | 1.52 |
| 8 | N | 1475 | SER | CA-C | -7.34 | 1.43 | 1.52 |
| 9 | Q | 64 | LYS | N-CA | -7.34 | 1.39 | 1.46 |
| 21 | t | 77 | VAL | CA-C | -7.34 | 1.43 | 1.52 |
| 20 | g | 123 | PRO | CA-CB | 7.34 | 1.63 | 1.53 |
| 20 | g | 421 | PRO | N-CA | -7.34 | 1.38 | 1.47 |
| 17 | d | 236 | GLN | N-CA | -7.34 | 1.37 | 1.46 |
| 15 | i | 161 | ARG | C-N | 7.33 | 1.41 | 1.34 |
| 12 | v | 187 | PHE | C-N | 7.33 | 1.43 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 14 | a | 313 | TYR | CA-C | -7.33 | 1.43 | 1.52 |
| 1 | Y | 912 | VAL | CA-C | -7.33 | 1.43 | 1.52 |
| 17 | k | 78 | LYS | N-CA | -7.33 | 1.37 | 1.46 |
| 2 | Z | 1198 | ARG | NE-CZ | 7.33 | 1.41 | 1.33 |
| 7 | O | 1049 | LEU | C-N | 7.33 | 1.43 | 1.33 |
| 10 | U | 274 | GLY | N-CA | -7.33 | 1.36 | 1.45 |
| 8 | N | 115 | SER | C-O | -7.32 | 1.15 | 1.24 |
| 12 | u | 293 | GLU | N-CA | -7.32 | 1.36 | 1.46 |
| 20 | n | 252 | PHE | CA-C | 7.32 | 1.62 | 1.52 |
| 1 | Y | 289 | SER | C-N | 7.32 | 1.42 | 1.33 |
| 16 | c | 600 | ASN | C-O | -7.32 | 1.14 | 1.24 |
| 2 | 1 | 506 | ILE | CA-CB | -7.32 | 1.45 | 1.54 |
| 9 | Q | 764 | ASP | C-N | 7.32 | 1.44 | 1.33 |
| 9 | T | 577 | ARG | C-O | -7.32 | 1.15 | 1.24 |
| 18 | l | 8 | HIS | ND1-CE1 | 7.32 | 1.39 | 1.32 |
| 20 | n | 111 | HIS | ND1-CE1 | 7.32 | 1.39 | 1.32 |
| 17 | d | 65 | LYS | N-CA | -7.32 | 1.37 | 1.46 |
| 8 | P | 1467 | SER | C-N | 7.31 | 1.43 | 1.33 |
| 20 | n | 629 | LEU | CA-C | -7.31 | 1.43 | 1.52 |
| 9 | S | 497 | THR | CA-C | -7.31 | 1.42 | 1.52 |
| 13 | x | 1282 | GLN | C-N | 7.31 | 1.43 | 1.33 |
| 1 | Y | 371 | LEU | C-N | 7.31 | 1.43 | 1.33 |
| 8 | N | 558 | LYS | C-N | 7.31 | 1.42 | 1.33 |
| 13 | w | 1297 | ASP | C-N | 7.31 | 1.44 | 1.34 |
| 15 | i | 255 | ARG | CZ-NH2 | 7.30 | 1.43 | 1.33 |
| 1 | Y | 1146 | TYR | C-N | 7.30 | 1.43 | 1.34 |
| 19 | m | 157 | ASP | C-N | 7.30 | 1.43 | 1.33 |
| 8 | N | 1488 | SER | C-N | 7.30 | 1.40 | 1.33 |
| 15 | b | 155 | LEU | CA-CB | 7.29 | 1.66 | 1.53 |
| 19 | f | 13 | THR | CA-C | -7.29 | 1.43 | 1.52 |
| 1 | Y | 1348 | ARG | CD-NE | 7.29 | 1.56 | 1.46 |
| 14 | h | 901 | ARG | CA-C | -7.29 | 1.44 | 1.52 |
| 21 | p | 65 | PHE | C-N | 7.29 | 1.39 | 1.33 |
| 9 | S | 693 | ALA | CA-C | -7.29 | 1.46 | 1.52 |
| 1 | Y | 203 | VAL | C-O | 7.29 | 1.31 | 1.23 |
| 18 | e | 224 | ILE | N-CA | -7.29 | 1.35 | 1.46 |
| 6 | F | 314 | TYR | N-CA | -7.29 | 1.37 | 1.46 |
| 9 | T | 245 | ALA | CA-C | -7.29 | 1.43 | 1.52 |
| 20 | n | 1085 | CYS | N-CA | -7.29 | 1.36 | 1.46 |
| 7 | M | 722 | ARG | C-N | 7.28 | 1.43 | 1.33 |
| 7 | O | 120 | ILE | CA-CB | -7.28 | 1.46 | 1.54 |
| 14 | h | 359 | THR | CA-C | -7.28 | 1.43 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | n | 818 | LEU | C-N | 7.28 | 1.43 | 1.33 |
| 9 | S | 488 | TYR | CA-C | -7.28 | 1.43 | 1.52 |
| 7 | M | 70 | PHE | C-N | 7.28 | 1.42 | 1.34 |
| 7 | M | 1363 | ILE | N-CA | -7.28 | 1.40 | 1.46 |
| 7 | O | 1490 | ARG | NE-CZ | 7.28 | 1.41 | 1.33 |
| 20 | n | 271 | ARG | NE-CZ | 7.28 | 1.41 | 1.33 |
| 20 | n | 991 | LEU | CA-C | -7.28 | 1.43 | 1.52 |
| 16 | c | 522 | THR | CA-C | 7.28 | 1.62 | 1.52 |
| 8 | P | 1494 | ILE | CA-CB | 7.27 | 1.62 | 1.54 |
| 21 | o | 76 | PHE | CA-C | -7.27 | 1.44 | 1.52 |
| 2 | Z | 773 | PHE | CA-CB | 7.27 | 1.63 | 1.53 |
| 19 | m | 647 | ALA | CA-C | -7.27 | 1.43 | 1.52 |
| 14 | h | 977 | ALA | C-N | 7.27 | 1.43 | 1.33 |
| 15 | i | 650 | LEU | N-CA | -7.27 | 1.37 | 1.46 |
| 7 | O | 236 | ALA | CA-C | -7.27 | 1.43 | 1.52 |
| 15 | b | 590 | VAL | CA-C | -7.27 | 1.44 | 1.52 |
| 2 | 1 | 1348 | LYS | C-N | 7.26 | 1.44 | 1.34 |
| 8 | P | 696 | GLY | C-N | 7.26 | 1.43 | 1.33 |
| 14 | a | 638 | VAL | CA-C | -7.26 | 1.44 | 1.52 |
| 8 | P | 1076 | SER | C-N | 7.26 | 1.43 | 1.34 |
| 21 | o | 42 | ALA | CA-C | -7.26 | 1.43 | 1.52 |
| 9 | Q | 298 | LEU | CA-C | -7.26 | 1.44 | 1.52 |
| 14 | h | 731 | ASN | CA-C | -7.26 | 1.46 | 1.53 |
| 14 | h | 848 | SER | N-CA | -7.26 | 1.37 | 1.46 |
| 21 | r | 33 | ASP | CA-C | 7.25 | 1.65 | 1.52 |
| 8 | N | 1000 | LYS | CA-CB | 7.25 | 1.64 | 1.53 |
| 14 | a | 570 | LEU | CA-C | -7.25 | 1.43 | 1.52 |
| 1 | 0 | 1012 | ARG | CD-NE | 7.25 | 1.56 | 1.46 |
| 2 | 1 | 985 | SER | CA-CB | 7.25 | 1.64 | 1.53 |
| 5 | K | 518 | ARG | NE-CZ | 7.25 | 1.41 | 1.33 |
| 7 | O | 126 | GLU | CA-C | -7.25 | 1.43 | 1.52 |
| 9 | R | 435 | TRP | CA-CB | 7.25 | 1.64 | 1.53 |
| 15 | i | 274 | LEU | CA-C | -7.25 | 1.43 | 1.52 |
| 8 | N | 1062 | ARG | NE-CZ | 7.24 | 1.41 | 1.33 |
| 16 | j | 319 | SER | C-N | 7.24 | 1.42 | 1.33 |
| 2 | Z | 749 | ARG | C-N | 7.24 | 1.39 | 1.33 |
| 8 | P | 474 | ASP | C-N | 7.24 | 1.42 | 1.33 |
| 21 | t | 15 | ASP | CA-C | -7.24 | 1.45 | 1.53 |
| 15 | b | 735 | LEU | CA-C | -7.24 | 1.42 | 1.52 |
| 8 | P | 149 | ILE | CA-CB | -7.24 | 1.45 | 1.54 |
| 8 | P | 736 | ILE | CA-CB | 7.24 | 1.64 | 1.54 |
| 14 | a | 258 | ASP | C-N | 7.24 | 1.43 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1437 | PRO | C-N | 7.24 | 1.43 | 1.33 |
| 17 | k | 206 | TRP | CA-CB | 7.24 | 1.65 | 1.53 |
| 8 | P | 50 | ASN | N-CA | -7.24 | 1.36 | 1.46 |
| 9 | Q | 599 | ARG | C-N | 7.24 | 1.41 | 1.33 |
| 12 | u | 58 | ASN | CA-C | 7.24 | 1.61 | 1.52 |
| 16 | j | 293 | GLN | N-CA | -7.24 | 1.37 | 1.46 |
| 15 | b | 95 | ILE | CA-C | 7.24 | 1.60 | 1.52 |
| 14 | h | 108 | LEU | CA-C | -7.23 | 1.44 | 1.52 |
| 1 | Y | 767 | SER | CA-C | 7.23 | 1.61 | 1.52 |
| 18 | l | 134 | LEU | CA-CB | 7.23 | 1.62 | 1.53 |
| 4 | D | 774 | ASN | C-N | 7.23 | 1.43 | 1.33 |
| 9 | T | 213 | GLU | C-N | 7.23 | 1.44 | 1.34 |
| 19 | m | 342 | PRO | C-N | 7.23 | 1.42 | 1.33 |
| 20 | g | 282 | LEU | CA-C | -7.23 | 1.44 | 1.52 |
| 14 | h | 803 | HIS | CB-CG | 7.22 | 1.60 | 1.50 |
| 7 | M | 1345 | PHE | CA-C | -7.22 | 1.43 | 1.52 |
| 8 | P | 1497 | ASN | CA-C | -7.22 | 1.43 | 1.52 |
| 12 | u | 65 | LEU | CA-C | -7.22 | 1.43 | 1.52 |
| 14 | h | 656 | ASP | N-CA | -7.22 | 1.37 | 1.46 |
| 15 | i | 48 | LEU | CA-CB | 7.22 | 1.63 | 1.53 |
| 18 | l | 54 | HIS | CG-ND1 | -7.22 | 1.30 | 1.38 |
| 19 | m | 416 | TYR | CA-C | -7.22 | 1.43 | 1.52 |
| 14 | a | 412 | LYS | N-CA | -7.22 | 1.37 | 1.46 |
| 8 | P | 898 | VAL | N-CA | 7.22 | 1.53 | 1.46 |
| 15 | i | 49 | VAL | CA-C | -7.22 | 1.46 | 1.52 |
| 20 | g | 140 | LEU | CA-CB | 7.22 | 1.64 | 1.53 |
| 2 | Z | 1268 | THR | CA-C | -7.22 | 1.43 | 1.52 |
| 20 | g | 1033 | VAL | N-CA | -7.22 | 1.37 | 1.46 |
| 14 | a | 88 | TYR | CA-CB | 7.22 | 1.64 | 1.53 |
| 18 | e | 339 | PHE | CA-C | -7.21 | 1.43 | 1.52 |
| 6 | I | 446 | GLU | N-CA | -7.21 | 1.37 | 1.46 |
| 12 | u | 222 | ASP | C-N | 7.21 | 1.43 | 1.33 |
| 8 | N | 1062 | ARG | CD-NE | 7.21 | 1.56 | 1.46 |
| 12 | u | 184 | ASP | CA-C | -7.21 | 1.43 | 1.52 |
| 14 | h | 1023 | LYS | CA-C | -7.21 | 1.43 | 1.52 |
| 15 | b | 682 | LEU | CA-C | -7.21 | 1.43 | 1.52 |
| 19 | f | 697 | GLU | CA-CB | 7.21 | 1.63 | 1.53 |
| 2 | Z | 536 | HIS | N-CA | -7.21 | 1.37 | 1.46 |
| 10 | W | 329 | GLN | N-CA | 7.20 | 1.55 | 1.46 |
| 7 | O | 1301 | SER | C-N | 7.20 | 1.43 | 1.33 |
| 20 | n | 327 | ALA | N-CA | -7.20 | 1.36 | 1.45 |
| 18 | e | 52 | ARG | CA-CB | 7.20 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 726 | GLU | CA-C | -7.20 | 1.43 | 1.52 |
| 8 | P | 1122 | PHE | CA-CB | 7.20 | 1.62 | 1.53 |
| 21 | t | 28 | SER | CA-C | -7.20 | 1.43 | 1.52 |
| 7 | O | 299 | THR | N-CA | -7.20 | 1.36 | 1.46 |
| 2 | 1 | 824 | SER | CA-C | -7.19 | 1.43 | 1.52 |
| 9 | T | 107 | GLU | CA-C | 7.19 | 1.62 | 1.52 |
| 11 | X | 351 | THR | CA-C | -7.19 | 1.43 | 1.52 |
| 20 | n | 788 | TRP | N-CA | -7.19 | 1.37 | 1.46 |
| 2 | Z | 303 | CYS | CA-CB | 7.19 | 1.65 | 1.53 |
| 19 | m | 595 | ARG | CD-NE | 7.19 | 1.56 | 1.46 |
| 7 | O | 1517 | ALA | C-N | 7.19 | 1.43 | 1.33 |
| 8 | P | 265 | PHE | C-N | 7.19 | 1.42 | 1.33 |
| 19 | m | 230 | GLU | N-CA | -7.19 | 1.36 | 1.46 |
| 16 | c | 439 | ARG | NE-CZ | 7.18 | 1.41 | 1.33 |
| 13 | x | 1404 | GLU | C-N | 7.18 | 1.43 | 1.33 |
| 20 | g | 215 | GLU | CA-CB | 7.18 | 1.63 | 1.53 |
| 7 | M | 1472 | GLU | C-N | 7.18 | 1.42 | 1.33 |
| 7 | O | 873 | ASN | CA-CB | 7.18 | 1.64 | 1.53 |
| 18 | l | 302 | ASP | CA-CB | 7.18 | 1.65 | 1.53 |
| 1 | 0 | 595 | ASN | CA-CB | 7.17 | 1.61 | 1.52 |
| 7 | M | 835 | LYS | CA-C | -7.17 | 1.43 | 1.52 |
| 15 | i | 696 | GLU | CA-C | -7.17 | 1.43 | 1.52 |
| 14 | a | 89 | HIS | CB-CG | 7.17 | 1.60 | 1.50 |
| 14 | h | 236 | VAL | CA-CB | -7.17 | 1.45 | 1.54 |
| 20 | g | 906 | ILE | CA-CB | -7.17 | 1.45 | 1.54 |
| 15 | i | 188 | MET | CA-C | -7.17 | 1.43 | 1.52 |
| 14 | a | 592 | LYS | N-CA | -7.17 | 1.39 | 1.46 |
| 2 | Z | 727 | ARG | CD-NE | 7.16 | 1.56 | 1.46 |
| 9 | R | 158 | ASN | CA-C | -7.16 | 1.43 | 1.52 |
| 12 | u | 314 | ILE | CA-C | -7.16 | 1.43 | 1.52 |
| 12 | v | 209 | TYR | N-CA | -7.16 | 1.36 | 1.46 |
| 9 | T | 721 | SER | CA-C | -7.16 | 1.43 | 1.52 |
| 15 | i | 372 | ALA | CA-C | -7.16 | 1.47 | 1.52 |
| 16 | j | 449 | PHE | CA-CB | 7.16 | 1.64 | 1.53 |
| 8 | N | 670 | HIS | ND1-CE1 | 7.15 | 1.39 | 1.32 |
| 5 | H | 446 | ARG | CA-C | -7.15 | 1.42 | 1.52 |
| 7 | M | 495 | TYR | C-N | 7.15 | 1.43 | 1.34 |
| 7 | O | 239 | HIS | ND1-CE1 | 7.15 | 1.39 | 1.32 |
| 9 | T | 431 | SER | C-N | 7.15 | 1.41 | 1.34 |
| 1 | 0 | 1197 | SER | CA-C | -7.15 | 1.43 | 1.52 |
| 2 | Z | 829 | LEU | CA-C | -7.15 | 1.43 | 1.52 |
| 20 | g | 475 | LEU | C-N | 7.15 | 1.43 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 351 | HIS | CD2-NE2 | 7.15 | 1.45 | 1.37 |
| 2 | Z | 596 | ALA | N-CA | -7.15 | 1.37 | 1.46 |
| 20 | g | 268 | VAL | CA-C | -7.15 | 1.43 | 1.52 |
| 2 | 1 | 1241 | LEU | N-CA | -7.15 | 1.37 | 1.46 |
| 16 | j | 525 | HIS | CE1-NE2 | 7.15 | 1.39 | 1.32 |
| 2 | 1 | 1213 | LEU | CA-CB | 7.14 | 1.65 | 1.53 |
| 8 | P | 1456 | ILE | C-N | 7.14 | 1.43 | 1.33 |
| 8 | N | 967 | LEU | CA-C | -7.14 | 1.45 | 1.53 |
| 9 | R | 595 | ARG | CA-CB | 7.14 | 1.65 | 1.53 |
| 20 | n | 180 | SER | CA-C | -7.14 | 1.43 | 1.52 |
| 2 | 1 | 110 | ILE | CA-C | -7.14 | 1.44 | 1.52 |
| 8 | N | 854 | LEU | C-N | 7.14 | 1.42 | 1.33 |
| 4 | J | 694 | ASP | CA-CB | 7.14 | 1.64 | 1.53 |
| 8 | N | 636 | GLN | C-N | 7.14 | 1.42 | 1.33 |
| 10 | W | 261 | THR | N-CA | 7.13 | 1.55 | 1.46 |
| 8 | P | 589 | GLU | CA-C | -7.13 | 1.43 | 1.52 |
| 2 | Z | 1001 | ARG | CA-C | -7.13 | 1.43 | 1.52 |
| 6 | F | 295 | LYS | C-N | 7.13 | 1.43 | 1.33 |
| 17 | k | 39 | GLU | CA-C | -7.13 | 1.43 | 1.52 |
| 15 | b | 639 | ARG | CZ-NH2 | 7.13 | 1.42 | 1.33 |
| 7 | M | 1150 | PHE | CA-CB | 7.13 | 1.64 | 1.53 |
| 16 | c | 509 | ARG | C-N | 7.13 | 1.43 | 1.33 |
| 19 | f | 436 | LEU | CA-CB | 7.13 | 1.63 | 1.53 |
| 7 | M | 740 | LEU | CA-CB | 7.12 | 1.66 | 1.53 |
| 4 | A | 667 | GLN | CA-C | -7.12 | 1.43 | 1.52 |
| 7 | M | 836 | ILE | N-CA | -7.12 | 1.37 | 1.46 |
| 14 | h | 919 | PHE | C-N | 7.12 | 1.43 | 1.33 |
| 4 | G | 722 | LEU | CA-C | -7.12 | 1.43 | 1.52 |
| 8 | P | 647 | GLN | CA-C | -7.11 | 1.43 | 1.52 |
| 19 | m | 37 | ASN | N-CA | -7.11 | 1.37 | 1.46 |
| 21 | t | 34 | LYS | C-N | 7.11 | 1.43 | 1.33 |
| 18 | e | 56 | SER | C-N | 7.11 | 1.43 | 1.33 |
| 15 | b | 645 | ALA | C-N | 7.11 | 1.42 | 1.33 |
| 15 | b | 510 | HIS | ND1-CE1 | 7.11 | 1.39 | 1.32 |
| 1 | Y | 954 | ALA | CA-C | 7.11 | 1.61 | 1.52 |
| 9 | S | 768 | VAL | CA-CB | 7.10 | 1.62 | 1.54 |
| 1 | 0 | 463 | GLU | CA-CB | 7.10 | 1.65 | 1.53 |
| 9 | Q | 757 | ALA | N-CA | -7.10 | 1.37 | 1.46 |
| 1 | Y | 436 | LEU | N-CA | -7.10 | 1.37 | 1.45 |
| 19 | m | 339 | SER | C-N | 7.10 | 1.43 | 1.33 |
| 12 | u | 63 | LEU | CA-CB | 7.10 | 1.65 | 1.52 |
| 14 | h | 909 | LEU | CA-C | -7.09 | 1.42 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 450 | GLY | CA-C | -7.09 | 1.43 | 1.52 |
| 21 | q | 44 | THR | N-CA | -7.09 | 1.37 | 1.46 |
| 8 | N | 574 | HIS | CA-CB | 7.09 | 1.64 | 1.53 |
| 9 | S | 612 | HIS | ND1-CE1 | 7.09 | 1.39 | 1.32 |
| 19 | m | 390 | THR | N-CA | -7.09 | 1.37 | 1.46 |
| 7 | M | 793 | TYR | CA-C | -7.09 | 1.42 | 1.52 |
| 7 | O | 626 | ASP | N-CA | -7.09 | 1.38 | 1.46 |
| 7 | O | 749 | ILE | C-O | -7.08 | 1.15 | 1.24 |
| 16 | c | 355 | SER | N-CA | -7.08 | 1.37 | 1.46 |
| 8 | N | 204 | VAL | N-CA | -7.08 | 1.39 | 1.46 |
| 9 | Q | 71 | TYR | N-CA | -7.08 | 1.38 | 1.46 |
| 18 | l | 35 | VAL | CA-CB | -7.08 | 1.45 | 1.54 |
| 19 | m | 43 | ARG | N-CA | -7.08 | 1.37 | 1.46 |
| 20 | g | 1011 | ASP | C-O | -7.08 | 1.15 | 1.23 |
| 7 | M | 1497 | ALA | C-N | 7.08 | 1.43 | 1.33 |
| 8 | N | 577 | MET | CA-C | -7.08 | 1.38 | 1.52 |
| 14 | h | 461 | SER | C-N | 7.08 | 1.42 | 1.33 |
| 5 | H | 333 | GLU | CA-C | 7.08 | 1.62 | 1.52 |
| 9 | T | 120 | ASN | CA-C | 7.08 | 1.61 | 1.52 |
| 6 | I | 451 | MET | CA-C | 7.07 | 1.62 | 1.52 |
| 2 | 1 | 884 | ILE | C-N | 7.07 | 1.41 | 1.34 |
| 5 | H | 538 | LYS | CA-C | -7.07 | 1.43 | 1.52 |
| 11 | V | 285 | ILE | N-CA | 7.07 | 1.55 | 1.46 |
| 19 | m | 545 | ALA | CA-CB | 7.07 | 1.62 | 1.53 |
| 7 | O | 1206 | ILE | C-N | 7.07 | 1.43 | 1.33 |
| 12 | v | 284 | PRO | N-CA | -7.07 | 1.38 | 1.47 |
| 14 | a | 776 | ILE | C-N | 7.07 | 1.42 | 1.33 |
| 7 | M | 1272 | LEU | CA-CB | 7.07 | 1.67 | 1.53 |
| 9 | S | 796 | SER | N-CA | 7.07 | 1.54 | 1.45 |
| 4 | z | 817 | GLN | CA-CB | 7.07 | 1.64 | 1.53 |
| 20 | n | 717 | CYS | CA-C | -7.07 | 1.43 | 1.52 |
| 12 | u | 447 | PHE | N-CA | -7.06 | 1.37 | 1.46 |
| 1 | 0 | 1474 | LEU | CA-CB | 7.06 | 1.63 | 1.53 |
| 8 | N | 720 | ARG | NE-CZ | 7.06 | 1.40 | 1.33 |
| 18 | e | 317 | THR | N-CA | 7.06 | 1.55 | 1.46 |
| 2 | 1 | 439 | SER | N-CA | -7.06 | 1.37 | 1.46 |
| 4 | A | 704 | GLN | CA-CB | 7.06 | 1.64 | 1.53 |
| 7 | M | 663 | LYS | C-N | 7.06 | 1.43 | 1.33 |
| 8 | P | 268 | THR | CA-C | -7.06 | 1.43 | 1.52 |
| 16 | c | 631 | GLN | CA-C | -7.06 | 1.41 | 1.52 |
| 12 | u | 212 | LEU | CA-C | -7.05 | 1.44 | 1.52 |
| 20 | g | 1043 | ARG | NE-CZ | 7.05 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 1176 | LEU | N-CA | -7.05 | 1.40 | 1.46 |
| 1 | Y | 1360 | SER | CA-C | -7.05 | 1.43 | 1.52 |
| 16 | j | 160 | LEU | N-CA | -7.05 | 1.38 | 1.46 |
| 9 | S | 425 | ILE | C-O | -7.05 | 1.19 | 1.24 |
| 1 | Y | 260 | HIS | CD2-NE2 | 7.05 | 1.45 | 1.37 |
| 1 | Y | 1402 | LEU | CA-CB | 7.05 | 1.63 | 1.53 |
| 19 | f | 238 | LYS | N-CA | -7.05 | 1.37 | 1.46 |
| 14 | a | 705 | LEU | C-N | 7.05 | 1.43 | 1.33 |
| 7 | O | 1023 | LEU | CA-CB | 7.05 | 1.65 | 1.53 |
| 1 | Y | 1461 | LYS | C-N | 7.05 | 1.42 | 1.33 |
| 1 | 0 | 1367 | LEU | CA-C | -7.05 | 1.43 | 1.52 |
| 4 | G | 716 | THR | CA-CB | -7.04 | 1.42 | 1.53 |
| 7 | M | 825 | ILE | C-N | 7.04 | 1.39 | 1.33 |
| 7 | O | 1223 | LEU | CA-C | -7.04 | 1.43 | 1.52 |
| 8 | P | 497 | ILE | CA-C | 7.04 | 1.61 | 1.52 |
| 9 | Q | 210 | GLU | CA-C | -7.04 | 1.44 | 1.52 |
| 11 | V | 385 | ILE | C-O | -7.04 | 1.19 | 1.24 |
| 19 | m | 518 | ILE | CA-CB | -7.04 | 1.46 | 1.54 |
| 14 | a | 704 | SER | CA-C | -7.04 | 1.44 | 1.52 |
| 5 | K | 305 | LYS | CA-C | -7.03 | 1.44 | 1.52 |
| 16 | j | 380 | SER | CA-CB | 7.03 | 1.64 | 1.53 |
| 4 | D | 704 | GLN | CA-C | -7.03 | 1.43 | 1.52 |
| 9 | S | 459 | LEU | N-CA | -7.03 | 1.36 | 1.45 |
| 20 | g | 867 | GLN | C-N | 7.03 | 1.43 | 1.33 |
| 2 | 1 | 242 | HIS | CB-CG | 7.03 | 1.59 | 1.50 |
| 2 | 1 | 973 | LYS | CA-CB | 7.03 | 1.64 | 1.53 |
| 13 | w | 1293 | GLU | N-CA | -7.03 | 1.37 | 1.46 |
| 1 | 0 | 206 | ASP | CA-CB | 7.03 | 1.65 | 1.53 |
| 7 | M | 786 | THR | N-CA | -7.03 | 1.38 | 1.46 |
| 7 | M | 1443 | ASN | C-N | 7.03 | 1.44 | 1.33 |
| 2 | Z | 240 | ARG | CD-NE | 7.03 | 1.56 | 1.46 |
| 17 | k | 17 | LEU | C-N | 7.03 | 1.43 | 1.33 |
| 9 | S | 262 | SER | C-N | -7.02 | 1.24 | 1.33 |
| 2 | Z | 232 | ILE | CA-CB | 7.02 | 1.60 | 1.53 |
| 15 | i | 57 | PRO | CA-C | 7.02 | 1.62 | 1.52 |
| 14 | a | 425 | GLN | C-N | 7.02 | 1.42 | 1.33 |
| 19 | m | 440 | ASP | CA-CB | 7.02 | 1.63 | 1.53 |
| 7 | O | 984 | THR | N-CA | 7.02 | 1.54 | 1.46 |
| 20 | n | 429 | VAL | N-CA | -7.02 | 1.38 | 1.46 |
| 20 | g | 379 | SER | CA-CB | 7.02 | 1.65 | 1.53 |
| 9 | R | 534 | PHE | CA-C | -7.02 | 1.43 | 1.52 |
| 9 | Q | 320 | TRP | CA-CB | 7.01 | 1.64 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 14 | h | 107 | THR | N-CA | -7.01 | 1.37 | 1.46 |
| 15 | b | 385 | ASP | N-CA | -7.01 | 1.38 | 1.46 |
| 16 | c | 614 | ILE | CA-C | -7.01 | 1.43 | 1.52 |
| 5 | E | 300 | ASP | CA-CB | 7.01 | 1.64 | 1.54 |
| 7 | M | 142 | SER | CA-CB | 7.01 | 1.62 | 1.53 |
| 8 | N | 469 | SER | CA-C | -7.01 | 1.44 | 1.52 |
| 8 | N | 1490 | ARG | N-CA | 7.01 | 1.54 | 1.46 |
| 20 | n | 257 | TRP | CA-CB | 7.01 | 1.65 | 1.53 |
| 9 | Q | 462 | PHE | CA-C | -7.01 | 1.45 | 1.53 |
| 19 | f | 611 | SER | N-CA | -7.01 | 1.37 | 1.46 |
| 14 | a | 270 | PHE | N-CA | -7.01 | 1.37 | 1.46 |
| 8 | P | 723 | LEU | N-CA | -7.01 | 1.36 | 1.46 |
| 12 | v | 297 | TYR | CA-C | -7.01 | 1.44 | 1.52 |
| 16 | j | 291 | ILE | N-CA | -7.00 | 1.38 | 1.46 |
| 20 | g | 260 | ILE | CA-C | 7.00 | 1.60 | 1.53 |
| 5 | H | 411 | ARG | CD-NE | 7.00 | 1.56 | 1.46 |
| 1 | Y | 972 | ASN | CA-CB | 7.00 | 1.64 | 1.53 |
| 4 | J | 770 | ASN | N-CA | -7.00 | 1.37 | 1.46 |
| 10 | W | 284 | LYS | CA-C | 7.00 | 1.67 | 1.52 |
| 6 | C | 378 | HIS | ND1-CE1 | 7.00 | 1.39 | 1.32 |
| 9 | S | 73 | LEU | CA-C | -7.00 | 1.43 | 1.52 |
| 2 | 1 | 355 | HIS | N-CA | -6.99 | 1.37 | 1.46 |
| 5 | K | 462 | ARG | CD-NE | 6.99 | 1.56 | 1.46 |
| 6 | L | 391 | LEU | C-N | 6.99 | 1.43 | 1.33 |
| 2 | 1 | 405 | LYS | C-N | 6.99 | 1.41 | 1.33 |
| 7 | O | 516 | ARG | CA-C | -6.99 | 1.44 | 1.52 |
| 2 | Z | 574 | THR | CA-C | -6.99 | 1.44 | 1.52 |
| 4 | J | 658 | TYR | C-N | 6.99 | 1.42 | 1.33 |
| 1 | Y | 916 | GLU | C-N | 6.99 | 1.40 | 1.33 |
| 15 | b | 662 | TYR | N-CA | -6.99 | 1.38 | 1.46 |
| 8 | N | 752 | SER | C-N | 6.99 | 1.42 | 1.33 |
| 7 | O | 1291 | SER | N-CA | -6.99 | 1.38 | 1.46 |
| 16 | j | 343 | TRP | C-O | -6.99 | 1.15 | 1.24 |
| 19 | m | 432 | TYR | N-CA | -6.99 | 1.38 | 1.46 |
| 20 | g | 499 | ASP | N-CA | 6.99 | 1.55 | 1.46 |
| 12 | v | 388 | SER | N-CA | 6.98 | 1.54 | 1.46 |
| 19 | m | 51 | LEU | N-CA | -6.98 | 1.37 | 1.46 |
| 12 | u | 270 | VAL | CA-C | -6.98 | 1.44 | 1.52 |
| 12 | v | 73 | SER | N-CA | -6.98 | 1.37 | 1.46 |
| 18 | l | 193 | ILE | CA-C | 6.98 | 1.60 | 1.53 |
| 1 | Y | 530 | ILE | CA-CB | -6.98 | 1.46 | 1.54 |
| 14 | h | 498 | HIS | CG-CD2 | 6.98 | 1.43 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | g | 313 | TYR | N-CA | -6.98 | 1.37 | 1.46 |
| 1 | 0 | 1060 | TYR | N-CA | -6.98 | 1.37 | 1.46 |
| 2 | 1 | 1115 | LEU | CA-C | -6.98 | 1.43 | 1.52 |
| 4 | G | 727 | SER | CA-C | -6.98 | 1.38 | 1.52 |
| 19 | m | 477 | ARG | NE-CZ | 6.98 | 1.40 | 1.33 |
| 19 | f | 325 | GLN | N-CA | -6.98 | 1.37 | 1.46 |
| 9 | T | 422 | ARG | NE-CZ | 6.97 | 1.40 | 1.33 |
| 19 | m | 700 | LYS | CA-CB | 6.97 | 1.65 | 1.53 |
| 8 | N | 210 | ASN | N-CA | -6.97 | 1.37 | 1.46 |
| 8 | N | 1533 | ILE | CA-CB | -6.97 | 1.46 | 1.54 |
| 17 | k | 206 | TRP | NE1-CE2 | -6.97 | 1.29 | 1.37 |
| 21 | t | 90 | LYS | C-N | 6.97 | 1.43 | 1.33 |
| 1 | 0 | 252 | ASN | C-N | 6.97 | 1.43 | 1.33 |
| 4 | D | 688 | HIS | ND1-CE1 | 6.97 | 1.39 | 1.32 |
| 8 | P | 860 | ALA | C-N | 6.97 | 1.42 | 1.33 |
| 2 | Z | 129 | VAL | CA-C | 6.97 | 1.61 | 1.52 |
| 19 | m | 595 | ARG | C-N | 6.97 | 1.43 | 1.33 |
| 6 | C | 330 | LEU | CA-C | -6.97 | 1.43 | 1.52 |
| 2 | Z | 231 | TYR | C-N | 6.97 | 1.40 | 1.33 |
| 19 | f | 319 | SER | N-CA | -6.96 | 1.36 | 1.45 |
| 8 | P | 1321 | LEU | CA-C | -6.96 | 1.43 | 1.52 |
| 7 | M | 301 | ASP | C-N | 6.96 | 1.42 | 1.33 |
| 8 | N | 1602 | LEU | C-N | 6.96 | 1.43 | 1.33 |
| 7 | O | 566 | THR | CA-C | -6.96 | 1.43 | 1.52 |
| 14 | a | 932 | ASN | N-CA | -6.96 | 1.37 | 1.46 |
| 12 | v | 363 | LEU | CA-C | -6.96 | 1.44 | 1.52 |
| 20 | n | 1100 | GLY | C-N | 6.96 | 1.42 | 1.33 |
| 2 | Z | 358 | SER | CA-C | -6.96 | 1.43 | 1.53 |
| 12 | v | 401 | ASP | CA-C | -6.96 | 1.43 | 1.52 |
| 14 | h | 762 | MET | C-N | 6.96 | 1.43 | 1.33 |
| 6 | L | 281 | ASP | CA-C | -6.95 | 1.44 | 1.52 |
| 8 | P | 151 | ASN | CA-C | -6.95 | 1.43 | 1.52 |
| 20 | n | 520 | ILE | CA-CB | 6.95 | 1.62 | 1.54 |
| 15 | b | 699 | TRP | CA-C | -6.95 | 1.43 | 1.52 |
| 13 | w | 1104 | SER | CA-C | -6.95 | 1.44 | 1.52 |
| 20 | g | 400 | PHE | CA-C | -6.95 | 1.44 | 1.52 |
| 9 | R | 595 | ARG | CZ-NH2 | 6.95 | 1.42 | 1.33 |
| 19 | f | 289 | HIS | ND1-CE1 | 6.95 | 1.39 | 1.32 |
| 6 | I | 382 | LYS | CA-CB | 6.95 | 1.62 | 1.53 |
| 1 | 0 | 1147 | GLU | CA-CB | 6.95 | 1.64 | 1.53 |
| 17 | d | 280 | LEU | N-CA | 6.95 | 1.54 | 1.46 |
| 1 | Y | 199 | ASN | CA-CB | 6.94 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 12 | u | 566 | SER | CA-CB | 6.94 | 1.64 | 1.53 |
| 12 | v | 207 | ALA | CA-C | -6.94 | 1.43 | 1.52 |
| 15 | i | 208 | LEU | CA-C | 6.94 | 1.62 | 1.52 |
| 20 | g | 250 | LYS | N-CA | -6.94 | 1.41 | 1.46 |
| 4 | J | 798 | ASN | C-O | 6.94 | 1.32 | 1.24 |
| 12 | v | 650 | SER | CA-C | -6.94 | 1.43 | 1.52 |
| 14 | h | 370 | ASP | CA-CB | 6.94 | 1.62 | 1.53 |
| 12 | v | 144 | VAL | CA-C | -6.94 | 1.44 | 1.52 |
| 20 | n | 577 | TYR | CA-C | -6.94 | 1.44 | 1.52 |
| 7 | M | 984 | THR | CA-C | -6.94 | 1.43 | 1.52 |
| 1 | 0 | 1318 | HIS | ND1-CE1 | 6.94 | 1.39 | 1.32 |
| 7 | M | 705 | ASP | CA-C | -6.94 | 1.43 | 1.52 |
| 18 | l | 88 | PRO | CA-C | 6.94 | 1.59 | 1.52 |
| 15 | b | 140 | HIS | ND1-CE1 | 6.94 | 1.39 | 1.32 |
| 14 | a | 151 | HIS | CA-C | -6.94 | 1.44 | 1.52 |
| 4 | y | 721 | LEU | CA-C | -6.94 | 1.43 | 1.52 |
| 8 | N | 994 | ILE | N-CA | -6.93 | 1.38 | 1.46 |
| 9 | T | 326 | THR | CA-CB | -6.93 | 1.44 | 1.52 |
| 7 | M | 618 | SER | CA-CB | 6.93 | 1.64 | 1.53 |
| 12 | u | 171 | ASN | C-N | 6.93 | 1.42 | 1.33 |
| 20 | n | 1049 | ASN | CA-C | -6.93 | 1.43 | 1.52 |
| 18 | e | 132 | GLY | C-N | 6.93 | 1.42 | 1.33 |
| 7 | M | 907 | HIS | CB-CG | -6.93 | 1.40 | 1.50 |
| 12 | v | 703 | GLN | N-CA | -6.93 | 1.37 | 1.46 |
| 1 | 0 | 845 | SER | N-CA | -6.93 | 1.39 | 1.46 |
| 9 | Q | 811 | ARG | NE-CZ | 6.93 | 1.40 | 1.33 |
| 4 | G | 765 | LEU | CA-C | -6.92 | 1.43 | 1.52 |
| 19 | m | 139 | VAL | CA-CB | -6.92 | 1.45 | 1.54 |
| 9 | R | 605 | GLU | CA-CB | 6.92 | 1.63 | 1.53 |
| 16 | j | 406 | HIS | CE1-NE2 | -6.92 | 1.25 | 1.32 |
| 8 | P | 256 | THR | N-CA | -6.92 | 1.33 | 1.46 |
| 8 | P | 956 | PHE | N-CA | 6.92 | 1.55 | 1.46 |
| 20 | g | 860 | LEU | C-N | 6.92 | 1.41 | 1.33 |
| 9 | Q | 680 | ASN | CA-CB | 6.92 | 1.64 | 1.53 |
| 2 | 1 | 989 | ASN | CA-CB | 6.92 | 1.63 | 1.53 |
| 7 | M | 1067 | ASN | C-N | 6.92 | 1.43 | 1.33 |
| 21 | o | 39 | ARG | NE-CZ | 6.92 | 1.40 | 1.33 |
| 2 | 1 | 1077 | SER | C-N | 6.91 | 1.43 | 1.33 |
| 7 | O | 259 | PHE | CA-C | -6.91 | 1.43 | 1.52 |
| 7 | M | 870 | LYS | CA-CB | 6.91 | 1.65 | 1.53 |
| 9 | R | 640 | SER | C-N | 6.91 | 1.42 | 1.33 |
| 15 | b | 594 | ILE | C-N | 6.91 | 1.43 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | g | 264 | ASN | N-CA | -6.91 | 1.37 | 1.46 |
| 1 | 0 | 1415 | ILE | C-N | 6.91 | 1.42 | 1.33 |
| 18 | l | 185 | VAL | CA-C | -6.91 | 1.43 | 1.52 |
| 9 | R | 711 | LYS | CA-CB | 6.91 | 1.62 | 1.53 |
| 5 | H | 295 | CYS | CA-C | 6.90 | 1.58 | 1.52 |
| 5 | B | 377 | ASN | N-CA | -6.90 | 1.38 | 1.46 |
| 8 | P | 1640 | ILE | C-N | 6.90 | 1.43 | 1.33 |
| 1 | Y | 595 | ASN | N-CA | -6.90 | 1.37 | 1.46 |
| 1 | Y | 1450 | TRP | NE1-CE2 | -6.90 | 1.29 | 1.37 |
| 19 | f | 509 | HIS | ND1-CE1 | 6.90 | 1.39 | 1.32 |
| 19 | f | 599 | GLU | C-N | 6.90 | 1.43 | 1.33 |
| 4 | z | 675 | GLN | C-N | 6.90 | 1.42 | 1.33 |
| 2 | 1 | 1164 | PHE | CA-CB | 6.89 | 1.64 | 1.53 |
| 12 | v | 268 | GLY | C-N | 6.89 | 1.42 | 1.33 |
| 9 | R | 416 | GLY | C-N | 6.89 | 1.43 | 1.33 |
| 1 | 0 | 590 | GLY | C-N | 6.89 | 1.43 | 1.33 |
| 16 | j | 419 | GLY | CA-C | -6.89 | 1.42 | 1.51 |
| 15 | b | 525 | ILE | N-CA | 6.89 | 1.54 | 1.46 |
| 4 | A | 643 | LYS | CA-C | -6.89 | 1.44 | 1.52 |
| 21 | o | 46 | LYS | CA-CB | 6.89 | 1.64 | 1.53 |
| 11 | V | 285 | ILE | C-N | 6.89 | 1.43 | 1.34 |
| 21 | r | 39 | ARG | C-N | 6.89 | 1.43 | 1.33 |
| 5 | E | 411 | ARG | C-N | 6.88 | 1.42 | 1.33 |
| 6 | I | 292 | HIS | CB-CG | 6.88 | 1.59 | 1.50 |
| 9 | Q | 555 | GLU | N-CA | -6.88 | 1.38 | 1.46 |
| 21 | t | 10 | ILE | CA-C | -6.88 | 1.43 | 1.52 |
| 15 | i | 570 | SER | CA-CB | 6.88 | 1.66 | 1.53 |
| 18 | l | 202 | LEU | C-N | 6.88 | 1.42 | 1.33 |
| 21 | o | 26 | THR | C-O | -6.88 | 1.16 | 1.24 |
| 17 | k | 141 | ILE | CA-C | -6.88 | 1.44 | 1.52 |
| 2 | 1 | 603 | VAL | CA-C | -6.88 | 1.44 | 1.52 |
| 1 | Y | 1063 | SER | CA-CB | 6.88 | 1.62 | 1.53 |
| 2 | Z | 425 | ILE | CA-C | -6.88 | 1.44 | 1.52 |
| 2 | Z | 1348 | LYS | CA-C | -6.88 | 1.44 | 1.52 |
| 12 | u | 447 | PHE | CA-CB | 6.88 | 1.64 | 1.53 |
| 14 | h | 609 | GLY | C-N | 6.88 | 1.44 | 1.33 |
| 17 | k | 121 | SER | CA-CB | 6.88 | 1.61 | 1.52 |
| 15 | b | 338 | VAL | CA-C | -6.88 | 1.43 | 1.52 |
| 20 | g | 285 | ILE | CA-CB | -6.88 | 1.47 | 1.55 |
| 19 | f | 290 | LEU | C-N | 6.88 | 1.43 | 1.33 |
| 5 | B | 472 | ASN | CA-C | -6.87 | 1.44 | 1.53 |
| 8 | P | 1627 | LEU | CA-CB | 6.87 | 1.65 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 14 | a | 451 | ARG | NE-CZ | 6.87 | 1.40 | 1.33 |
| 7 | O | 419 | THR | C-N | 6.87 | 1.42 | 1.33 |
| 16 | j | 165 | VAL | C-N | 6.87 | 1.39 | 1.33 |
| 20 | g | 395 | PHE | N-CA | -6.87 | 1.37 | 1.46 |
| 14 | a | 122 | ILE | CA-C | -6.87 | 1.45 | 1.53 |
| 8 | P | 1565 | ASN | N-CA | -6.87 | 1.38 | 1.46 |
| 1 | Y | 200 | GLU | N-CA | -6.87 | 1.37 | 1.46 |
| 12 | v | 202 | GLY | N-CA | -6.87 | 1.36 | 1.46 |
| 14 | h | 67 | TYR | C-N | 6.87 | 1.41 | 1.33 |
| 14 | a | 847 | LYS | CA-C | -6.87 | 1.43 | 1.52 |
| 6 | C | 297 | ASP | N-CA | -6.86 | 1.37 | 1.46 |
| 5 | E | 446 | ARG | CD-NE | 6.86 | 1.55 | 1.46 |
| 14 | h | 440 | GLU | CA-CB | 6.86 | 1.62 | 1.53 |
| 15 | i | 512 | PRO | N-CA | -6.86 | 1.38 | 1.47 |
| 19 | m | 597 | TYR | N-CA | -6.86 | 1.38 | 1.46 |
| 2 | Z | 379 | ILE | C-N | 6.86 | 1.42 | 1.33 |
| 14 | h | 723 | PHE | CA-C | -6.86 | 1.44 | 1.52 |
| 14 | a | 151 | HIS | ND1-CE1 | 6.86 | 1.39 | 1.32 |
| 8 | N | 281 | GLN | C-N | 6.86 | 1.43 | 1.33 |
| 14 | h | 799 | SER | CA-C | -6.86 | 1.44 | 1.52 |
| 15 | i | 454 | LEU | CA-CB | 6.86 | 1.65 | 1.53 |
| 2 | 1 | 1358 | ARG | NE-CZ | 6.86 | 1.40 | 1.33 |
| 6 | F | 274 | ARG | CD-NE | 6.86 | 1.55 | 1.46 |
| 7 | O | 490 | ALA | C-N | 6.86 | 1.43 | 1.33 |
| 15 | i | 63 | ASP | N-CA | -6.86 | 1.37 | 1.46 |
| 19 | f | 288 | ILE | C-N | 6.86 | 1.43 | 1.33 |
| 7 | M | 1327 | PHE | CA-CB | 6.85 | 1.64 | 1.53 |
| 9 | Q | 821 | GLN | N-CA | -6.85 | 1.38 | 1.46 |
| 8 | N | 221 | VAL | CA-C | 6.85 | 1.61 | 1.52 |
| 8 | P | 106 | ARG | NE-CZ | 6.85 | 1.40 | 1.33 |
| 15 | i | 719 | SER | CA-C | -6.85 | 1.45 | 1.53 |
| 20 | n | 854 | HIS | ND1-CE1 | 6.85 | 1.39 | 1.32 |
| 21 | t | 65 | PHE | C-N | 6.85 | 1.39 | 1.33 |
| 17 | d | 115 | LEU | N-CA | -6.85 | 1.37 | 1.46 |
| 8 | P | 983 | ASN | CA-CB | 6.85 | 1.58 | 1.53 |
| 13 | w | 1227 | VAL | N-CA | 6.85 | 1.54 | 1.46 |
| 14 | h | 540 | LEU | C-N | 6.85 | 1.41 | 1.33 |
| 7 | M | 1111 | ILE | N-CA | 6.85 | 1.54 | 1.46 |
| 8 | P | 411 | PHE | C-N | 6.85 | 1.42 | 1.33 |
| 9 | S | 745 | LEU | CA-C | -6.85 | 1.47 | 1.52 |
| 14 | h | 1031 | ARG | CZ-NH1 | 6.85 | 1.42 | 1.32 |
| 16 | c | 218 | LYS | CA-C | -6.85 | 1.43 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | C | 320 | SER | CA-C | -6.84 | 1.43 | 1.52 |
| 12 | v | 438 | ALA | N-CA | -6.84 | 1.37 | 1.46 |
| 15 | b | 508 | LEU | CA-C | 6.84 | 1.61 | 1.52 |
| 16 | c | 138 | ILE | CA-C | -6.84 | 1.44 | 1.52 |
| 14 | a | 243 | LEU | CA-CB | 6.84 | 1.61 | 1.52 |
| 15 | b | 426 | ALA | CA-C | -6.84 | 1.43 | 1.52 |
| 2 | Z | 865 | GLU | CA-C | -6.84 | 1.43 | 1.52 |
| 20 | n | 571 | VAL | C-N | 6.84 | 1.43 | 1.33 |
| 6 | I | 337 | LYS | CA-CB | 6.84 | 1.64 | 1.53 |
| 8 | N | 159 | SER | C-N | 6.84 | 1.43 | 1.33 |
| 9 | R | 780 | SER | CA-C | -6.84 | 1.44 | 1.52 |
| 15 | i | 732 | ARG | CZ-NH2 | 6.84 | 1.42 | 1.33 |
| 20 | n | 303 | HIS | ND1-CE1 | 6.84 | 1.39 | 1.32 |
| 12 | u | 354 | VAL | CA-C | -6.84 | 1.44 | 1.52 |
| 17 | d | 118 | VAL | CA-CB | -6.84 | 1.46 | 1.54 |
| 13 | w | 1119 | GLU | C-N | 6.83 | 1.41 | 1.33 |
| 8 | N | 930 | ALA | CA-C | -6.83 | 1.43 | 1.52 |
| 8 | P | 299 | ASN | CA-CB | 6.83 | 1.64 | 1.53 |
| 12 | u | 383 | GLN | CA-C | -6.83 | 1.44 | 1.52 |
| 2 | 1 | 362 | ILE | N-CA | -6.83 | 1.38 | 1.46 |
| 7 | M | 220 | VAL | N-CA | -6.83 | 1.37 | 1.46 |
| 9 | Q | 251 | ALA | N-CA | -6.83 | 1.38 | 1.46 |
| 1 | Y | 151 | GLN | N-CA | 6.83 | 1.50 | 1.46 |
| 12 | v | 437 | LEU | CA-C | -6.83 | 1.44 | 1.52 |
| 20 | n | 408 | ASN | CG-ND2 | 6.83 | 1.47 | 1.33 |
| 20 | g | 785 | HIS | ND1-CE1 | 6.83 | 1.39 | 1.32 |
| 7 | M | 1472 | GLU | C-O | -6.83 | 1.18 | 1.23 |
| 9 | R | 658 | ASN | N-CA | -6.83 | 1.38 | 1.46 |
| 5 | B | 474 | SER | CA-C | -6.83 | 1.43 | 1.52 |
| 7 | O | 1519 | LYS | C-N | 6.83 | 1.42 | 1.33 |
| 13 | x | 1452 | PHE | C-N | 6.83 | 1.42 | 1.33 |
| 14 | a | 966 | CYS | CA-C | -6.83 | 1.43 | 1.52 |
| 7 | M | 193 | LEU | N-CA | -6.83 | 1.38 | 1.46 |
| 14 | h | 893 | HIS | ND1-CE1 | 6.83 | 1.39 | 1.32 |
| 21 | q | 15 | ASP | CA-C | -6.83 | 1.45 | 1.53 |
| 2 | Z | 656 | HIS | CD2-NE2 | 6.82 | 1.45 | 1.37 |
| 20 | g | 776 | ASN | C-N | 6.82 | 1.41 | 1.33 |
| 7 | O | 1516 | THR | CA-C | 6.82 | 1.61 | 1.52 |
| 15 | i | 120 | ASP | C-N | 6.82 | 1.42 | 1.33 |
| 20 | g | 621 | TYR | N-CA | -6.82 | 1.36 | 1.45 |
| 1 | 0 | 1257 | GLN | CA-CB | 6.82 | 1.67 | 1.53 |
| 5 | B | 329 | HIS | N-CA | -6.82 | 1.37 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | f | 178 | HIS | ND1-CE1 | 6.82 | 1.39 | 1.32 |
| 6 | F | 283 | TYR | C-O | 6.82 | 1.29 | 1.23 |
| 7 | M | 1063 | ILE | CA-C | -6.82 | 1.44 | 1.52 |
| 1 | Y | 153 | VAL | CA-C | -6.82 | 1.44 | 1.52 |
| 1 | Y | 154 | PHE | CA-C | -6.82 | 1.44 | 1.52 |
| 16 | c | 339 | GLN | C-N | 6.82 | 1.42 | 1.33 |
| 17 | d | 144 | HIS | ND1-CE1 | 6.82 | 1.39 | 1.32 |
| 1 | 0 | 937 | SER | CA-CB | 6.82 | 1.63 | 1.53 |
| 6 | L | 389 | ARG | NE-CZ | 6.82 | 1.40 | 1.33 |
| 9 | T | 761 | SER | C-N | 6.82 | 1.43 | 1.33 |
| 15 | b | 466 | LEU | C-O | -6.81 | 1.16 | 1.24 |
| 19 | m | 535 | ARG | CD-NE | 6.81 | 1.55 | 1.46 |
| 15 | b | 677 | LEU | CA-C | -6.81 | 1.44 | 1.52 |
| 14 | a | 771 | ASP | C-N | 6.81 | 1.43 | 1.33 |
| 7 | M | 221 | SER | CA-CB | 6.81 | 1.62 | 1.53 |
| 19 | f | 63 | ILE | CA-CB | 6.81 | 1.63 | 1.54 |
| 20 | n | 685 | GLY | CA-C | -6.81 | 1.42 | 1.51 |
| 14 | a | 161 | ARG | NE-CZ | 6.81 | 1.40 | 1.33 |
| 8 | P | 1491 | LEU | N-CA | -6.80 | 1.38 | 1.46 |
| 19 | m | 43 | ARG | NE-CZ | 6.80 | 1.40 | 1.33 |
| 14 | a | 886 | LEU | C-N | 6.80 | 1.43 | 1.33 |
| 1 | 0 | 173 | MET | N-CA | -6.80 | 1.37 | 1.46 |
| 20 | n | 376 | THR | C-N | 6.80 | 1.42 | 1.33 |
| 15 | b | 97 | ARG | NE-CZ | 6.80 | 1.40 | 1.33 |
| 6 | F | 456 | ARG | CD-NE | 6.80 | 1.55 | 1.46 |
| 1 | Y | 265 | VAL | C-N | 6.80 | 1.43 | 1.33 |
| 21 | q | 72 | GLU | N-CA | -6.80 | 1.37 | 1.46 |
| 1 | 0 | 1207 | ARG | CZ-NH2 | 6.80 | 1.42 | 1.33 |
| 12 | v | 272 | ILE | CA-C | -6.80 | 1.44 | 1.52 |
| 12 | v | 575 | ASP | CA-C | -6.80 | 1.44 | 1.52 |
| 14 | a | 282 | LEU | CA-C | -6.80 | 1.44 | 1.52 |
| 4 | A | 751 | LEU | C-N | 6.79 | 1.43 | 1.33 |
| 6 | C | 356 | GLN | CA-CB | 6.79 | 1.65 | 1.53 |
| 17 | k | 247 | LEU | N-CA | -6.79 | 1.36 | 1.46 |
| 20 | g | 477 | PHE | CA-C | -6.79 | 1.45 | 1.53 |
| 2 | 1 | 590 | PHE | CA-CB | 6.79 | 1.64 | 1.53 |
| 2 | 1 | 1188 | ARG | NE-CZ | 6.79 | 1.40 | 1.33 |
| 1 | Y | 832 | VAL | CA-C | 6.79 | 1.61 | 1.52 |
| 5 | K | 297 | GLU | N-CA | -6.79 | 1.37 | 1.46 |
| 8 | P | 717 | VAL | CA-C | -6.79 | 1.42 | 1.52 |
| 4 | A | 662 | ILE | N-CA | -6.79 | 1.37 | 1.46 |
| 14 | h | 177 | PHE | CA-C | -6.79 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | q | 55 | ASN | CA-CB | 6.79 | 1.65 | 1.53 |
| 9 | T | 441 | MET | SD-CE | 6.78 | 1.96 | 1.79 |
| 13 | w | 1106 | ASP | CA-C | -6.78 | 1.44 | 1.52 |
| 20 | g | 97 | GLY | CA-C | -6.78 | 1.45 | 1.52 |
| 20 | g | 545 | TYR | N-CA | -6.78 | 1.37 | 1.46 |
| 14 | a | 160 | VAL | CA-C | -6.78 | 1.44 | 1.52 |
| 9 | R | 270 | ILE | CA-CB | 6.78 | 1.63 | 1.54 |
| 2 | Z | 1119 | ALA | CA-C | -6.78 | 1.44 | 1.52 |
| 13 | x | 1338 | GLN | C-O | -6.78 | 1.16 | 1.24 |
| 20 | n | 556 | HIS | CG-ND1 | -6.78 | 1.30 | 1.38 |
| 6 | I | 471 | SER | N-CA | -6.78 | 1.36 | 1.46 |
| 1 | Y | 984 | THR | CA-CB | 6.78 | 1.63 | 1.53 |
| 2 | Z | 191 | TYR | N-CA | -6.78 | 1.38 | 1.46 |
| 12 | u | 392 | THR | CA-CB | 6.78 | 1.64 | 1.53 |
| 14 | h | 375 | ASN | N-CA | -6.78 | 1.37 | 1.46 |
| 9 | T | 22 | LEU | CA-CB | 6.78 | 1.63 | 1.53 |
| 7 | O | 544 | TYR | C-N | 6.78 | 1.43 | 1.34 |
| 12 | v | 323 | SER | CA-C | -6.78 | 1.44 | 1.52 |
| 15 | i | 489 | ILE | CA-C | -6.78 | 1.44 | 1.52 |
| 17 | d | 196 | LEU | CA-CB | 6.78 | 1.61 | 1.52 |
| 9 | Q | 700 | ALA | N-CA | 6.77 | 1.54 | 1.46 |
| 15 | b | 581 | MET | CA-C | -6.77 | 1.43 | 1.52 |
| 14 | h | 916 | ARG | CD-NE | 6.77 | 1.55 | 1.46 |
| 7 | O | 672 | TRP | N-CA | -6.77 | 1.38 | 1.46 |
| 20 | n | 866 | GLN | C-N | 6.77 | 1.43 | 1.33 |
| 2 | Z | 1171 | ASP | CA-CB | 6.77 | 1.64 | 1.53 |
| 21 | o | 14 | SER | N-CA | -6.77 | 1.37 | 1.46 |
| 1 | 0 | 441 | VAL | C-N | 6.77 | 1.42 | 1.33 |
| 1 | Y | 952 | LEU | N-CA | -6.77 | 1.38 | 1.46 |
| 12 | v | 285 | PHE | N-CA | -6.77 | 1.37 | 1.46 |
| 7 | O | 1438 | VAL | CA-CB | -6.76 | 1.46 | 1.54 |
| 1 | Y | 964 | ARG | CD-NE | 6.76 | 1.55 | 1.46 |
| 12 | v | 155 | ASP | C-N | 6.76 | 1.42 | 1.33 |
| 17 | d | 76 | ASP | C-N | 6.76 | 1.43 | 1.33 |
| 4 | A | 772 | VAL | N-CA | -6.76 | 1.37 | 1.46 |
| 7 | M | 768 | VAL | N-CA | -6.76 | 1.37 | 1.46 |
| 9 | S | 136 | PHE | CA-C | -6.76 | 1.44 | 1.52 |
| 2 | Z | 1267 | ASN | CA-CB | 6.76 | 1.64 | 1.53 |
| 7 | M | 1398 | SER | CA-C | 6.76 | 1.61 | 1.53 |
| 7 | O | 150 | PHE | CA-CB | 6.76 | 1.63 | 1.53 |
| 8 | P | 1598 | LEU | C-N | 6.76 | 1.43 | 1.33 |
| 10 | U | 276 | ILE | CA-CB | -6.76 | 1.45 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | q | 88 | VAL | N-CA | -6.76 | 1.37 | 1.46 |
| 10 | U | 273 | PHE | CA-C | -6.76 | 1.44 | 1.52 |
| 17 | k | 198 | SER | CA-C | -6.76 | 1.44 | 1.52 |
| 8 | P | 937 | SER | CA-CB | 6.75 | 1.64 | 1.53 |
| 9 | T | 712 | GLU | CA-CB | 6.75 | 1.64 | 1.53 |
| 15 | b | 121 | ASP | N-CA | -6.75 | 1.38 | 1.46 |
| 19 | m | 441 | CYS | CA-C | 6.75 | 1.61 | 1.52 |
| 1 | 0 | 1004 | PHE | CA-CB | 6.75 | 1.64 | 1.53 |
| 7 | O | 156 | SER | CA-CB | 6.75 | 1.64 | 1.53 |
| 7 | O | 1627 | LYS | N-CA | -6.75 | 1.38 | 1.46 |
| 1 | Y | 458 | GLU | N-CA | -6.75 | 1.37 | 1.45 |
| 2 | Z | 951 | VAL | CA-CB | -6.75 | 1.45 | 1.54 |
| 5 | E | 349 | PRO | CA-C | -6.75 | 1.42 | 1.52 |
| 16 | c | 539 | PHE | CA-C | 6.75 | 1.61 | 1.52 |
| 19 | f | 279 | TYR | CA-C | -6.75 | 1.43 | 1.52 |
| 1 | Y | 907 | LEU | CA-C | -6.75 | 1.44 | 1.52 |
| 2 | Z | 1270 | ILE | CA-C | -6.74 | 1.44 | 1.52 |
| 20 | g | 149 | SER | CA-CB | 6.74 | 1.63 | 1.53 |
| 8 | N | 518 | LEU | CA-C | -6.74 | 1.43 | 1.52 |
| 1 | Y | 1207 | ARG | CZ-NH2 | 6.74 | 1.42 | 1.33 |
| 20 | n | 838 | GLU | CA-C | -6.74 | 1.43 | 1.52 |
| 7 | O | 55 | GLU | CA-CB | 6.74 | 1.63 | 1.53 |
| 7 | M | 13 | ARG | NE-CZ | 6.74 | 1.40 | 1.33 |
| 7 | O | 486 | TYR | CA-C | -6.74 | 1.44 | 1.52 |
| 8 | P | 989 | ASP | N-CA | -6.74 | 1.38 | 1.46 |
| 1 | Y | 1328 | ALA | CA-C | -6.74 | 1.44 | 1.52 |
| 2 | Z | 301 | LYS | C-N | 6.74 | 1.42 | 1.33 |
| 15 | b | 726 | THR | N-CA | -6.74 | 1.37 | 1.45 |
| 14 | a | 805 | ASP | N-CA | -6.74 | 1.37 | 1.46 |
| 14 | h | 271 | ARG | C-O | -6.74 | 1.16 | 1.24 |
| 20 | g | 465 | LEU | CA-C | 6.73 | 1.61 | 1.52 |
| 4 | D | 808 | ASP | N-CA | -6.73 | 1.37 | 1.46 |
| 19 | f | 287 | HIS | N-CA | -6.73 | 1.37 | 1.46 |
| 1 | 0 | 179 | LEU | CA-C | -6.73 | 1.45 | 1.52 |
| 6 | F | 286 | LYS | CA-C | -6.73 | 1.43 | 1.52 |
| 1 | Y | 1326 | LYS | C-N | 6.73 | 1.41 | 1.33 |
| 12 | v | 246 | LYS | CA-CB | 6.73 | 1.63 | 1.53 |
| 8 | N | 820 | LEU | CA-CB | 6.73 | 1.63 | 1.53 |
| 20 | n | 227 | ARG | CA-CB | 6.73 | 1.63 | 1.53 |
| 1 | 0 | 262 | SER | C-N | 6.73 | 1.41 | 1.33 |
| 9 | Q | 669 | ASP | C-N | 6.73 | 1.43 | 1.33 |
| 1 | Y | 1097 | TYR | CA-C | -6.73 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | o | 16 | ILE | N-CA | -6.73 | 1.39 | 1.46 |
| 5 | H | 437 | TRP | NE1-CE2 | -6.72 | 1.30 | 1.37 |
| 12 | v | 366 | LEU | N-CA | -6.72 | 1.40 | 1.45 |
| 20 | g | 556 | HIS | CG-CD2 | 6.72 | 1.43 | 1.35 |
| 14 | a | 422 | ARG | CA-CB | 6.72 | 1.63 | 1.53 |
| 6 | I | 452 | ASP | CA-C | -6.72 | 1.44 | 1.52 |
| 10 | W | 349 | ALA | CA-CB | 6.72 | 1.64 | 1.53 |
| 1 | Y | 128 | ASN | CA-C | -6.72 | 1.44 | 1.52 |
| 17 | d | 200 | LEU | C-N | 6.72 | 1.39 | 1.33 |
| 9 | T | 763 | LEU | CA-C | -6.72 | 1.46 | 1.53 |
| 1 | 0 | 145 | PHE | CA-C | -6.72 | 1.44 | 1.52 |
| 5 | K | 530 | ASP | CA-C | -6.72 | 1.44 | 1.52 |
| 7 | O | 925 | HIS | ND1-CE1 | 6.72 | 1.39 | 1.32 |
| 7 | O | 1034 | LEU | CA-C | -6.72 | 1.43 | 1.52 |
| 14 | a | 316 | GLN | N-CA | -6.72 | 1.37 | 1.45 |
| 8 | N | 1000 | LYS | C-N | 6.72 | 1.44 | 1.33 |
| 9 | S | 832 | LEU | CA-CB | 6.72 | 1.61 | 1.52 |
| 2 | Z | 1242 | LEU | CA-C | -6.72 | 1.43 | 1.52 |
| 15 | i | 548 | SER | C-O | 6.72 | 1.32 | 1.24 |
| 19 | m | 49 | LEU | CA-C | -6.72 | 1.44 | 1.52 |
| 21 | o | 80 | TYR | C-N | 6.72 | 1.41 | 1.33 |
| 20 | g | 946 | LYS | C-N | 6.72 | 1.42 | 1.33 |
| 6 | I | 307 | SER | C-N | 6.71 | 1.41 | 1.33 |
| 2 | 1 | 1355 | SER | CA-C | -6.71 | 1.43 | 1.52 |
| 8 | N | 992 | SER | C-N | 6.71 | 1.42 | 1.33 |
| 11 | V | 300 | VAL | CA-C | -6.71 | 1.44 | 1.52 |
| 14 | h | 628 | ARG | C-N | 6.71 | 1.42 | 1.33 |
| 1 | 0 | 244 | ALA | CA-C | -6.71 | 1.44 | 1.52 |
| 4 | D | 765 | LEU | C-N | 6.71 | 1.42 | 1.33 |
| 14 | h | 929 | HIS | CB-CG | 6.71 | 1.59 | 1.50 |
| 19 | f | 435 | PHE | CA-C | -6.71 | 1.44 | 1.52 |
| 4 | y | 673 | GLY | CA-C | 6.71 | 1.59 | 1.52 |
| 20 | n | 812 | SER | C-N | 6.71 | 1.43 | 1.33 |
| 20 | g | 1133 | LEU | N-CA | -6.71 | 1.37 | 1.46 |
| 1 | 0 | 767 | SER | CA-C | -6.71 | 1.45 | 1.52 |
| 2 | Z | 929 | ASP | C-N | 6.71 | 1.43 | 1.33 |
| 12 | v | 353 | ARG | CA-C | -6.71 | 1.44 | 1.52 |
| 16 | j | 660 | VAL | CA-C | 6.71 | 1.61 | 1.52 |
| 5 | E | 397 | ARG | CD-NE | 6.70 | 1.55 | 1.46 |
| 4 | D | 757 | SER | N-CA | -6.70 | 1.38 | 1.46 |
| 6 | I | 461 | HIS | ND1-CE1 | 6.70 | 1.39 | 1.32 |
| 8 | P | 364 | THR | CA-C | -6.70 | 1.44 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 16 | j | 317 | HIS | ND1-CE1 | 6.70 | 1.39 | 1.32 |
| 15 | b | 661 | HIS | CA-C | -6.70 | 1.43 | 1.52 |
| 16 | c | 186 | ASP | C-N | 6.70 | 1.43 | 1.34 |
| 16 | c | 529 | ARG | CZ-NH1 | 6.70 | 1.42 | 1.32 |
| 9 | T | 826 | ARG | N-CA | -6.70 | 1.38 | 1.46 |
| 14 | h | 973 | SER | N-CA | -6.70 | 1.38 | 1.46 |
| 9 | R | 235 | ALA | N-CA | -6.69 | 1.38 | 1.46 |
| 1 | Y | 364 | GLN | CA-CB | 6.69 | 1.62 | 1.53 |
| 21 | o | 70 | THR | N-CA | -6.69 | 1.37 | 1.46 |
| 16 | c | 561 | LEU | CA-C | -6.69 | 1.43 | 1.52 |
| 7 | M | 1248 | LEU | CA-CB | 6.69 | 1.64 | 1.53 |
| 7 | M | 1316 | ASP | N-CA | 6.69 | 1.55 | 1.45 |
| 18 | l | 127 | CYS | CA-C | -6.69 | 1.44 | 1.52 |
| 17 | d | 20 | TYR | C-N | 6.69 | 1.42 | 1.33 |
| 5 | B | 451 | ALA | N-CA | -6.69 | 1.38 | 1.46 |
| 21 | q | 19 | LYS | C-N | 6.69 | 1.42 | 1.33 |
| 14 | a | 85 | SER | CA-C | -6.69 | 1.44 | 1.52 |
| 14 | a | 607 | PHE | CA-CB | 6.69 | 1.64 | 1.53 |
| 18 | l | 10 | ASP | CA-C | -6.69 | 1.44 | 1.52 |
| 14 | a | 271 | ARG | NE-CZ | 6.69 | 1.40 | 1.33 |
| 2 | Z | 1128 | SER | C-N | 6.68 | 1.42 | 1.33 |
| 20 | n | 992 | LYS | CA-C | 6.68 | 1.61 | 1.52 |
| 8 | P | 1617 | ILE | CA-C | 6.68 | 1.58 | 1.52 |
| 9 | Q | 767 | ILE | N-CA | -6.68 | 1.37 | 1.46 |
| 9 | S | 120 | ASN | C-N | 6.68 | 1.42 | 1.33 |
| 18 | l | 308 | TRP | C-N | 6.68 | 1.42 | 1.33 |
| 1 | 0 | 534 | ALA | CA-CB | 6.68 | 1.63 | 1.53 |
| 4 | y | 681 | SER | C-N | 6.68 | 1.42 | 1.33 |
| 21 | s | 81 | ILE | N-CA | -6.68 | 1.36 | 1.46 |
| 9 | T | 408 | ARG | CA-C | -6.68 | 1.44 | 1.52 |
| 2 | Z | 983 | TYR | N-CA | -6.68 | 1.38 | 1.46 |
| 7 | M | 1024 | LEU | CA-C | -6.67 | 1.43 | 1.52 |
| 9 | Q | 95 | PHE | N-CA | 6.67 | 1.54 | 1.46 |
| 14 | h | 948 | ILE | N-CA | -6.67 | 1.38 | 1.46 |
| 21 | p | 43 | GLY | CA-C | -6.67 | 1.44 | 1.52 |
| 4 | A | 800 | HIS | ND1-CE1 | 6.67 | 1.39 | 1.32 |
| 9 | S | 427 | ALA | C-N | 6.67 | 1.41 | 1.34 |
| 19 | m | 178 | HIS | ND1-CE1 | 6.67 | 1.39 | 1.32 |
| 8 | P | 1006 | ASP | C-N | 6.67 | 1.42 | 1.33 |
| 9 | S | 624 | THR | CA-C | -6.67 | 1.43 | 1.52 |
| 1 | Y | 647 | ILE | CA-C | -6.67 | 1.45 | 1.52 |
| 17 | k | 53 | GLU | CA-C | -6.67 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | O | 475 | LYS | CA-C | -6.67 | 1.44 | 1.52 |
| 7 | O | 1194 | LEU | C-N | 6.67 | 1.42 | 1.33 |
| 2 | Z | 573 | LEU | C-N | 6.67 | 1.42 | 1.33 |
| 20 | n | 1034 | LYS | CA-C | -6.67 | 1.44 | 1.52 |
| 4 | G | 654 | HIS | CB-CG | 6.66 | 1.59 | 1.50 |
| 8 | P | 856 | THR | C-N | 6.66 | 1.42 | 1.33 |
| 12 | u | 690 | ASP | C-N | 6.66 | 1.42 | 1.33 |
| 16 | j | 317 | HIS | CB-CG | 6.66 | 1.59 | 1.50 |
| 1 | 0 | 938 | LEU | CA-C | -6.66 | 1.43 | 1.52 |
| 8 | P | 347 | THR | CA-C | -6.66 | 1.44 | 1.52 |
| 2 | Z | 279 | ASP | CA-CB | 6.66 | 1.64 | 1.53 |
| 20 | g | 731 | GLU | CA-C | -6.66 | 1.44 | 1.52 |
| 5 | B | 446 | ARG | CD-NE | 6.66 | 1.55 | 1.46 |
| 7 | O | 1085 | LYS | N-CA | 6.66 | 1.54 | 1.46 |
| 9 | Q | 758 | GLN | C-N | 6.66 | 1.43 | 1.33 |
| 9 | R | 121 | ILE | N-CA | 6.66 | 1.54 | 1.46 |
| 18 | l | 238 | GLY | CA-C | -6.66 | 1.42 | 1.51 |
| 12 | u | 412 | SER | N-CA | -6.66 | 1.38 | 1.46 |
| 20 | g | 526 | SER | CA-CB | 6.66 | 1.61 | 1.52 |
| 5 | H | 365 | GLN | CA-C | -6.66 | 1.43 | 1.52 |
| 7 | O | 198 | TYR | CA-C | -6.66 | 1.43 | 1.52 |
| 9 | T | 629 | ARG | CD-NE | 6.66 | 1.55 | 1.46 |
| 14 | h | 498 | HIS | N-CA | -6.66 | 1.38 | 1.46 |
| 16 | j | 783 | ARG | CD-NE | 6.66 | 1.55 | 1.46 |
| 14 | a | 793 | PHE | CA-C | -6.66 | 1.44 | 1.52 |
| 8 | N | 332 | ARG | CA-C | -6.65 | 1.43 | 1.52 |
| 14 | h | 164 | HIS | ND1-CE1 | 6.65 | 1.39 | 1.32 |
| 20 | g | 472 | MET | CA-C | 6.65 | 1.60 | 1.52 |
| 8 | P | 1024 | LEU | C-N | 6.65 | 1.41 | 1.33 |
| 11 | X | 384 | CYS | C-N | 6.65 | 1.40 | 1.33 |
| 20 | g | 467 | VAL | CA-CB | -6.65 | 1.45 | 1.54 |
| 20 | g | 506 | LYS | C-N | 6.65 | 1.41 | 1.33 |
| 9 | T | 26 | LEU | CA-C | 6.65 | 1.61 | 1.52 |
| 1 | Y | 260 | HIS | ND1-CE1 | 6.65 | 1.39 | 1.32 |
| 19 | m | 258 | PRO | CA-CB | 6.65 | 1.63 | 1.53 |
| 12 | v | 55 | HIS | ND1-CE1 | 6.65 | 1.39 | 1.32 |
| 18 | e | 308 | TRP | CA-C | -6.65 | 1.44 | 1.52 |
| 2 | Z | 573 | LEU | CA-C | -6.65 | 1.44 | 1.52 |
| 17 | k | 63 | HIS | ND1-CE1 | 6.64 | 1.39 | 1.32 |
| 20 | g | 672 | LEU | CA-C | 6.64 | 1.59 | 1.53 |
| 14 | a | 624 | SER | CA-C | 6.64 | 1.61 | 1.52 |
| 1 | 0 | 1294 | ILE | C-O | -6.64 | 1.16 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 1108 | ARG | CZ-NH1 | 6.64 | 1.42 | 1.32 |
| 16 | j | 518 | LEU | C-N | 6.64 | 1.42 | 1.33 |
| 18 | l | 340 | LYS | CA-C | -6.64 | 1.45 | 1.52 |
| 16 | c | 418 | ILE | CA-C | -6.64 | 1.43 | 1.52 |
| 20 | g | 603 | ILE | C-N | 6.64 | 1.41 | 1.33 |
| 1 | Y | 124 | ARG | CZ-NH1 | 6.64 | 1.42 | 1.32 |
| 15 | i | 351 | ARG | C-N | 6.64 | 1.41 | 1.33 |
| 20 | n | 326 | PHE | CA-CB | 6.64 | 1.64 | 1.53 |
| 2 | Z | 1380 | GLN | N-CA | -6.64 | 1.37 | 1.46 |
| 20 | n | 805 | ALA | N-CA | -6.64 | 1.38 | 1.46 |
| 7 | M | 1520 | ALA | C-N | 6.64 | 1.42 | 1.33 |
| 7 | O | 208 | LYS | CA-CB | 6.64 | 1.64 | 1.53 |
| 7 | M | 1492 | LEU | N-CA | -6.63 | 1.38 | 1.46 |
| 1 | Y | 417 | TYR | CA-C | -6.63 | 1.44 | 1.52 |
| 12 | v | 372 | LYS | CA-C | -6.63 | 1.44 | 1.52 |
| 20 | n | 688 | THR | C-N | 6.63 | 1.41 | 1.33 |
| 20 | n | 909 | ASP | CA-CB | 6.63 | 1.62 | 1.53 |
| 1 | 0 | 1094 | ARG | CD-NE | 6.63 | 1.55 | 1.46 |
| 6 | I | 469 | SER | N-CA | -6.63 | 1.39 | 1.46 |
| 7 | O | 1389 | ILE | N-CA | -6.63 | 1.38 | 1.46 |
| 9 | R | 660 | LEU | C-N | 6.63 | 1.42 | 1.33 |
| 18 | e | 27 | CYS | C-N | 6.63 | 1.41 | 1.33 |
| 20 | g | 556 | HIS | ND1-CE1 | 6.63 | 1.39 | 1.32 |
| 5 | K | 320 | GLU | CA-C | -6.63 | 1.43 | 1.52 |
| 8 | N | 57 | THR | C-N | 6.63 | 1.42 | 1.33 |
| 12 | u | 439 | LEU | CA-CB | 6.63 | 1.61 | 1.53 |
| 14 | h | 509 | TYR | N-CA | -6.63 | 1.38 | 1.46 |
| 20 | n | 589 | GLU | CA-C | -6.63 | 1.44 | 1.52 |
| 19 | f | 239 | LYS | N-CA | -6.63 | 1.38 | 1.46 |
| 19 | f | 315 | LEU | N-CA | -6.63 | 1.36 | 1.46 |
| 6 | C | 460 | LEU | CA-CB | 6.62 | 1.63 | 1.53 |
| 9 | Q | 236 | ASN | CA-CB | 6.62 | 1.64 | 1.53 |
| 21 | q | 47 | LYS | CA-CB | 6.62 | 1.63 | 1.53 |
| 18 | l | 332 | LYS | N-CA | -6.62 | 1.38 | 1.46 |
| 5 | B | 415 | LEU | C-N | 6.62 | 1.43 | 1.33 |
| 7 | O | 181 | PHE | CA-CB | 6.62 | 1.65 | 1.53 |
| 20 | n | 1001 | ASP | CA-CB | 6.62 | 1.64 | 1.53 |
| 19 | f | 475 | ILE | CA-CB | 6.62 | 1.64 | 1.54 |
| 8 | P | 1598 | LEU | CA-C | -6.62 | 1.43 | 1.52 |
| 8 | P | 266 | THR | CA-C | -6.62 | 1.44 | 1.52 |
| 2 | Z | 1177 | VAL | CA-CB | 6.62 | 1.63 | 1.54 |
| 6 | I | 293 | HIS | CA-C | -6.62 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | Q | 264 | LYS | C-O | -6.62 | 1.16 | 1.24 |
| 9 | S | 609 | PRO | CA-CB | 6.62 | 1.63 | 1.53 |
| 1 | Y | 1161 | MET | CA-CB | 6.62 | 1.63 | 1.53 |
| 20 | g | 628 | HIS | ND1-CE1 | 6.62 | 1.39 | 1.32 |
| 2 | 1 | 235 | ILE | CA-CB | 6.61 | 1.61 | 1.54 |
| 1 | Y | 973 | ARG | CA-CB | 6.61 | 1.61 | 1.52 |
| 20 | n | 538 | ILE | CA-C | -6.61 | 1.43 | 1.52 |
| 21 | t | 87 | LEU | CB-CG | 6.61 | 1.66 | 1.53 |
| 5 | H | 304 | THR | C-N | 6.61 | 1.43 | 1.33 |
| 5 | H | 462 | ARG | N-CA | -6.61 | 1.38 | 1.46 |
| 17 | k | 52 | HIS | CA-C | -6.61 | 1.44 | 1.53 |
| 9 | T | 42 | ILE | N-CA | -6.61 | 1.38 | 1.46 |
| 16 | j | 144 | PHE | C-N | 6.61 | 1.42 | 1.33 |
| 16 | j | 324 | TYR | N-CA | -6.61 | 1.38 | 1.46 |
| 2 | 1 | 1240 | ARG | CD-NE | 6.61 | 1.55 | 1.46 |
| 19 | f | 390 | THR | N-CA | -6.61 | 1.38 | 1.46 |
| 4 | D | 709 | ASN | CA-C | -6.61 | 1.43 | 1.52 |
| 7 | M | 709 | PHE | CA-CB | 6.61 | 1.63 | 1.53 |
| 9 | S | 551 | ARG | NE-CZ | 6.61 | 1.40 | 1.33 |
| 15 | i | 170 | ASN | CA-C | -6.61 | 1.43 | 1.52 |
| 5 | E | 471 | LYS | N-CA | -6.61 | 1.37 | 1.46 |
| 2 | Z | 1308 | CYS | CA-CB | 6.61 | 1.63 | 1.53 |
| 17 | d | 69 | ILE | N-CA | -6.61 | 1.38 | 1.46 |
| 8 | N | 1566 | TYR | C-N | 6.60 | 1.42 | 1.33 |
| 7 | M | 27 | GLU | CA-CB | 6.60 | 1.63 | 1.54 |
| 18 | l | 23 | HIS | ND1-CE1 | 6.60 | 1.39 | 1.32 |
| 7 | O | 1462 | SER | CA-CB | 6.60 | 1.63 | 1.53 |
| 20 | n | 212 | LEU | CA-C | -6.60 | 1.44 | 1.52 |
| 9 | R | 48 | GLU | CA-C | -6.60 | 1.44 | 1.52 |
| 12 | v | 412 | SER | CA-CB | 6.60 | 1.63 | 1.53 |
| 2 | 1 | 144 | THR | CA-CB | 6.59 | 1.64 | 1.53 |
| 7 | M | 42 | LEU | C-N | 6.59 | 1.42 | 1.33 |
| 8 | N | 833 | LYS | CA-CB | 6.59 | 1.65 | 1.53 |
| 7 | O | 493 | PRO | C-N | 6.59 | 1.42 | 1.34 |
| 16 | j | 616 | VAL | CA-CB | -6.59 | 1.46 | 1.54 |
| 9 | S | 700 | ALA | CA-C | -6.59 | 1.43 | 1.52 |
| 17 | d | 41 | GLU | C-N | 6.59 | 1.42 | 1.33 |
| 20 | g | 503 | TYR | C-N | 6.59 | 1.42 | 1.33 |
| 8 | N | 1522 | VAL | C-N | 6.59 | 1.42 | 1.33 |
| 9 | S | 333 | ILE | N-CA | 6.59 | 1.55 | 1.46 |
| 4 | y | 772 | VAL | CA-CB | -6.59 | 1.46 | 1.54 |
| 6 | I | 386 | ASP | CA-CB | 6.59 | 1.64 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | O | 356 | ILE | N-CA | -6.59 | 1.38 | 1.46 |
| 14 | h | 299 | GLN | CA-CB | 6.59 | 1.62 | 1.53 |
| 17 | k | 292 | ALA | CA-C | -6.59 | 1.44 | 1.52 |
| 2 | 1 | 1133 | CYS | N-CA | -6.58 | 1.37 | 1.46 |
| 21 | q | 38 | GLU | N-CA | -6.58 | 1.38 | 1.46 |
| 8 | N | 323 | TYR | CA-C | -6.58 | 1.47 | 1.53 |
| 7 | O | 713 | PHE | N-CA | -6.58 | 1.38 | 1.46 |
| 7 | O | 1575 | PHE | N-CA | -6.58 | 1.37 | 1.46 |
| 7 | O | 1666 | MET | C-N | 6.58 | 1.39 | 1.33 |
| 19 | m | 73 | ARG | NE-CZ | 6.58 | 1.40 | 1.33 |
| 2 | 1 | 500 | THR | CA-C | -6.58 | 1.44 | 1.52 |
| 8 | P | 1633 | ARG | CD-NE | 6.58 | 1.55 | 1.46 |
| 1 | Y | 947 | LEU | CA-C | -6.58 | 1.46 | 1.53 |
| 9 | R | 418 | CYS | CA-C | -6.58 | 1.45 | 1.52 |
| 1 | 0 | 909 | PHE | C-N | 6.57 | 1.42 | 1.33 |
| 21 | t | 50 | ASP | C-N | 6.57 | 1.42 | 1.33 |
| 19 | f | 67 | ASP | N-CA | -6.57 | 1.38 | 1.46 |
| 20 | g | 445 | ASP | C-N | 6.57 | 1.42 | 1.33 |
| 8 | P | 1348 | VAL | C-N | 6.57 | 1.42 | 1.33 |
| 9 | T | 237 | GLU | N-CA | -6.57 | 1.38 | 1.46 |
| 8 | N | 198 | MET | N-CA | -6.57 | 1.38 | 1.46 |
| 7 | M | 943 | ARG | NE-CZ | 6.57 | 1.40 | 1.33 |
| 9 | T | 421 | SER | CA-C | -6.57 | 1.43 | 1.53 |
| 6 | L | 287 | GLN | C-O | -6.57 | 1.16 | 1.24 |
| 7 | M | 259 | PHE | CA-CB | 6.57 | 1.64 | 1.53 |
| 7 | O | 1671 | VAL | CA-CB | 6.57 | 1.62 | 1.54 |
| 17 | k | 36 | PHE | C-N | 6.57 | 1.42 | 1.33 |
| 2 | 1 | 540 | VAL | C-O | -6.57 | 1.17 | 1.24 |
| 2 | 1 | 1250 | SER | C-N | 6.57 | 1.39 | 1.33 |
| 6 | I | 370 | ASP | C-N | 6.57 | 1.43 | 1.33 |
| 7 | M | 149 | LYS | CA-C | -6.57 | 1.44 | 1.52 |
| 14 | h | 276 | VAL | CA-C | 6.57 | 1.61 | 1.52 |
| 16 | j | 151 | ALA | N-CA | -6.57 | 1.38 | 1.46 |
| 14 | a | 881 | MET | N-CA | 6.57 | 1.54 | 1.46 |
| 7 | M | 41 | LYS | CA-C | -6.56 | 1.44 | 1.52 |
| 8 | P | 1649 | ASP | CA-C | -6.56 | 1.44 | 1.52 |
| 9 | Q | 808 | ASN | C-N | 6.56 | 1.42 | 1.33 |
| 15 | b | 70 | LYS | CA-C | -6.56 | 1.44 | 1.52 |
| 7 | M | 20 | PHE | C-N | 6.56 | 1.42 | 1.33 |
| 8 | N | 1427 | SER | C-N | 6.56 | 1.43 | 1.33 |
| 9 | S | 215 | TYR | CA-C | -6.56 | 1.44 | 1.52 |
| 14 | h | 252 | THR | C-N | 6.56 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | b | 486 | ILE | N-CA | -6.56 | 1.37 | 1.46 |
| 1 | Y | 439 | LEU | N-CA | -6.56 | 1.38 | 1.46 |
| 20 | n | 874 | PHE | C-N | 6.56 | 1.42 | 1.33 |
| 6 | F | 357 | LEU | CA-CB | 6.56 | 1.65 | 1.53 |
| 7 | O | 420 | THR | CA-C | -6.56 | 1.44 | 1.52 |
| 20 | n | 632 | LYS | CA-C | -6.56 | 1.44 | 1.52 |
| 19 | f | 431 | ILE | C-N | 6.56 | 1.42 | 1.33 |
| 6 | C | 398 | VAL | C-N | 6.55 | 1.43 | 1.34 |
| 8 | N | 1217 | ARG | C-N | 6.55 | 1.42 | 1.33 |
| 7 | O | 621 | TYR | N-CA | 6.55 | 1.53 | 1.46 |
| 4 | y | 668 | VAL | CA-CB | 6.55 | 1.62 | 1.54 |
| 6 | C | 373 | PHE | C-N | 6.55 | 1.43 | 1.34 |
| 14 | a | 25 | ASP | CA-CB | 6.55 | 1.62 | 1.53 |
| 14 | a | 602 | ILE | CA-CB | -6.55 | 1.46 | 1.54 |
| 7 | M | 1664 | ASN | N-CA | 6.55 | 1.54 | 1.46 |
| 1 | 0 | 1022 | ASP | CA-C | -6.55 | 1.44 | 1.52 |
| 9 | T | 593 | ILE | CA-C | -6.55 | 1.44 | 1.52 |
| 14 | a | 92 | THR | CA-C | -6.55 | 1.44 | 1.52 |
| 1 | 0 | 609 | ILE | CA-C | 6.54 | 1.59 | 1.52 |
| 1 | 0 | 1068 | LEU | CA-C | 6.54 | 1.61 | 1.52 |
| 5 | K | 532 | ALA | C-N | 6.54 | 1.41 | 1.33 |
| 7 | M | 1511 | LEU | CA-CB | 6.54 | 1.65 | 1.53 |
| 19 | m | 447 | PHE | C-N | 6.54 | 1.42 | 1.33 |
| 7 | M | 125 | HIS | ND1-CE1 | 6.54 | 1.39 | 1.32 |
| 1 | Y | 137 | ARG | CD-NE | 6.54 | 1.55 | 1.46 |
| 14 | h | 414 | ARG | N-CA | -6.54 | 1.37 | 1.46 |
| 15 | i | 647 | ARG | CZ-NH1 | 6.54 | 1.42 | 1.32 |
| 18 | e | 121 | LEU | CA-C | -6.54 | 1.44 | 1.52 |
| 19 | f | 628 | PHE | CA-C | 6.54 | 1.61 | 1.52 |
| 6 | L | 271 | PRO | N-CA | -6.54 | 1.38 | 1.47 |
| 9 | S | 247 | GLY | CA-C | 6.54 | 1.58 | 1.51 |
| 12 | u | 87 | GLU | CA-C | -6.54 | 1.44 | 1.52 |
| 14 | a | 618 | SER | CA-CB | 6.54 | 1.64 | 1.53 |
| 5 | K | 320 | GLU | N-CA | -6.54 | 1.37 | 1.46 |
| 8 | N | 948 | LEU | CA-C | -6.54 | 1.44 | 1.52 |
| 7 | M | 130 | LEU | CA-C | -6.54 | 1.43 | 1.52 |
| 7 | M | 249 | ASP | CA-CB | 6.54 | 1.63 | 1.53 |
| 8 | P | 1596 | LYS | C-N | 6.54 | 1.42 | 1.33 |
| 9 | T | 703 | SER | C-N | 6.54 | 1.43 | 1.33 |
| 9 | T | 825 | PRO | C-N | 6.54 | 1.42 | 1.33 |
| 2 | Z | 846 | ASP | CA-C | 6.54 | 1.61 | 1.52 |
| 20 | g | 840 | PRO | CA-C | -6.54 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 14 | a | 55 | GLU | N-CA | -6.54 | 1.37 | 1.46 |
| 7 | M | 1288 | ASN | N-CA | -6.53 | 1.38 | 1.46 |
| 17 | k | 249 | LYS | CA-C | -6.53 | 1.44 | 1.52 |
| 21 | o | 22 | GLU | C-N | 6.53 | 1.42 | 1.33 |
| 1 | 0 | 1335 | VAL | C-N | 6.53 | 1.42 | 1.33 |
| 9 | R | 93 | ASN | N-CA | -6.53 | 1.38 | 1.46 |
| 13 | w | 1433 | GLY | C-O | 6.53 | 1.31 | 1.23 |
| 17 | d | 105 | VAL | CA-CB | -6.53 | 1.46 | 1.54 |
| 1 | 0 | 1374 | ILE | C-N | 6.53 | 1.41 | 1.34 |
| 9 | R | 553 | ALA | CA-C | 6.53 | 1.61 | 1.52 |
| 2 | Z | 353 | VAL | CA-CB | 6.53 | 1.61 | 1.53 |
| 2 | Z | 493 | ILE | CA-C | -6.53 | 1.44 | 1.52 |
| 12 | u | 63 | LEU | CA-C | -6.53 | 1.45 | 1.52 |
| 13 | w | 1125 | ASP | N-CA | -6.53 | 1.38 | 1.46 |
| 16 | j | 512 | MET | C-N | 6.53 | 1.42 | 1.33 |
| 16 | c | 202 | ARG | CD-NE | 6.53 | 1.55 | 1.46 |
| 7 | M | 712 | LEU | N-CA | -6.53 | 1.38 | 1.46 |
| 8 | N | 839 | ILE | CA-CB | -6.53 | 1.46 | 1.54 |
| 20 | g | 994 | THR | N-CA | -6.52 | 1.38 | 1.46 |
| 7 | M | 69 | GLU | CA-C | -6.52 | 1.43 | 1.52 |
| 8 | P | 217 | GLN | N-CA | -6.52 | 1.38 | 1.46 |
| 9 | Q | 68 | LYS | N-CA | -6.52 | 1.38 | 1.46 |
| 9 | T | 247 | GLY | CA-C | -6.52 | 1.45 | 1.52 |
| 21 | q | 32 | LEU | C-N | 6.52 | 1.43 | 1.33 |
| 18 | l | 145 | LEU | CA-C | -6.52 | 1.42 | 1.52 |
| 9 | S | 633 | GLU | C-N | 6.52 | 1.43 | 1.33 |
| 20 | n | 223 | THR | CA-C | -6.52 | 1.44 | 1.52 |
| 19 | f | 103 | GLY | N-CA | -6.52 | 1.36 | 1.45 |
| 2 | Z | 634 | SER | CA-C | -6.52 | 1.47 | 1.52 |
| 12 | u | 422 | ARG | CA-C | -6.52 | 1.44 | 1.52 |
| 15 | b | 264 | CYS | N-CA | 6.52 | 1.54 | 1.46 |
| 20 | g | 557 | LEU | CA-C | 6.52 | 1.61 | 1.52 |
| 9 | Q | 327 | VAL | N-CA | -6.52 | 1.38 | 1.46 |
| 2 | Z | 571 | VAL | CA-C | -6.52 | 1.44 | 1.52 |
| 7 | M | 1048 | LEU | CA-C | -6.51 | 1.43 | 1.52 |
| 15 | i | 186 | ARG | CD-NE | 6.51 | 1.55 | 1.46 |
| 17 | d | 177 | GLY | C-N | 6.51 | 1.42 | 1.33 |
| 2 | Z | 997 | PHE | CA-CB | 6.51 | 1.63 | 1.53 |
| 14 | h | 779 | LEU | CB-CG | 6.51 | 1.66 | 1.53 |
| 19 | f | 99 | TYR | C-O | -6.51 | 1.15 | 1.24 |
| 14 | a | 932 | ASN | CA-CB | 6.51 | 1.64 | 1.53 |
| 2 | 1 | 1078 | GLN | CA-CB | 6.51 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | C | 350 | PHE | CA-CB | 6.51 | 1.64 | 1.53 |
| 8 | P | 845 | SER | CA-C | -6.51 | 1.44 | 1.52 |
| 9 | Q | 80 | PHE | C-N | 6.51 | 1.42 | 1.33 |
| 15 | i | 683 | MET | CA-C | -6.51 | 1.44 | 1.52 |
| 2 | 1 | 867 | LEU | C-N | 6.51 | 1.41 | 1.33 |
| 7 | M | 1496 | ASP | CA-CB | 6.51 | 1.66 | 1.53 |
| 16 | j | 447 | VAL | C-N | 6.51 | 1.42 | 1.33 |
| 2 | 1 | 961 | PRO | CA-C | -6.51 | 1.43 | 1.52 |
| 9 | S | 424 | ASN | C-N | 6.51 | 1.39 | 1.33 |
| 14 | h | 728 | ILE | N-CA | 6.51 | 1.55 | 1.46 |
| 8 | N | 1214 | PHE | C-N | 6.50 | 1.42 | 1.33 |
| 9 | Q | 712 | GLU | N-CA | -6.50 | 1.38 | 1.46 |
| 18 | e | 300 | HIS | C-N | 6.50 | 1.42 | 1.33 |
| 8 | P | 52 | ILE | CA-C | 6.50 | 1.60 | 1.53 |
| 9 | Q | 647 | ALA | CA-C | -6.50 | 1.44 | 1.52 |
| 9 | S | 267 | ASP | CA-CB | 6.50 | 1.65 | 1.53 |
| 18 | l | 50 | SER | C-N | 6.50 | 1.42 | 1.33 |
| 14 | a | 94 | ASN | C-N | 6.50 | 1.46 | 1.33 |
| 14 | a | 278 | GLU | CA-C | -6.50 | 1.45 | 1.52 |
| 5 | B | 383 | SER | CA-C | -6.50 | 1.44 | 1.52 |
| 2 | Z | 1188 | ARG | N-CA | -6.50 | 1.37 | 1.46 |
| 8 | P | 1600 | ALA | C-N | 6.50 | 1.42 | 1.33 |
| 9 | T | 808 | ASN | CA-C | 6.50 | 1.61 | 1.52 |
| 14 | h | 991 | LEU | CA-CB | 6.50 | 1.63 | 1.53 |
| 2 | 1 | 793 | ILE | C-N | 6.50 | 1.43 | 1.33 |
| 4 | J | 665 | TRP | CA-CB | 6.50 | 1.63 | 1.53 |
| 7 | M | 1667 | VAL | CA-CB | 6.50 | 1.62 | 1.54 |
| 16 | j | 570 | MET | N-CA | -6.50 | 1.40 | 1.46 |
| 16 | c | 657 | CYS | N-CA | -6.50 | 1.37 | 1.46 |
| 2 | 1 | 110 | ILE | C-N | 6.49 | 1.41 | 1.33 |
| 7 | M | 423 | LEU | CA-C | -6.49 | 1.44 | 1.52 |
| 9 | T | 806 | LEU | CA-C | -6.49 | 1.44 | 1.52 |
| 2 | Z | 1005 | TYR | CA-CB | 6.49 | 1.63 | 1.53 |
| 12 | v | 62 | HIS | C-N | 6.49 | 1.41 | 1.33 |
| 20 | n | 180 | SER | N-CA | -6.49 | 1.38 | 1.46 |
| 20 | n | 702 | ASP | N-CA | -6.49 | 1.38 | 1.46 |
| 17 | d | 59 | VAL | N-CA | -6.49 | 1.38 | 1.46 |
| 15 | i | 495 | GLY | C-N | 6.49 | 1.42 | 1.33 |
| 14 | a | 882 | PHE | CG-CD2 | 6.49 | 1.52 | 1.38 |
| 4 | D | 652 | ALA | N-CA | -6.49 | 1.38 | 1.46 |
| 4 | J | 677 | SER | CA-CB | 6.49 | 1.63 | 1.53 |
| 8 | N | 949 | LEU | CA-C | -6.49 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1595 | VAL | C-N | 6.49 | 1.42 | 1.33 |
| 12 | u | 446 | THR | C-N | 6.49 | 1.42 | 1.33 |
| 2 | 1 | 347 | VAL | CA-C | -6.49 | 1.45 | 1.52 |
| 2 | 1 | 874 | ASN | CA-CB | 6.49 | 1.63 | 1.53 |
| 10 | W | 329 | GLN | C-N | 6.49 | 1.42 | 1.33 |
| 12 | v | 209 | TYR | CA-C | 6.49 | 1.61 | 1.52 |
| 19 | m | 62 | VAL | CA-C | -6.49 | 1.44 | 1.52 |
| 6 | F | 442 | THR | C-N | 6.49 | 1.41 | 1.33 |
| 4 | J | 764 | SER | N-CA | -6.49 | 1.38 | 1.46 |
| 5 | H | 361 | ARG | CD-NE | 6.48 | 1.55 | 1.46 |
| 7 | O | 991 | THR | C-N | 6.48 | 1.42 | 1.33 |
| 2 | Z | 1238 | TRP | NE1-CE2 | 6.48 | 1.44 | 1.37 |
| 16 | j | 181 | ARG | NE-CZ | 6.48 | 1.40 | 1.33 |
| 9 | S | 579 | LEU | C-N | 6.48 | 1.42 | 1.33 |
| 19 | f | 473 | SER | CA-C | -6.48 | 1.44 | 1.52 |
| 6 | L | 389 | ARG | CD-NE | 6.48 | 1.55 | 1.46 |
| 20 | n | 598 | ILE | N-CA | 6.48 | 1.54 | 1.46 |
| 9 | Q | 40 | GLY | C-N | 6.48 | 1.42 | 1.33 |
| 17 | k | 252 | LYS | CA-C | 6.48 | 1.61 | 1.52 |
| 21 | t | 39 | ARG | CD-NE | 6.48 | 1.55 | 1.46 |
| 4 | J | 698 | GLN | CA-C | -6.48 | 1.43 | 1.52 |
| 8 | P | 695 | LEU | CA-CB | 6.48 | 1.62 | 1.53 |
| 19 | m | 601 | GLN | CA-CB | 6.48 | 1.63 | 1.53 |
| 18 | e | 17 | TYR | CA-C | -6.48 | 1.45 | 1.52 |
| 7 | O | 441 | THR | N-CA | -6.48 | 1.38 | 1.46 |
| 16 | j | 253 | ASP | CA-CB | 6.48 | 1.64 | 1.53 |
| 8 | P | 60 | GLN | CA-CB | 6.47 | 1.64 | 1.53 |
| 16 | j | 214 | SER | C-N | 6.47 | 1.42 | 1.33 |
| 20 | n | 519 | GLU | N-CA | -6.47 | 1.38 | 1.46 |
| 8 | N | 805 | LEU | C-N | 6.47 | 1.43 | 1.33 |
| 8 | N | 857 | LEU | CA-C | -6.47 | 1.44 | 1.52 |
| 15 | i | 122 | ARG | C-N | 6.47 | 1.42 | 1.33 |
| 19 | m | 424 | GLY | N-CA | -6.47 | 1.36 | 1.45 |
| 20 | g | 1020 | ARG | CD-NE | 6.47 | 1.55 | 1.46 |
| 1 | 0 | 1471 | ILE | CA-C | -6.47 | 1.45 | 1.52 |
| 5 | E | 443 | LEU | CA-CB | 6.47 | 1.63 | 1.53 |
| 7 | M | 861 | GLN | CA-C | -6.47 | 1.44 | 1.52 |
| 7 | M | 1251 | ARG | CZ-NH1 | 6.47 | 1.41 | 1.32 |
| 8 | N | 476 | ASP | CA-C | -6.47 | 1.45 | 1.52 |
| 8 | N | 597 | LEU | CA-CB | 6.47 | 1.63 | 1.53 |
| 7 | O | 437 | ASP | C-N | 6.47 | 1.42 | 1.33 |
| 8 | P | 469 | SER | CA-C | -6.47 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | Q | 342 | ARG | CD-NE | 6.47 | 1.55 | 1.46 |
| 20 | n | 399 | ILE | N-CA | -6.47 | 1.38 | 1.46 |
| 7 | M | 234 | THR | N-CA | 6.47 | 1.53 | 1.46 |
| 9 | Q | 320 | TRP | NE1-CE2 | 6.47 | 1.44 | 1.37 |
| 1 | Y | 1393 | ILE | C-N | 6.47 | 1.41 | 1.33 |
| 1 | 0 | 123 | GLU | CA-CB | 6.46 | 1.64 | 1.53 |
| 9 | Q | 652 | ILE | CA-C | 6.46 | 1.59 | 1.52 |
| 9 | Q | 773 | ASN | N-CA | -6.46 | 1.37 | 1.46 |
| 14 | h | 19 | GLU | CA-CB | 6.46 | 1.62 | 1.53 |
| 14 | h | 958 | TRP | CA-C | -6.46 | 1.44 | 1.52 |
| 14 | a | 113 | VAL | N-CA | 6.46 | 1.53 | 1.46 |
| 7 | M | 126 | GLU | CA-CB | 6.46 | 1.61 | 1.52 |
| 5 | B | 397 | ARG | CA-C | 6.46 | 1.61 | 1.52 |
| 5 | B | 529 | LYS | CA-CB | 6.46 | 1.63 | 1.53 |
| 8 | N | 1163 | LEU | CA-CB | 6.46 | 1.60 | 1.53 |
| 12 | u | 313 | GLU | C-N | 6.46 | 1.41 | 1.33 |
| 15 | i | 190 | PHE | CA-CB | 6.46 | 1.61 | 1.52 |
| 20 | n | 336 | SER | C-N | 6.46 | 1.39 | 1.33 |
| 20 | n | 523 | ASP | CA-CB | 6.46 | 1.64 | 1.53 |
| 20 | n | 790 | HIS | C-N | 6.46 | 1.41 | 1.33 |
| 21 | q | 24 | ILE | C-N | 6.46 | 1.42 | 1.33 |
| 1 | Y | 446 | LEU | CA-C | -6.46 | 1.45 | 1.52 |
| 2 | Z | 1390 | LEU | C-O | -6.46 | 1.15 | 1.24 |
| 17 | k | 76 | ASP | CA-CB | 6.46 | 1.64 | 1.53 |
| 15 | i | 275 | SER | N-CA | -6.46 | 1.37 | 1.46 |
| 21 | r | 80 | TYR | CA-C | -6.46 | 1.45 | 1.52 |
| 21 | s | 62 | GLY | C-N | 6.46 | 1.42 | 1.33 |
| 17 | d | 118 | VAL | C-N | 6.46 | 1.41 | 1.33 |
| 1 | 0 | 1333 | HIS | N-CA | -6.46 | 1.38 | 1.46 |
| 8 | P | 1171 | ARG | CA-CB | 6.46 | 1.61 | 1.53 |
| 14 | h | 1036 | GLY | N-CA | -6.46 | 1.35 | 1.45 |
| 21 | p | 27 | ILE | CA-C | -6.46 | 1.44 | 1.52 |
| 17 | d | 119 | ALA | CA-C | -6.46 | 1.44 | 1.52 |
| 14 | a | 725 | ARG | C-N | 6.46 | 1.42 | 1.33 |
| 2 | 1 | 707 | PRO | CA-C | 6.46 | 1.62 | 1.52 |
| 9 | T | 640 | SER | C-N | 6.46 | 1.41 | 1.33 |
| 1 | Y | 297 | HIS | CB-CG | 6.46 | 1.59 | 1.50 |
| 5 | E | 472 | ASN | C-N | 6.45 | 1.41 | 1.33 |
| 7 | O | 962 | ARG | CZ-NH1 | 6.45 | 1.41 | 1.32 |
| 16 | j | 638 | ILE | N-CA | 6.45 | 1.54 | 1.46 |
| 18 | e | 315 | THR | C-N | 6.45 | 1.42 | 1.33 |
| 7 | O | 844 | VAL | C-N | 6.45 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | Q | 358 | ALA | CA-C | -6.45 | 1.45 | 1.52 |
| 1 | Y | 712 | ASP | CA-CB | 6.45 | 1.64 | 1.53 |
| 1 | 0 | 1015 | GLU | CA-C | -6.45 | 1.44 | 1.52 |
| 4 | A | 693 | ILE | CA-C | -6.45 | 1.46 | 1.52 |
| 5 | E | 305 | LYS | CA-CB | 6.45 | 1.64 | 1.53 |
| 7 | M | 152 | HIS | C-N | 6.45 | 1.42 | 1.33 |
| 9 | R | 103 | ILE | N-CA | 6.45 | 1.54 | 1.46 |
| 9 | T | 626 | GLN | CA-C | -6.45 | 1.44 | 1.52 |
| 1 | Y | 1227 | ILE | N-CA | -6.45 | 1.38 | 1.46 |
| 8 | N | 453 | ALA | CA-C | -6.44 | 1.44 | 1.52 |
| 2 | 1 | 1371 | LYS | CA-C | -6.44 | 1.44 | 1.52 |
| 5 | K | 331 | LEU | CA-CB | 6.44 | 1.63 | 1.53 |
| 8 | P | 61 | ASN | N-CA | 6.44 | 1.54 | 1.46 |
| 21 | q | 89 | PHE | CA-CB | 6.44 | 1.65 | 1.53 |
| 2 | 1 | 302 | ILE | CA-C | -6.44 | 1.46 | 1.53 |
| 4 | D | 766 | ILE | N-CA | 6.44 | 1.54 | 1.46 |
| 7 | M | 910 | ARG | NE-CZ | 6.44 | 1.40 | 1.33 |
| 1 | Y | 1100 | LYS | C-N | -6.44 | 1.25 | 1.33 |
| 21 | r | 48 | GLN | CA-C | -6.44 | 1.44 | 1.52 |
| 11 | V | 384 | CYS | CA-CB | 6.44 | 1.65 | 1.53 |
| 7 | O | 1251 | ARG | CD-NE | 6.44 | 1.55 | 1.46 |
| 8 | P | 427 | ILE | CA-C | -6.44 | 1.44 | 1.52 |
| 7 | M | 70 | PHE | N-CA | 6.44 | 1.54 | 1.46 |
| 7 | O | 635 | PHE | CA-C | -6.43 | 1.43 | 1.52 |
| 9 | S | 704 | ARG | CZ-NH2 | 6.43 | 1.41 | 1.33 |
| 1 | Y | 1146 | TYR | CA-C | -6.43 | 1.44 | 1.52 |
| 14 | h | 692 | PHE | CA-CB | 6.43 | 1.63 | 1.53 |
| 1 | 0 | 1105 | TYR | CA-C | -6.43 | 1.44 | 1.52 |
| 15 | i | 525 | ILE | CA-CB | -6.43 | 1.46 | 1.54 |
| 16 | j | 139 | MET | N-CA | 6.43 | 1.53 | 1.46 |
| 8 | N | 682 | LEU | CA-C | -6.43 | 1.44 | 1.52 |
| 14 | h | 812 | LEU | CA-C | 6.43 | 1.61 | 1.52 |
| 21 | p | 61 | VAL | CA-C | -6.43 | 1.44 | 1.52 |
| 20 | g | 1058 | LEU | CA-C | -6.43 | 1.44 | 1.52 |
| 14 | a | 91 | LYS | CA-C | -6.43 | 1.44 | 1.52 |
| 8 | N | 1160 | ILE | C-N | 6.43 | 1.41 | 1.33 |
| 9 | Q | 334 | TRP | C-N | 6.43 | 1.42 | 1.34 |
| 9 | T | 17 | GLY | N-CA | 6.43 | 1.53 | 1.45 |
| 14 | h | 436 | HIS | CG-ND1 | 6.43 | 1.45 | 1.38 |
| 17 | d | 204 | SER | C-N | 6.43 | 1.42 | 1.33 |
| 7 | M | 1048 | LEU | N-CA | 6.43 | 1.54 | 1.46 |
| 10 | U | 347 | PRO | CA-C | -6.43 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 205 | ASP | C-N | 6.43 | 1.42 | 1.33 |
| 10 | W | 272 | ASN | C-N | 6.42 | 1.42 | 1.33 |
| 15 | i | 97 | ARG | C-N | 6.42 | 1.42 | 1.33 |
| 21 | r | 90 | LYS | CA-CB | 6.42 | 1.64 | 1.53 |
| 9 | S | 303 | ASN | CA-CB | 6.42 | 1.63 | 1.53 |
| 2 | Z | 880 | SER | CA-CB | 6.42 | 1.64 | 1.54 |
| 12 | u | 691 | SER | C-N | 6.42 | 1.42 | 1.33 |
| 12 | v | 649 | LYS | N-CA | -6.42 | 1.38 | 1.46 |
| 19 | m | 63 | ILE | CA-C | -6.42 | 1.44 | 1.52 |
| 2 | Z | 930 | THR | N-CA | -6.42 | 1.38 | 1.46 |
| 7 | O | 85 | GLU | C-N | 6.42 | 1.42 | 1.33 |
| 13 | w | 1276 | ILE | CA-C | -6.42 | 1.44 | 1.52 |
| 9 | T | 741 | LEU | C-N | 6.42 | 1.42 | 1.33 |
| 2 | Z | 750 | PRO | CA-C | -6.42 | 1.46 | 1.52 |
| 18 | l | 123 | LEU | CA-CB | 6.42 | 1.61 | 1.52 |
| 21 | s | 68 | TYR | N-CA | -6.42 | 1.39 | 1.46 |
| 15 | b | 403 | HIS | C-N | 6.42 | 1.42 | 1.33 |
| 5 | K | 348 | ILE | N-CA | 6.42 | 1.50 | 1.45 |
| 7 | O | 492 | ARG | CA-CB | 6.42 | 1.60 | 1.53 |
| 7 | O | 555 | TRP | NE1-CE2 | -6.42 | 1.30 | 1.37 |
| 9 | S | 19 | ASN | CA-CB | 6.42 | 1.63 | 1.53 |
| 9 | T | 547 | TYR | N-CA | -6.42 | 1.38 | 1.46 |
| 9 | T | 580 | VAL | C-N | 6.42 | 1.42 | 1.33 |
| 15 | b | 654 | GLU | CA-C | -6.42 | 1.44 | 1.53 |
| 16 | c | 181 | ARG | CA-C | -6.42 | 1.44 | 1.52 |
| 16 | j | 430 | ASN | CA-CB | 6.42 | 1.62 | 1.53 |
| 2 | 1 | 708 | ARG | CD-NE | 6.41 | 1.55 | 1.46 |
| 9 | R | 259 | ILE | CA-CB | -6.41 | 1.47 | 1.54 |
| 2 | Z | 1322 | TYR | C-N | 6.41 | 1.43 | 1.33 |
| 18 | e | 68 | TYR | CA-CB | 6.41 | 1.61 | 1.53 |
| 18 | e | 295 | GLU | N-CA | -6.41 | 1.38 | 1.46 |
| 20 | g | 275 | ILE | CA-C | 6.41 | 1.60 | 1.52 |
| 1 | 0 | 685 | VAL | CA-C | 6.41 | 1.60 | 1.52 |
| 15 | b | 399 | SER | N-CA | -6.41 | 1.38 | 1.46 |
| 8 | P | 347 | THR | CA-CB | 6.41 | 1.63 | 1.53 |
| 9 | Q | 492 | ILE | N-CA | -6.41 | 1.38 | 1.46 |
| 9 | R | 414 | LEU | CA-C | -6.41 | 1.46 | 1.53 |
| 2 | Z | 665 | PHE | CA-CB | 6.41 | 1.63 | 1.53 |
| 5 | B | 371 | GLN | N-CA | 6.41 | 1.54 | 1.46 |
| 5 | H | 453 | LEU | CA-C | -6.41 | 1.45 | 1.52 |
| 12 | v | 304 | THR | CA-C | -6.41 | 1.45 | 1.52 |
| 14 | h | 650 | HIS | N-CA | -6.41 | 1.38 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | n | 927 | ALA | N-CA | -6.41 | 1.38 | 1.46 |
| 7 | M | 1273 | LYS | CA-C | -6.41 | 1.44 | 1.52 |
| 7 | O | 1474 | PHE | N-CA | -6.41 | 1.37 | 1.46 |
| 7 | O | 1657 | ASP | CA-C | 6.41 | 1.60 | 1.52 |
| 9 | R | 606 | GLU | CA-CB | 6.41 | 1.63 | 1.53 |
| 12 | u | 400 | SER | C-N | 6.41 | 1.42 | 1.33 |
| 13 | x | 1391 | ALA | C-N | 6.41 | 1.42 | 1.33 |
| 5 | E | 530 | ASP | N-CA | -6.40 | 1.38 | 1.46 |
| 1 | 0 | 1383 | PHE | CA-CB | 6.40 | 1.63 | 1.53 |
| 8 | N | 1066 | VAL | CA-C | 6.40 | 1.60 | 1.52 |
| 8 | P | 876 | LEU | N-CA | -6.40 | 1.37 | 1.46 |
| 9 | R | 331 | VAL | CA-C | -6.40 | 1.46 | 1.52 |
| 9 | T | 714 | CYS | CA-C | -6.40 | 1.44 | 1.52 |
| 1 | Y | 638 | ARG | CA-C | -6.40 | 1.44 | 1.52 |
| 11 | X | 386 | PRO | CA-C | -6.40 | 1.45 | 1.52 |
| 12 | u | 147 | GLU | N-CA | -6.40 | 1.37 | 1.46 |
| 21 | r | 75 | HIS | ND1-CE1 | 6.40 | 1.39 | 1.32 |
| 15 | b | 187 | THR | CA-C | -6.40 | 1.45 | 1.52 |
| 7 | O | 34 | ASN | CA-C | -6.40 | 1.44 | 1.52 |
| 9 | Q | 501 | MET | N-CA | 6.40 | 1.54 | 1.46 |
| 14 | a | 852 | SER | N-CA | -6.40 | 1.38 | 1.45 |
| 2 | 1 | 1387 | HIS | ND1-CE1 | 6.39 | 1.39 | 1.32 |
| 7 | M | 893 | HIS | CB-CG | -6.39 | 1.41 | 1.50 |
| 8 | N | 529 | LEU | C-N | 6.39 | 1.42 | 1.33 |
| 9 | T | 660 | LEU | CA-CB | 6.39 | 1.63 | 1.53 |
| 8 | P | 176 | LEU | N-CA | -6.39 | 1.40 | 1.46 |
| 16 | j | 529 | ARG | NE-CZ | 6.39 | 1.40 | 1.33 |
| 16 | c | 640 | GLY | CA-C | 6.39 | 1.59 | 1.52 |
| 8 | P | 641 | ILE | CA-CB | -6.39 | 1.47 | 1.54 |
| 20 | n | 396 | LYS | CA-CB | 6.39 | 1.63 | 1.53 |
| 4 | A | 666 | ASP | CA-CB | 6.39 | 1.63 | 1.53 |
| 7 | O | 211 | ASP | N-CA | -6.39 | 1.38 | 1.46 |
| 9 | S | 718 | LEU | CA-C | -6.39 | 1.44 | 1.52 |
| 2 | Z | 901 | ILE | N-CA | 6.39 | 1.54 | 1.46 |
| 12 | u | 266 | ARG | CD-NE | 6.39 | 1.55 | 1.46 |
| 16 | c | 224 | MET | CA-C | 6.39 | 1.60 | 1.52 |
| 14 | a | 507 | PHE | CA-C | -6.39 | 1.44 | 1.52 |
| 9 | R | 432 | ILE | N-CA | 6.39 | 1.54 | 1.46 |
| 9 | S | 498 | PHE | C-N | 6.39 | 1.41 | 1.33 |
| 14 | h | 925 | LEU | C-N | 6.39 | 1.42 | 1.33 |
| 18 | l | 98 | TRP | C-N | 6.39 | 1.43 | 1.33 |
| 7 | M | 500 | TRP | NE1-CE2 | -6.39 | 1.30 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | N | 262 | SER | N-CA | -6.39 | 1.38 | 1.46 |
| 9 | T | 564 | GLU | N-CA | -6.39 | 1.38 | 1.46 |
| 10 | U | 280 | PHE | CA-C | -6.39 | 1.44 | 1.52 |
| 1 | Y | 714 | LYS | CA-CB | 6.39 | 1.63 | 1.53 |
| 21 | r | 57 | TRP | N-CA | -6.39 | 1.38 | 1.45 |
| 19 | f | 346 | LEU | CA-C | -6.39 | 1.44 | 1.52 |
| 14 | a | 974 | GLU | N-CA | 6.39 | 1.53 | 1.45 |
| 1 | 0 | 423 | ILE | N-CA | -6.38 | 1.38 | 1.46 |
| 2 | 1 | 399 | LEU | CA-CB | 6.38 | 1.62 | 1.53 |
| 9 | S | 232 | PHE | CA-C | -6.38 | 1.44 | 1.52 |
| 16 | c | 604 | ASP | CA-C | -6.38 | 1.45 | 1.52 |
| 14 | a | 820 | ARG | CA-C | -6.38 | 1.44 | 1.52 |
| 17 | k | 133 | ASN | C-N | 6.38 | 1.42 | 1.33 |
| 6 | F | 276 | GLU | CA-CB | 6.38 | 1.63 | 1.53 |
| 8 | N | 758 | TYR | CA-CB | 6.38 | 1.64 | 1.53 |
| 8 | N | 826 | SER | CA-C | 6.38 | 1.60 | 1.52 |
| 1 | Y | 1266 | CYS | CA-C | -6.38 | 1.44 | 1.52 |
| 4 | y | 798 | ASN | CA-C | 6.38 | 1.61 | 1.52 |
| 14 | a | 616 | LEU | C-N | 6.38 | 1.42 | 1.33 |
| 5 | B | 453 | LEU | CB-CG | 6.38 | 1.66 | 1.53 |
| 15 | i | 182 | LEU | N-CA | -6.38 | 1.38 | 1.46 |
| 17 | k | 289 | TRP | NE1-CE2 | -6.38 | 1.30 | 1.37 |
| 20 | n | 647 | LYS | C-N | 6.38 | 1.42 | 1.34 |
| 18 | e | 90 | GLN | CA-CB | 6.38 | 1.63 | 1.53 |
| 20 | g | 1023 | SER | CA-C | -6.38 | 1.45 | 1.53 |
| 7 | O | 654 | PHE | N-CA | -6.38 | 1.38 | 1.46 |
| 16 | j | 479 | ALA | CA-C | -6.38 | 1.44 | 1.52 |
| 19 | f | 658 | LEU | N-CA | -6.38 | 1.38 | 1.46 |
| 2 | 1 | 1096 | ASN | CA-CB | 6.38 | 1.63 | 1.53 |
| 7 | M | 320 | GLU | CA-C | -6.38 | 1.44 | 1.52 |
| 9 | R | 330 | GLY | CA-C | -6.38 | 1.42 | 1.51 |
| 12 | v | 128 | LYS | CA-CB | 6.38 | 1.63 | 1.54 |
| 12 | v | 529 | THR | C-N | 6.37 | 1.42 | 1.33 |
| 8 | P | 1427 | SER | C-N | 6.37 | 1.41 | 1.33 |
| 9 | T | 805 | SER | CA-CB | 6.37 | 1.64 | 1.53 |
| 1 | Y | 1164 | TRP | NE1-CE2 | -6.37 | 1.30 | 1.37 |
| 16 | c | 764 | LEU | N-CA | -6.37 | 1.38 | 1.46 |
| 19 | f | 515 | GLU | N-CA | -6.37 | 1.38 | 1.46 |
| 8 | P | 141 | LEU | C-N | 6.37 | 1.42 | 1.33 |
| 12 | v | 424 | PRO | CA-C | 6.37 | 1.58 | 1.53 |
| 4 | y | 754 | ASN | CA-C | -6.37 | 1.44 | 1.52 |
| 5 | B | 303 | THR | CA-CB | 6.37 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | K | 355 | PHE | N-CA | -6.37 | 1.38 | 1.46 |
| 1 | Y | 1466 | ILE | N-CA | -6.37 | 1.38 | 1.46 |
| 14 | a | 121 | VAL | N-CA | -6.37 | 1.38 | 1.46 |
| 1 | 0 | 607 | GLN | CA-C | -6.36 | 1.44 | 1.52 |
| 7 | M | 64 | PHE | CA-CB | 6.36 | 1.64 | 1.53 |
| 2 | Z | 1130 | ARG | NE-CZ | 6.36 | 1.40 | 1.33 |
| 17 | k | 60 | ASP | C-N | 6.36 | 1.41 | 1.33 |
| 7 | O | 1445 | VAL | C-N | 6.36 | 1.40 | 1.33 |
| 9 | Q | 754 | ARG | NE-CZ | 6.36 | 1.40 | 1.33 |
| 10 | W | 262 | ILE | N-CA | -6.36 | 1.38 | 1.46 |
| 20 | n | 519 | GLU | CA-CB | 6.36 | 1.63 | 1.53 |
| 20 | g | 284 | TYR | CA-CB | 6.36 | 1.62 | 1.53 |
| 1 | 0 | 119 | PRO | N-CD | -6.36 | 1.38 | 1.47 |
| 20 | n | 158 | GLN | CA-CB | 6.36 | 1.63 | 1.53 |
| 20 | g | 830 | SER | C-O | 6.36 | 1.31 | 1.23 |
| 4 | G | 687 | GLU | C-N | 6.36 | 1.42 | 1.33 |
| 6 | L | 456 | ARG | C-N | 6.36 | 1.41 | 1.34 |
| 8 | N | 693 | MET | C-N | 6.36 | 1.41 | 1.33 |
| 9 | S | 573 | HIS | ND1-CE1 | 6.36 | 1.39 | 1.32 |
| 9 | T | 536 | ASN | C-N | 6.36 | 1.42 | 1.33 |
| 13 | x | 1302 | ASP | N-CA | -6.36 | 1.38 | 1.46 |
| 15 | i | 257 | LEU | C-N | 6.36 | 1.41 | 1.33 |
| 2 | 1 | 922 | LYS | CA-C | -6.36 | 1.44 | 1.52 |
| 8 | P | 921 | SER | CA-CB | 6.36 | 1.63 | 1.53 |
| 2 | Z | 909 | HIS | ND1-CE1 | 6.36 | 1.39 | 1.32 |
| 20 | n | 808 | TYR | C-N | 6.36 | 1.43 | 1.33 |
| 15 | b | 383 | VAL | C-N | 6.36 | 1.42 | 1.33 |
| 17 | d | 44 | LYS | C-N | 6.36 | 1.41 | 1.33 |
| 18 | e | 328 | VAL | CA-CB | 6.36 | 1.62 | 1.54 |
| 7 | M | 337 | SER | C-N | 6.35 | 1.43 | 1.33 |
| 8 | P | 502 | ASP | CA-CB | 6.35 | 1.64 | 1.53 |
| 16 | j | 152 | LYS | CA-C | -6.35 | 1.44 | 1.52 |
| 14 | a | 56 | TYR | CA-C | -6.35 | 1.45 | 1.52 |
| 14 | a | 872 | TYR | CB-CG | -6.35 | 1.37 | 1.51 |
| 1 | Y | 1170 | ARG | CA-CB | 6.35 | 1.61 | 1.53 |
| 12 | v | 439 | LEU | CA-CB | 6.35 | 1.61 | 1.53 |
| 14 | h | 975 | ARG | NE-CZ | 6.35 | 1.40 | 1.33 |
| 15 | b | 431 | GLU | CA-C | 6.35 | 1.60 | 1.52 |
| 7 | M | 945 | LEU | CA-C | -6.35 | 1.44 | 1.52 |
| 14 | a | 688 | PHE | CA-C | 6.35 | 1.61 | 1.52 |
| 1 | 0 | 171 | THR | C-N | 6.35 | 1.42 | 1.33 |
| 7 | M | 1313 | ILE | N-CA | -6.35 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1498 | GLY | N-CA | 6.35 | 1.52 | 1.45 |
| 9 | T | 74 | ALA | CA-C | -6.35 | 1.44 | 1.52 |
| 14 | h | 593 | PRO | CA-C | -6.35 | 1.46 | 1.52 |
| 20 | n | 790 | HIS | ND1-CE1 | 6.35 | 1.38 | 1.32 |
| 16 | c | 277 | GLY | CA-C | -6.35 | 1.42 | 1.51 |
| 7 | O | 1362 | ASP | N-CA | -6.35 | 1.37 | 1.46 |
| 9 | T | 608 | GLN | N-CA | -6.35 | 1.37 | 1.46 |
| 14 | h | 438 | GLU | N-CA | -6.35 | 1.38 | 1.46 |
| 18 | l | 186 | SER | CA-CB | 6.35 | 1.61 | 1.53 |
| 20 | n | 826 | SER | N-CA | -6.35 | 1.37 | 1.46 |
| 8 | N | 795 | ILE | C-N | 6.34 | 1.42 | 1.33 |
| 9 | R | 439 | HIS | CB-CG | -6.34 | 1.41 | 1.50 |
| 9 | T | 537 | ILE | CA-C | -6.34 | 1.44 | 1.52 |
| 1 | Y | 681 | THR | CA-C | 6.34 | 1.61 | 1.52 |
| 13 | x | 1270 | LEU | CA-C | -6.34 | 1.44 | 1.52 |
| 14 | a | 484 | TYR | CA-CB | 6.34 | 1.62 | 1.53 |
| 7 | M | 1561 | LEU | C-N | 6.34 | 1.41 | 1.33 |
| 8 | N | 318 | HIS | ND1-CE1 | 6.34 | 1.38 | 1.32 |
| 16 | j | 575 | SER | N-CA | 6.34 | 1.54 | 1.46 |
| 19 | m | 205 | ASN | C-N | 6.34 | 1.40 | 1.33 |
| 20 | n | 610 | LEU | CA-C | -6.34 | 1.44 | 1.52 |
| 9 | Q | 694 | SER | C-N | 6.34 | 1.39 | 1.33 |
| 10 | U | 269 | HIS | ND1-CE1 | 6.34 | 1.38 | 1.32 |
| 2 | Z | 558 | THR | CA-C | -6.34 | 1.44 | 1.52 |
| 14 | a | 628 | ARG | CD-NE | 6.34 | 1.55 | 1.46 |
| 8 | N | 602 | VAL | N-CA | -6.34 | 1.38 | 1.46 |
| 7 | O | 32 | LEU | C-N | 6.34 | 1.42 | 1.33 |
| 2 | Z | 1233 | VAL | C-N | 6.34 | 1.41 | 1.33 |
| 12 | u | 86 | ASN | C-N | -6.34 | 1.25 | 1.33 |
| 20 | n | 1114 | TYR | CA-C | -6.34 | 1.44 | 1.52 |
| 14 | a | 104 | GLN | N-CA | -6.34 | 1.38 | 1.46 |
| 6 | C | 326 | LEU | C-N | 6.33 | 1.42 | 1.33 |
| 4 | z | 642 | THR | C-N | 6.33 | 1.42 | 1.33 |
| 15 | b | 532 | PRO | CA-C | -6.33 | 1.45 | 1.52 |
| 7 | M | 649 | LEU | N-CA | 6.33 | 1.53 | 1.46 |
| 9 | R | 724 | ARG | CD-NE | 6.33 | 1.55 | 1.46 |
| 17 | k | 201 | GLU | N-CA | -6.33 | 1.38 | 1.46 |
| 19 | f | 664 | LEU | N-CA | -6.33 | 1.38 | 1.46 |
| 7 | O | 1396 | LEU | C-N | 6.33 | 1.42 | 1.33 |
| 10 | W | 308 | TYR | C-N | 6.33 | 1.42 | 1.33 |
| 13 | x | 1366 | LEU | CA-C | -6.33 | 1.43 | 1.52 |
| 14 | h | 641 | ASP | C-N | 6.33 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | q | 71 | HIS | C-N | 6.33 | 1.42 | 1.33 |
| 18 | e | 168 | ASP | CA-C | -6.33 | 1.44 | 1.52 |
| 6 | C | 387 | TYR | C-N | 6.33 | 1.42 | 1.33 |
| 6 | L | 344 | LEU | CA-C | -6.33 | 1.46 | 1.52 |
| 8 | N | 1260 | TYR | CA-C | -6.33 | 1.44 | 1.52 |
| 8 | P | 449 | ASP | C-N | 6.33 | 1.41 | 1.33 |
| 1 | Y | 984 | THR | C-N | 6.33 | 1.42 | 1.33 |
| 14 | a | 924 | ARG | CA-CB | 6.33 | 1.61 | 1.53 |
| 9 | R | 713 | ILE | N-CA | -6.33 | 1.39 | 1.46 |
| 21 | p | 78 | TYR | C-O | -6.33 | 1.17 | 1.24 |
| 9 | S | 43 | GLN | CA-C | -6.32 | 1.44 | 1.52 |
| 9 | T | 426 | PRO | CA-C | -6.32 | 1.46 | 1.53 |
| 20 | n | 1005 | LEU | N-CA | -6.32 | 1.38 | 1.46 |
| 5 | B | 411 | ARG | CA-C | -6.32 | 1.44 | 1.52 |
| 8 | P | 1622 | GLU | CA-CB | 6.32 | 1.63 | 1.53 |
| 4 | y | 792 | GLN | CA-C | -6.32 | 1.44 | 1.52 |
| 16 | j | 208 | PRO | C-N | 6.32 | 1.38 | 1.33 |
| 9 | Q | 304 | LYS | N-CA | 6.32 | 1.54 | 1.46 |
| 9 | R | 155 | VAL | C-N | 6.32 | 1.41 | 1.33 |
| 18 | l | 80 | THR | CA-CB | 6.32 | 1.64 | 1.53 |
| 1 | 0 | 175 | ILE | CA-C | 6.32 | 1.59 | 1.52 |
| 6 | I | 470 | LEU | CA-C | -6.32 | 1.43 | 1.52 |
| 7 | M | 1444 | ASP | CA-CB | 6.32 | 1.63 | 1.53 |
| 8 | N | 1007 | SER | CA-CB | 6.32 | 1.63 | 1.54 |
| 11 | X | 355 | TRP | CA-C | -6.32 | 1.45 | 1.52 |
| 1 | Y | 417 | TYR | CA-CB | 6.32 | 1.63 | 1.53 |
| 14 | h | 880 | ARG | NE-CZ | 6.32 | 1.40 | 1.33 |
| 19 | f | 245 | ARG | NE-CZ | 6.32 | 1.40 | 1.33 |
| 12 | u | 332 | GLU | N-CA | -6.32 | 1.38 | 1.46 |
| 16 | j | 775 | GLY | N-CA | -6.32 | 1.39 | 1.45 |
| 6 | I | 369 | LEU | N-CA | 6.31 | 1.58 | 1.46 |
| 2 | Z | 425 | ILE | C-N | 6.31 | 1.41 | 1.33 |
| 7 | M | 1195 | PHE | CA-C | -6.31 | 1.45 | 1.53 |
| 19 | m | 683 | PHE | CA-CB | 6.31 | 1.64 | 1.53 |
| 6 | C | 293 | HIS | ND1-CE1 | 6.31 | 1.38 | 1.32 |
| 8 | N | 828 | LEU | CA-C | -6.31 | 1.44 | 1.52 |
| 1 | 0 | 1261 | ARG | NE-CZ | 6.31 | 1.40 | 1.33 |
| 8 | P | 1028 | THR | C-N | 6.31 | 1.42 | 1.33 |
| 14 | h | 426 | ILE | N-CA | -6.31 | 1.38 | 1.46 |
| 20 | n | 400 | PHE | CA-C | 6.31 | 1.60 | 1.52 |
| 9 | R | 60 | ASN | CA-C | -6.31 | 1.44 | 1.53 |
| 17 | k | 259 | ARG | CD-NE | 6.31 | 1.55 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 18 | e | 221 | ALA | N-CA | -6.31 | 1.38 | 1.45 |
| 4 | J | 667 | GLN | C-N | 6.30 | 1.41 | 1.33 |
| 7 | O | 245 | ARG | CD-NE | 6.30 | 1.55 | 1.46 |
| 12 | u | 705 | SER | C-N | 6.30 | 1.42 | 1.33 |
| 4 | y | 656 | GLU | N-CA | 6.30 | 1.53 | 1.46 |
| 14 | h | 797 | LEU | N-CA | 6.30 | 1.54 | 1.46 |
| 7 | O | 1009 | ASN | CA-C | 6.30 | 1.61 | 1.52 |
| 4 | y | 812 | THR | C-N | 6.30 | 1.41 | 1.33 |
| 1 | 0 | 895 | ALA | N-CA | -6.30 | 1.38 | 1.46 |
| 9 | R | 805 | SER | C-N | 6.30 | 1.42 | 1.33 |
| 11 | X | 350 | PHE | CB-CG | 6.30 | 1.65 | 1.50 |
| 1 | Y | 1011 | ARG | NE-CZ | 6.30 | 1.40 | 1.33 |
| 20 | g | 1042 | TRP | CA-CB | 6.30 | 1.63 | 1.53 |
| 14 | h | 1000 | TYR | N-CA | 6.30 | 1.53 | 1.46 |
| 1 | 0 | 1465 | ILE | CA-C | -6.30 | 1.45 | 1.53 |
| 8 | N | 762 | LEU | C-N | 6.30 | 1.42 | 1.33 |
| 9 | Q | 616 | GLU | CA-C | -6.30 | 1.44 | 1.52 |
| 2 | 1 | 723 | ILE | CA-C | -6.29 | 1.44 | 1.52 |
| 17 | k | 20 | TYR | C-N | 6.29 | 1.42 | 1.33 |
| 19 | f | 671 | LEU | C-N | 6.29 | 1.41 | 1.33 |
| 9 | R | 139 | PHE | CA-C | -6.29 | 1.44 | 1.52 |
| 5 | B | 364 | VAL | N-CA | -6.29 | 1.38 | 1.46 |
| 10 | U | 348 | ALA | N-CA | -6.29 | 1.38 | 1.46 |
| 20 | n | 86 | LEU | CA-CB | 6.29 | 1.64 | 1.53 |
| 20 | n | 984 | PHE | C-N | -6.29 | 1.25 | 1.34 |
| 19 | f | 589 | HIS | C-N | 6.29 | 1.42 | 1.33 |
| 7 | M | 783 | ILE | C-N | 6.29 | 1.41 | 1.33 |
| 8 | P | 746 | ALA | C-N | 6.29 | 1.42 | 1.33 |
| 7 | M | 1411 | HIS | C-O | -6.29 | 1.16 | 1.24 |
| 1 | Y | 778 | THR | CA-C | -6.29 | 1.45 | 1.52 |
| 13 | w | 1146 | SER | CA-C | -6.29 | 1.45 | 1.52 |
| 16 | j | 218 | LYS | CA-CB | 6.29 | 1.63 | 1.53 |
| 20 | n | 786 | LEU | CA-C | -6.29 | 1.44 | 1.52 |
| 15 | b | 253 | VAL | C-N | 6.29 | 1.42 | 1.33 |
| 9 | Q | 64 | LYS | C-O | -6.29 | 1.17 | 1.24 |
| 9 | T | 757 | ALA | CA-C | -6.29 | 1.44 | 1.52 |
| 10 | U | 265 | SER | CA-C | -6.29 | 1.44 | 1.52 |
| 7 | O | 89 | CYS | CA-C | -6.29 | 1.43 | 1.52 |
| 7 | O | 152 | HIS | CA-CB | 6.29 | 1.63 | 1.53 |
| 9 | T | 294 | MET | CA-C | -6.29 | 1.43 | 1.52 |
| 1 | Y | 172 | ASP | C-N | 6.29 | 1.42 | 1.33 |
| 14 | h | 191 | GLY | CA-C | -6.29 | 1.43 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 18 | l | 124 | LYS | CA-C | -6.29 | 1.45 | 1.52 |
| 6 | F | 348 | GLN | CA-C | -6.28 | 1.44 | 1.52 |
| 13 | w | 1226 | THR | C-N | 6.28 | 1.41 | 1.33 |
| 16 | j | 308 | LYS | N-CA | -6.28 | 1.38 | 1.46 |
| 9 | R | 355 | GLU | N-CA | -6.28 | 1.37 | 1.46 |
| 14 | h | 839 | GLU | CA-C | -6.28 | 1.45 | 1.52 |
| 16 | j | 639 | SER | CA-C | -6.28 | 1.44 | 1.52 |
| 14 | a | 132 | GLN | CA-CB | 6.28 | 1.63 | 1.53 |
| 1 | Y | 1006 | ALA | C-N | 6.28 | 1.40 | 1.33 |
| 1 | Y | 1236 | LEU | CA-CB | 6.28 | 1.61 | 1.53 |
| 8 | N | 522 | LYS | C-N | 6.28 | 1.42 | 1.33 |
| 17 | d | 152 | SER | N-CA | -6.28 | 1.38 | 1.46 |
| 2 | 1 | 1177 | VAL | C-N | 6.28 | 1.42 | 1.33 |
| 7 | O | 183 | ARG | CA-C | -6.28 | 1.44 | 1.52 |
| 7 | O | 1435 | LYS | CA-C | -6.28 | 1.44 | 1.52 |
| 20 | n | 234 | ARG | C-N | 6.28 | 1.42 | 1.33 |
| 14 | h | 652 | SER | N-CA | -6.27 | 1.38 | 1.46 |
| 19 | m | 114 | LYS | N-CA | -6.27 | 1.38 | 1.46 |
| 19 | f | 524 | VAL | CA-C | -6.27 | 1.44 | 1.52 |
| 14 | a | 930 | SER | C-N | 6.27 | 1.42 | 1.33 |
| 2 | Z | 1160 | ILE | C-N | 6.27 | 1.42 | 1.34 |
| 20 | n | 596 | CYS | N-CA | -6.27 | 1.37 | 1.46 |
| 6 | C | 401 | ILE | C-N | 6.27 | 1.41 | 1.33 |
| 2 | Z | 849 | PHE | C-N | 6.27 | 1.42 | 1.33 |
| 16 | c | 473 | ALA | CA-C | -6.27 | 1.44 | 1.52 |
| 8 | N | 981 | LYS | N-CA | -6.27 | 1.40 | 1.46 |
| 2 | Z | 1126 | LYS | CA-CB | 6.27 | 1.64 | 1.53 |
| 17 | k | 16 | VAL | CA-CB | 6.27 | 1.63 | 1.54 |
| 20 | n | 220 | VAL | CA-CB | -6.27 | 1.46 | 1.54 |
| 1 | 0 | 963 | ILE | C-N | 6.27 | 1.42 | 1.33 |
| 9 | S | 792 | SER | C-N | 6.27 | 1.41 | 1.33 |
| 5 | K | 507 | ASN | CA-CB | 6.26 | 1.64 | 1.53 |
| 7 | O | 932 | VAL | CA-C | -6.26 | 1.46 | 1.52 |
| 9 | R | 112 | TYR | CA-C | -6.26 | 1.45 | 1.52 |
| 15 | i | 308 | ASN | CA-CB | 6.26 | 1.63 | 1.53 |
| 4 | A | 717 | LYS | N-CA | -6.26 | 1.38 | 1.46 |
| 20 | g | 580 | SER | CA-C | -6.26 | 1.45 | 1.52 |
| 2 | 1 | 820 | ASP | CA-CB | 6.26 | 1.63 | 1.53 |
| 6 | C | 395 | GLU | N-CA | -6.26 | 1.38 | 1.46 |
| 5 | E | 445 | GLN | N-CA | -6.26 | 1.38 | 1.46 |
| 8 | N | 348 | LYS | N-CA | -6.26 | 1.38 | 1.46 |
| 2 | Z | 1012 | VAL | C-N | 6.26 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | n | 289 | LYS | C-N | 6.26 | 1.41 | 1.33 |
| 1 | 0 | 265 | VAL | N-CA | -6.26 | 1.38 | 1.46 |
| 2 | 1 | 540 | VAL | CA-C | -6.26 | 1.45 | 1.52 |
| 8 | N | 466 | THR | CA-C | -6.26 | 1.44 | 1.52 |
| 7 | O | 998 | LEU | CA-C | -6.26 | 1.44 | 1.52 |
| 8 | P | 1229 | LEU | CA-CB | 6.26 | 1.63 | 1.53 |
| 15 | i | 654 | GLU | C-O | -6.26 | 1.19 | 1.23 |
| 2 | 1 | 1107 | HIS | ND1-CE1 | 6.26 | 1.38 | 1.32 |
| 9 | R | 668 | SER | CA-CB | 6.26 | 1.61 | 1.53 |
| 9 | T | 756 | LYS | CA-CB | 6.26 | 1.64 | 1.53 |
| 7 | M | 1147 | PHE | N-CA | -6.26 | 1.38 | 1.46 |
| 12 | u | 165 | VAL | CA-C | -6.26 | 1.45 | 1.52 |
| 12 | u | 301 | ASN | CA-CB | 6.26 | 1.64 | 1.53 |
| 14 | h | 161 | ARG | C-N | 6.26 | 1.39 | 1.33 |
| 16 | c | 571 | ALA | N-CA | -6.26 | 1.37 | 1.46 |
| 9 | R | 480 | GLN | N-CA | -6.25 | 1.38 | 1.46 |
| 1 | Y | 453 | GLY | N-CA | -6.25 | 1.38 | 1.45 |
| 14 | h | 872 | TYR | C-N | 6.25 | 1.43 | 1.33 |
| 2 | 1 | 1318 | HIS | CB-CG | 6.25 | 1.58 | 1.50 |
| 8 | P | 1518 | THR | N-CA | 6.25 | 1.54 | 1.46 |
| 14 | h | 96 | HIS | C-N | 6.25 | 1.42 | 1.33 |
| 15 | i | 225 | GLU | N-CA | -6.25 | 1.38 | 1.46 |
| 15 | i | 652 | LEU | C-N | 6.25 | 1.42 | 1.33 |
| 15 | i | 734 | LYS | C-N | 6.25 | 1.42 | 1.33 |
| 8 | N | 1189 | ASP | C-N | 6.25 | 1.42 | 1.33 |
| 8 | P | 19 | ALA | N-CA | -6.25 | 1.37 | 1.46 |
| 9 | T | 281 | GLN | CA-C | -6.25 | 1.44 | 1.52 |
| 16 | j | 652 | ARG | CA-C | -6.25 | 1.44 | 1.52 |
| 6 | C | 274 | ARG | CA-CB | -6.25 | 1.43 | 1.53 |
| 2 | 1 | 561 | LEU | N-CA | -6.25 | 1.38 | 1.46 |
| 9 | R | 221 | GLN | N-CA | -6.25 | 1.39 | 1.46 |
| 9 | T | 562 | LEU | C-N | 6.25 | 1.41 | 1.33 |
| 21 | p | 13 | ALA | CA-C | -6.25 | 1.44 | 1.52 |
| 7 | M | 648 | PRO | C-O | -6.25 | 1.17 | 1.23 |
| 8 | P | 1222 | LEU | CA-CB | 6.25 | 1.62 | 1.53 |
| 8 | P | 1638 | LYS | C-N | 6.25 | 1.41 | 1.33 |
| 9 | R | 505 | HIS | N-CA | -6.25 | 1.38 | 1.46 |
| 9 | Q | 18 | ALA | CA-C | 6.24 | 1.60 | 1.52 |
| 15 | i | 104 | PHE | CA-CB | 6.24 | 1.63 | 1.53 |
| 21 | p | 71 | HIS | N-CA | -6.24 | 1.37 | 1.46 |
| 19 | f | 273 | ASN | CA-CB | 6.24 | 1.64 | 1.53 |
| 2 | 1 | 747 | ILE | CA-C | -6.24 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 455 | PHE | CA-CB | 6.24 | 1.63 | 1.54 |
| 16 | j | 153 | PHE | CA-C | -6.24 | 1.45 | 1.52 |
| 18 | l | 149 | THR | CA-CB | -6.24 | 1.45 | 1.53 |
| 7 | M | 1099 | TYR | CA-C | -6.24 | 1.45 | 1.52 |
| 7 | O | 837 | TYR | CA-CB | 6.24 | 1.63 | 1.53 |
| 16 | c | 173 | LYS | N-CA | -6.24 | 1.38 | 1.46 |
| 9 | S | 217 | ARG | CA-C | -6.24 | 1.45 | 1.52 |
| 2 | Z | 1204 | ASP | CA-C | -6.24 | 1.45 | 1.53 |
| 12 | u | 379 | ASN | N-CA | -6.24 | 1.38 | 1.46 |
| 14 | h | 314 | THR | CA-CB | 6.24 | 1.63 | 1.53 |
| 17 | k | 249 | LYS | CA-CB | 6.24 | 1.63 | 1.53 |
| 20 | n | 1040 | LEU | CA-C | -6.24 | 1.45 | 1.52 |
| 2 | 1 | 662 | LEU | CA-CB | 6.24 | 1.63 | 1.53 |
| 7 | M | 774 | ARG | NE-CZ | 6.24 | 1.40 | 1.33 |
| 19 | f | 278 | GLN | CA-CB | 6.24 | 1.63 | 1.53 |
| 2 | 1 | 970 | PHE | C-N | 6.24 | 1.42 | 1.33 |
| 9 | Q | 81 | GLU | C-N | 6.24 | 1.41 | 1.33 |
| 2 | Z | 1163 | LEU | N-CA | -6.24 | 1.38 | 1.46 |
| 12 | v | 445 | LEU | CA-C | -6.24 | 1.45 | 1.52 |
| 12 | v | 631 | PHE | C-N | 6.24 | 1.41 | 1.33 |
| 18 | l | 318 | ILE | CA-CB | 6.24 | 1.60 | 1.53 |
| 19 | m | 534 | SER | CA-C | -6.24 | 1.45 | 1.52 |
| 19 | m | 330 | ARG | CA-C | -6.23 | 1.44 | 1.52 |
| 7 | O | 1342 | TYR | CA-C | -6.23 | 1.45 | 1.52 |
| 12 | v | 43 | ILE | CA-C | 6.23 | 1.60 | 1.52 |
| 12 | v | 113 | HIS | ND1-CE1 | 6.23 | 1.38 | 1.32 |
| 21 | o | 86 | PHE | CA-C | -6.23 | 1.45 | 1.52 |
| 18 | e | 319 | LEU | CA-C | -6.23 | 1.45 | 1.52 |
| 4 | G | 822 | LYS | CA-C | -6.23 | 1.44 | 1.52 |
| 7 | M | 478 | LEU | CA-C | -6.23 | 1.44 | 1.52 |
| 9 | S | 320 | TRP | C-N | 6.23 | 1.40 | 1.33 |
| 12 | v | 346 | ASN | CA-CB | 6.23 | 1.61 | 1.53 |
| 4 | z | 654 | HIS | CA-C | -6.23 | 1.44 | 1.52 |
| 17 | d | 98 | HIS | CE1-NE2 | -6.23 | 1.26 | 1.32 |
| 1 | Y | 967 | LEU | CB-CG | 6.23 | 1.66 | 1.53 |
| 12 | u | 443 | LYS | N-CA | -6.23 | 1.39 | 1.46 |
| 13 | w | 1221 | VAL | CA-C | -6.23 | 1.45 | 1.52 |
| 15 | b | 70 | LYS | N-CA | -6.23 | 1.38 | 1.46 |
| 18 | e | 177 | ARG | NE-CZ | 6.23 | 1.40 | 1.33 |
| 10 | U | 349 | ALA | CA-C | -6.23 | 1.45 | 1.53 |
| 12 | u | 441 | SER | N-CA | -6.23 | 1.37 | 1.46 |
| 12 | v | 64 | VAL | C-N | 6.23 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 16 | j | 298 | LEU | CA-C | 6.23 | 1.60 | 1.52 |
| 8 | N | 159 | SER | CA-C | 6.23 | 1.61 | 1.53 |
| 12 | v | 711 | LYS | N-CA | -6.23 | 1.38 | 1.46 |
| 20 | g | 333 | ILE | N-CA | -6.23 | 1.39 | 1.46 |
| 7 | O | 1436 | LYS | C-N | -6.22 | 1.25 | 1.33 |
| 15 | i | 351 | ARG | CA-CB | 6.22 | 1.64 | 1.53 |
| 19 | m | 631 | ILE | CA-C | 6.22 | 1.60 | 1.52 |
| 21 | s | 68 | TYR | CA-CB | 6.22 | 1.63 | 1.53 |
| 6 | C | 439 | ILE | C-N | 6.22 | 1.42 | 1.34 |
| 7 | O | 207 | MET | CA-CB | 6.22 | 1.61 | 1.53 |
| 7 | O | 943 | ARG | C-N | 6.22 | 1.41 | 1.33 |
| 9 | T | 485 | SER | C-N | 6.22 | 1.40 | 1.33 |
| 14 | h | 140 | SER | CA-C | 6.22 | 1.60 | 1.52 |
| 19 | f | 187 | LEU | CA-C | -6.22 | 1.44 | 1.52 |
| 20 | g | 316 | ILE | C-N | 6.22 | 1.42 | 1.33 |
| 7 | O | 1202 | ASN | N-CA | -6.22 | 1.38 | 1.46 |
| 14 | h | 71 | HIS | ND1-CE1 | 6.22 | 1.38 | 1.32 |
| 7 | O | 762 | ALA | N-CA | -6.22 | 1.38 | 1.46 |
| 7 | O | 1102 | LYS | CA-CB | 6.22 | 1.63 | 1.53 |
| 4 | y | 674 | GLU | C-N | 6.22 | 1.42 | 1.33 |
| 18 | e | 147 | SER | CA-C | -6.22 | 1.45 | 1.52 |
| 7 | O | 691 | SER | CA-C | -6.22 | 1.44 | 1.52 |
| 12 | u | 246 | LYS | CA-C | -6.22 | 1.44 | 1.52 |
| 19 | m | 611 | SER | CA-C | 6.22 | 1.61 | 1.52 |
| 20 | n | 303 | HIS | CB-CG | 6.22 | 1.58 | 1.50 |
| 21 | t | 51 | VAL | C-N | 6.22 | 1.42 | 1.33 |
| 20 | g | 238 | GLY | CA-C | -6.22 | 1.43 | 1.52 |
| 8 | N | 409 | GLU | CA-CB | 6.21 | 1.64 | 1.53 |
| 9 | R | 744 | LEU | N-CA | -6.21 | 1.38 | 1.46 |
| 12 | u | 55 | HIS | CA-CB | 6.21 | 1.61 | 1.53 |
| 4 | z | 806 | SER | CA-C | 6.21 | 1.60 | 1.52 |
| 14 | h | 870 | ILE | CA-CB | 6.21 | 1.61 | 1.54 |
| 20 | g | 738 | TYR | N-CA | -6.21 | 1.38 | 1.46 |
| 11 | X | 276 | TYR | CA-C | -6.21 | 1.45 | 1.53 |
| 6 | F | 354 | LEU | C-N | 6.21 | 1.42 | 1.33 |
| 9 | T | 86 | PHE | C-N | -6.21 | 1.26 | 1.34 |
| 14 | h | 617 | GLU | CA-CB | 6.21 | 1.63 | 1.53 |
| 1 | 0 | 1027 | HIS | C-O | -6.21 | 1.16 | 1.23 |
| 2 | 1 | 1178 | ARG | CA-C | 6.21 | 1.60 | 1.52 |
| 6 | C | 286 | LYS | N-CA | -6.21 | 1.38 | 1.46 |
| 7 | M | 1551 | SER | CA-C | -6.21 | 1.45 | 1.53 |
| 7 | O | 315 | GLU | N-CA | 6.21 | 1.53 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | t | 71 | HIS | CA-C | -6.21 | 1.44 | 1.52 |
| 15 | b | 608 | PRO | CA-CB | 6.21 | 1.62 | 1.53 |
| 20 | g | 306 | LYS | CA-C | -6.21 | 1.45 | 1.52 |
| 5 | K | 373 | ARG | NE-CZ | 6.21 | 1.39 | 1.33 |
| 7 | O | 859 | LYS | CA-C | -6.21 | 1.44 | 1.52 |
| 2 | Z | 234 | THR | C-N | 6.21 | 1.41 | 1.33 |
| 12 | v | 190 | ASP | CA-CB | 6.21 | 1.63 | 1.53 |
| 15 | i | 583 | GLY | CA-C | -6.21 | 1.44 | 1.51 |
| 9 | R | 515 | LEU | CA-C | -6.21 | 1.40 | 1.52 |
| 9 | R | 827 | GLU | C-N | 6.21 | 1.41 | 1.33 |
| 1 | Y | 1095 | LYS | C-N | 6.21 | 1.42 | 1.34 |
| 7 | M | 608 | PHE | CA-C | 6.20 | 1.60 | 1.52 |
| 9 | R | 546 | ARG | CZ-NH2 | 6.20 | 1.41 | 1.33 |
| 9 | R | 614 | ARG | N-CA | -6.20 | 1.38 | 1.46 |
| 2 | Z | 1354 | ASP | CA-CB | 6.20 | 1.63 | 1.53 |
| 9 | R | 573 | HIS | CE1-NE2 | 6.20 | 1.38 | 1.32 |
| 14 | h | 992 | ASP | N-CA | -6.20 | 1.38 | 1.46 |
| 2 | 1 | 667 | ALA | CA-C | -6.20 | 1.43 | 1.52 |
| 8 | N | 1615 | ARG | NE-CZ | 6.20 | 1.39 | 1.33 |
| 9 | R | 439 | HIS | ND1-CE1 | 6.20 | 1.38 | 1.32 |
| 14 | h | 348 | TYR | C-N | 6.20 | 1.41 | 1.33 |
| 19 | f | 335 | HIS | C-N | 6.20 | 1.39 | 1.33 |
| 14 | a | 890 | ARG | CD-NE | 6.20 | 1.54 | 1.46 |
| 8 | N | 1608 | HIS | N-CA | 6.20 | 1.52 | 1.46 |
| 7 | O | 242 | ALA | C-N | 6.20 | 1.41 | 1.33 |
| 14 | a | 225 | SER | C-N | 6.20 | 1.41 | 1.33 |
| 2 | 1 | 108 | THR | N-CA | -6.20 | 1.37 | 1.45 |
| 5 | H | 341 | LYS | N-CA | -6.20 | 1.39 | 1.46 |
| 5 | H | 511 | GLU | N-CA | 6.20 | 1.53 | 1.46 |
| 15 | i | 168 | ARG | NE-CZ | 6.20 | 1.39 | 1.33 |
| 1 | 0 | 1224 | ASN | C-N | 6.19 | 1.41 | 1.33 |
| 8 | P | 1251 | TYR | C-N | 6.19 | 1.42 | 1.33 |
| 9 | S | 345 | LEU | CA-CB | 6.19 | 1.62 | 1.53 |
| 9 | S | 707 | HIS | N-CA | 6.19 | 1.54 | 1.46 |
| 1 | 0 | 1011 | ARG | N-CA | -6.19 | 1.38 | 1.46 |
| 2 | 1 | 1348 | LYS | CA-CB | 6.19 | 1.63 | 1.53 |
| 7 | M | 728 | TYR | C-N | 6.19 | 1.42 | 1.33 |
| 7 | O | 1069 | ASP | C-N | 6.19 | 1.42 | 1.33 |
| 9 | R | 504 | VAL | CA-C | -6.19 | 1.45 | 1.52 |
| 15 | i | 692 | ILE | CA-C | 6.19 | 1.60 | 1.52 |
| 14 | a | 968 | ARG | CA-CB | 6.19 | 1.62 | 1.53 |
| 4 | D | 684 | VAL | CA-C | 6.19 | 1.60 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 635 | PHE | CA-C | -6.19 | 1.44 | 1.52 |
| 2 | Z | 601 | VAL | CA-CB | -6.19 | 1.46 | 1.54 |
| 4 | z | 814 | LEU | CA-C | -6.19 | 1.44 | 1.52 |
| 14 | a | 761 | ALA | N-CA | 6.19 | 1.53 | 1.46 |
| 20 | n | 80 | PHE | N-CA | -6.19 | 1.40 | 1.46 |
| 1 | 0 | 259 | THR | C-N | 6.19 | 1.42 | 1.33 |
| 4 | z | 654 | HIS | N-CA | -6.19 | 1.38 | 1.46 |
| 16 | j | 524 | ASP | CA-C | -6.19 | 1.44 | 1.52 |
| 1 | 0 | 249 | LYS | N-CA | -6.18 | 1.37 | 1.46 |
| 8 | P | 223 | PHE | N-CA | -6.18 | 1.39 | 1.46 |
| 8 | P | 749 | ILE | CA-CB | 6.18 | 1.62 | 1.54 |
| 12 | u | 531 | ILE | CA-CB | -6.18 | 1.46 | 1.54 |
| 12 | v | 432 | ASN | CA-C | 6.18 | 1.61 | 1.53 |
| 18 | e | 135 | ARG | CD-NE | 6.18 | 1.54 | 1.46 |
| 18 | e | 303 | HIS | ND1-CE1 | 6.18 | 1.38 | 1.32 |
| 20 | g | 220 | VAL | N-CA | -6.18 | 1.39 | 1.46 |
| 14 | a | 526 | ARG | CA-CB | 6.18 | 1.62 | 1.53 |
| 8 | N | 153 | ASP | CA-C | -6.18 | 1.45 | 1.52 |
| 7 | O | 328 | ASP | N-CA | -6.18 | 1.39 | 1.46 |
| 7 | O | 1016 | THR | CA-C | 6.18 | 1.60 | 1.52 |
| 7 | O | 1603 | PRO | N-CA | -6.18 | 1.39 | 1.47 |
| 9 | R | 300 | THR | CA-C | -6.18 | 1.45 | 1.52 |
| 20 | g | 997 | VAL | N-CA | -6.18 | 1.39 | 1.46 |
| 8 | N | 1232 | HIS | ND1-CE1 | 6.18 | 1.38 | 1.32 |
| 14 | h | 652 | SER | C-O | -6.18 | 1.17 | 1.24 |
| 1 | 0 | 460 | LEU | N-CA | 6.18 | 1.53 | 1.46 |
| 9 | R | 435 | TRP | C-N | 6.18 | 1.41 | 1.33 |
| 2 | Z | 1206 | PHE | CA-C | -6.18 | 1.44 | 1.52 |
| 12 | u | 217 | LEU | CA-CB | 6.18 | 1.61 | 1.53 |
| 20 | n | 1035 | LYS | N-CA | -6.18 | 1.38 | 1.46 |
| 8 | N | 296 | ASP | C-N | 6.18 | 1.42 | 1.33 |
| 7 | O | 199 | GLY | CA-C | -6.18 | 1.44 | 1.52 |
| 2 | 1 | 814 | VAL | CA-CB | 6.17 | 1.63 | 1.54 |
| 7 | M | 1287 | THR | C-N | 6.17 | 1.41 | 1.33 |
| 14 | h | 299 | GLN | CA-C | -6.17 | 1.45 | 1.52 |
| 8 | P | 929 | MET | N-CA | -6.17 | 1.39 | 1.46 |
| 9 | S | 132 | ALA | N-CA | -6.17 | 1.39 | 1.46 |
| 10 | W | 251 | HIS | CA-CB | 6.17 | 1.63 | 1.53 |
| 17 | k | 57 | TRP | CA-C | -6.17 | 1.46 | 1.53 |
| 2 | 1 | 159 | ILE | C-N | 6.17 | 1.42 | 1.33 |
| 4 | D | 817 | GLN | CA-CB | 6.17 | 1.61 | 1.53 |
| 8 | N | 152 | TYR | CA-CB | 6.17 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | R | 619 | PHE | CA-CB | 6.17 | 1.63 | 1.53 |
| 9 | T | 139 | PHE | CA-CB | 6.17 | 1.62 | 1.53 |
| 9 | T | 714 | CYS | CA-CB | 6.17 | 1.62 | 1.53 |
| 19 | m | 224 | ASP | C-O | -6.17 | 1.17 | 1.23 |
| 21 | s | 78 | TYR | CA-C | -6.17 | 1.45 | 1.52 |
| 2 | Z | 656 | HIS | ND1-CE1 | 6.17 | 1.38 | 1.32 |
| 9 | R | 634 | ASP | C-N | 6.17 | 1.40 | 1.33 |
| 20 | g | 571 | VAL | CA-C | 6.17 | 1.60 | 1.52 |
| 14 | a | 266 | ASP | N-CA | -6.17 | 1.38 | 1.46 |
| 9 | R | 510 | LEU | N-CA | -6.16 | 1.38 | 1.46 |
| 9 | Q | 430 | LEU | CA-CB | 6.16 | 1.61 | 1.53 |
| 9 | R | 408 | ARG | NE-CZ | 6.16 | 1.39 | 1.33 |
| 9 | T | 669 | ASP | N-CA | -6.16 | 1.37 | 1.46 |
| 19 | f | 402 | GLY | CA-C | -6.16 | 1.43 | 1.51 |
| 7 | M | 48 | ARG | C-N | 6.16 | 1.41 | 1.33 |
| 7 | O | 17 | SER | C-N | 6.16 | 1.40 | 1.33 |
| 8 | P | 1231 | GLU | C-N | 6.16 | 1.43 | 1.33 |
| 2 | Z | 495 | THR | N-CA | -6.16 | 1.38 | 1.46 |
| 2 | Z | 1048 | MET | CA-CB | 6.16 | 1.63 | 1.53 |
| 15 | i | 304 | ARG | NE-CZ | 6.16 | 1.39 | 1.33 |
| 16 | j | 181 | ARG | N-CA | -6.16 | 1.37 | 1.45 |
| 20 | g | 873 | GLN | C-N | 6.16 | 1.42 | 1.33 |
| 4 | G | 818 | ILE | C-N | 6.16 | 1.42 | 1.34 |
| 9 | Q | 311 | THR | CA-C | -6.16 | 1.44 | 1.52 |
| 4 | z | 692 | LYS | CA-CB | 6.16 | 1.62 | 1.53 |
| 14 | h | 921 | THR | N-CA | -6.16 | 1.38 | 1.46 |
| 7 | O | 473 | SER | CA-C | -6.16 | 1.44 | 1.52 |
| 15 | i | 635 | GLU | N-CA | 6.16 | 1.54 | 1.46 |
| 7 | M | 668 | ARG | CD-NE | 6.16 | 1.54 | 1.46 |
| 8 | N | 653 | SER | N-CA | 6.16 | 1.53 | 1.46 |
| 7 | O | 148 | PHE | C-N | 6.16 | 1.42 | 1.33 |
| 7 | O | 788 | LEU | N-CA | -6.16 | 1.38 | 1.46 |
| 9 | T | 316 | ALA | CA-C | -6.16 | 1.44 | 1.52 |
| 2 | Z | 604 | LEU | CA-CB | 6.16 | 1.62 | 1.53 |
| 12 | u | 534 | GLU | N-CA | -6.16 | 1.39 | 1.46 |
| 14 | h | 868 | GLN | N-CA | -6.16 | 1.38 | 1.46 |
| 16 | c | 643 | ILE | CA-CB | 6.16 | 1.62 | 1.54 |
| 9 | T | 305 | ILE | CA-C | -6.15 | 1.44 | 1.52 |
| 16 | j | 627 | ASN | N-CA | -6.15 | 1.38 | 1.46 |
| 18 | l | 313 | ASN | CA-CB | 6.15 | 1.62 | 1.53 |
| 18 | e | 247 | GLU | CA-C | -6.15 | 1.44 | 1.52 |
| 8 | N | 1626 | GLN | CA-C | -6.15 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | R | 332 | PRO | C-N | 6.15 | 1.41 | 1.34 |
| 9 | R | 785 | MET | CA-CB | 6.15 | 1.63 | 1.53 |
| 9 | T | 123 | MET | CA-C | 6.15 | 1.60 | 1.52 |
| 10 | U | 346 | SER | CA-C | -6.15 | 1.46 | 1.52 |
| 2 | Z | 503 | SER | C-N | 6.15 | 1.41 | 1.34 |
| 2 | Z | 622 | GLU | C-N | 6.15 | 1.42 | 1.33 |
| 12 | v | 375 | VAL | C-N | 6.15 | 1.40 | 1.33 |
| 7 | M | 1589 | ASP | C-N | 6.15 | 1.42 | 1.33 |
| 8 | P | 350 | ALA | N-CA | -6.15 | 1.39 | 1.46 |
| 9 | Q | 770 | ASN | C-N | 6.15 | 1.42 | 1.34 |
| 9 | R | 338 | PHE | CA-CB | 6.15 | 1.63 | 1.53 |
| 14 | h | 304 | LEU | N-CA | 6.15 | 1.53 | 1.45 |
| 16 | c | 144 | PHE | CA-C | -6.15 | 1.44 | 1.52 |
| 4 | J | 665 | TRP | CA-C | -6.15 | 1.45 | 1.52 |
| 8 | N | 796 | SER | CA-C | -6.15 | 1.44 | 1.52 |
| 1 | 0 | 512 | LYS | CA-C | -6.15 | 1.44 | 1.52 |
| 6 | C | 455 | GLU | CA-CB | 6.15 | 1.62 | 1.53 |
| 9 | R | 226 | ARG | CD-NE | 6.15 | 1.54 | 1.46 |
| 9 | R | 695 | ILE | CA-CB | -6.15 | 1.46 | 1.54 |
| 19 | m | 508 | MET | CA-C | -6.15 | 1.44 | 1.52 |
| 20 | n | 1104 | ILE | N-CA | 6.15 | 1.52 | 1.46 |
| 17 | d | 129 | GLU | CA-CB | 6.15 | 1.61 | 1.53 |
| 5 | H | 402 | GLN | C-N | 6.15 | 1.41 | 1.33 |
| 7 | O | 707 | LEU | CA-C | -6.15 | 1.44 | 1.52 |
| 14 | h | 631 | LEU | CA-C | -6.15 | 1.45 | 1.52 |
| 20 | g | 933 | LEU | C-N | 6.15 | 1.41 | 1.33 |
| 20 | g | 102 | HIS | CB-CG | 6.14 | 1.58 | 1.50 |
| 6 | I | 448 | THR | CA-C | -6.14 | 1.44 | 1.52 |
| 5 | K | 446 | ARG | CA-C | -6.14 | 1.44 | 1.52 |
| 9 | R | 100 | PRO | CA-C | -6.14 | 1.46 | 1.52 |
| 7 | O | 553 | ILE | CA-C | -6.14 | 1.45 | 1.52 |
| 4 | y | 653 | SER | N-CA | -6.14 | 1.39 | 1.46 |
| 14 | a | 758 | PHE | CA-CB | 6.14 | 1.63 | 1.53 |
| 11 | V | 401 | ASP | CA-CB | -6.14 | 1.45 | 1.53 |
| 15 | b | 458 | ARG | NE-CZ | 6.14 | 1.39 | 1.33 |
| 14 | a | 364 | GLN | N-CA | -6.14 | 1.38 | 1.46 |
| 5 | K | 522 | TYR | CA-C | -6.14 | 1.44 | 1.52 |
| 9 | S | 636 | ARG | NE-CZ | 6.14 | 1.39 | 1.33 |
| 16 | c | 493 | VAL | CA-CB | 6.14 | 1.62 | 1.54 |
| 1 | 0 | 888 | ALA | CA-C | 6.14 | 1.61 | 1.52 |
| 5 | B | 520 | ILE | C-N | 6.14 | 1.42 | 1.33 |
| 15 | i | 71 | LEU | CA-C | -6.14 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | n | 274 | PRO | C-N | 6.14 | 1.42 | 1.33 |
| 5 | H | 406 | VAL | CA-CB | 6.13 | 1.62 | 1.54 |
| 5 | K | 394 | THR | N-CA | -6.13 | 1.39 | 1.46 |
| 7 | O | 48 | ARG | CZ-NH2 | 6.13 | 1.41 | 1.33 |
| 7 | O | 615 | LEU | CA-C | -6.13 | 1.45 | 1.52 |
| 8 | P | 918 | PHE | C-N | 6.13 | 1.42 | 1.33 |
| 1 | 0 | 1369 | ASN | N-CA | -6.13 | 1.38 | 1.46 |
| 8 | P | 89 | PHE | CA-C | 6.13 | 1.60 | 1.52 |
| 9 | S | 131 | GLY | C-N | 6.13 | 1.41 | 1.33 |
| 2 | Z | 949 | ARG | CA-CB | 6.13 | 1.62 | 1.53 |
| 15 | i | 61 | ASN | CA-C | -6.13 | 1.43 | 1.52 |
| 14 | a | 585 | ASP | CA-C | -6.13 | 1.44 | 1.52 |
| 8 | N | 1643 | ASP | CA-C | 6.13 | 1.60 | 1.52 |
| 13 | x | 1304 | ALA | C-N | 6.13 | 1.42 | 1.33 |
| 18 | l | 193 | ILE | CA-CB | -6.13 | 1.46 | 1.53 |
| 8 | N | 426 | SER | C-N | 6.13 | 1.41 | 1.33 |
| 9 | R | 578 | GLU | N-CA | 6.13 | 1.53 | 1.46 |
| 7 | O | 1098 | SER | CA-C | -6.13 | 1.44 | 1.52 |
| 1 | Y | 657 | GLU | C-N | 6.13 | 1.41 | 1.33 |
| 2 | Z | 159 | ILE | CA-C | -6.13 | 1.45 | 1.52 |
| 20 | n | 76 | TYR | CZ-OH | 6.13 | 1.50 | 1.38 |
| 20 | g | 790 | HIS | C-N | 6.13 | 1.41 | 1.34 |
| 14 | a | 366 | LEU | N-CA | -6.13 | 1.38 | 1.46 |
| 14 | a | 929 | HIS | N-CA | -6.13 | 1.37 | 1.46 |
| 5 | H | 380 | LEU | CA-C | -6.13 | 1.44 | 1.52 |
| 12 | v | 547 | VAL | CA-C | -6.13 | 1.44 | 1.52 |
| 7 | O | 767 | ILE | C-N | 6.12 | 1.42 | 1.33 |
| 15 | i | 348 | GLN | N-CA | -6.12 | 1.38 | 1.46 |
| 14 | a | 837 | SER | CA-C | -6.12 | 1.44 | 1.52 |
| 7 | O | 709 | PHE | CA-C | -6.12 | 1.45 | 1.52 |
| 9 | T | 770 | ASN | N-CA | -6.12 | 1.38 | 1.45 |
| 2 | Z | 758 | SER | N-CA | -6.12 | 1.38 | 1.46 |
| 12 | u | 180 | ASN | CA-CB | 6.12 | 1.61 | 1.53 |
| 16 | j | 135 | ALA | CA-C | -6.12 | 1.44 | 1.52 |
| 19 | f | 327 | VAL | N-CA | -6.12 | 1.39 | 1.46 |
| 20 | g | 1056 | LYS | N-CA | -6.12 | 1.38 | 1.46 |
| 8 | P | 448 | ILE | N-CA | -6.12 | 1.38 | 1.46 |
| 9 | S | 155 | VAL | N-CA | -6.12 | 1.39 | 1.46 |
| 8 | N | 188 | ILE | CA-C | -6.12 | 1.45 | 1.52 |
| 1 | 0 | 1198 | ASN | CA-C | -6.12 | 1.44 | 1.52 |
| 2 | Z | 222 | LEU | C-N | 6.12 | 1.41 | 1.33 |
| 15 | b | 502 | MET | CA-C | -6.12 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 16 | c | 265 | HIS | N-CA | -6.12 | 1.38 | 1.46 |
| 20 | g | 327 | ALA | CA-C | -6.12 | 1.45 | 1.52 |
| 20 | g | 868 | HIS | C-N | 6.12 | 1.42 | 1.34 |
| 14 | a | 747 | PRO | N-CD | -6.12 | 1.39 | 1.47 |
| 2 | 1 | 1058 | CYS | C-N | 6.11 | 1.42 | 1.33 |
| 9 | S | 71 | TYR | N-CA | -6.11 | 1.39 | 1.46 |
| 20 | n | 286 | THR | CA-C | -6.11 | 1.45 | 1.52 |
| 15 | b | 585 | LYS | C-N | 6.11 | 1.42 | 1.33 |
| 19 | f | 38 | ILE | N-CA | -6.11 | 1.39 | 1.46 |
| 19 | f | 421 | LYS | CA-C | -6.11 | 1.44 | 1.52 |
| 20 | g | 546 | ILE | N-CA | -6.11 | 1.39 | 1.46 |
| 7 | M | 155 | LEU | CA-C | 6.11 | 1.60 | 1.52 |
| 7 | M | 868 | ALA | N-CA | -6.11 | 1.38 | 1.46 |
| 8 | N | 1489 | PRO | N-CA | -6.11 | 1.40 | 1.47 |
| 1 | Y | 160 | ILE | CA-CB | -6.11 | 1.46 | 1.54 |
| 1 | Y | 650 | TYR | C-N | 6.11 | 1.42 | 1.33 |
| 12 | u | 61 | ARG | CZ-NH1 | 6.11 | 1.41 | 1.32 |
| 14 | h | 894 | GLU | C-N | 6.11 | 1.41 | 1.33 |
| 20 | n | 1033 | VAL | N-CA | 6.11 | 1.53 | 1.46 |
| 14 | a | 378 | TRP | N-CA | -6.11 | 1.38 | 1.46 |
| 5 | K | 397 | ARG | NE-CZ | 6.11 | 1.39 | 1.33 |
| 7 | O | 227 | ASP | N-CA | -6.11 | 1.42 | 1.46 |
| 12 | u | 558 | PHE | C-N | 6.11 | 1.42 | 1.34 |
| 12 | v | 359 | GLU | CA-CB | 6.11 | 1.62 | 1.53 |
| 15 | i | 682 | LEU | N-CA | -6.11 | 1.38 | 1.46 |
| 15 | b | 79 | MET | C-N | 6.11 | 1.42 | 1.33 |
| 1 | 0 | 1100 | LYS | N-CA | 6.11 | 1.54 | 1.46 |
| 5 | B | 348 | ILE | CA-C | -6.11 | 1.48 | 1.53 |
| 5 | H | 308 | LEU | CA-C | 6.11 | 1.59 | 1.52 |
| 4 | J | 805 | ARG | CZ-NH2 | 6.11 | 1.41 | 1.33 |
| 7 | M | 893 | HIS | CA-C | -6.11 | 1.43 | 1.52 |
| 14 | a | 110 | ILE | N-CA | -6.11 | 1.39 | 1.46 |
| 7 | O | 1097 | TYR | C-N | 6.11 | 1.42 | 1.34 |
| 9 | Q | 69 | ALA | CA-C | -6.11 | 1.45 | 1.52 |
| 12 | v | 179 | VAL | CA-C | -6.11 | 1.45 | 1.52 |
| 19 | m | 459 | LYS | CA-CB | 6.11 | 1.63 | 1.53 |
| 16 | c | 653 | GLU | C-N | 6.11 | 1.40 | 1.34 |
| 19 | f | 40 | ARG | N-CA | -6.11 | 1.38 | 1.46 |
| 20 | g | 225 | MET | CA-C | -6.11 | 1.43 | 1.52 |
| 2 | 1 | 234 | THR | CA-CB | -6.10 | 1.43 | 1.53 |
| 9 | T | 342 | ARG | CD-NE | 6.10 | 1.54 | 1.46 |
| 14 | h | 584 | ASN | C-O | -6.10 | 1.16 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | H | 295 | CYS | C-N | 6.10 | 1.42 | 1.33 |
| 9 | Q | 790 | ASN | CA-CB | 6.10 | 1.64 | 1.53 |
| 9 | T | 581 | LEU | C-N | 6.10 | 1.41 | 1.33 |
| 19 | m | 511 | ILE | C-N | 6.10 | 1.42 | 1.33 |
| 20 | n | 599 | LYS | CA-C | -6.10 | 1.45 | 1.52 |
| 20 | g | 141 | THR | CA-C | -6.10 | 1.45 | 1.52 |
| 7 | M | 893 | HIS | ND1-CE1 | 6.10 | 1.38 | 1.32 |
| 15 | i | 239 | VAL | N-CA | -6.10 | 1.38 | 1.46 |
| 20 | n | 699 | MET | CA-CB | 6.10 | 1.63 | 1.53 |
| 9 | R | 338 | PHE | C-N | 6.10 | 1.42 | 1.33 |
| 2 | Z | 548 | LEU | N-CA | -6.10 | 1.38 | 1.46 |
| 15 | i | 738 | LYS | CA-CB | 6.10 | 1.63 | 1.53 |
| 21 | t | 50 | ASP | N-CA | -6.10 | 1.39 | 1.46 |
| 20 | g | 99 | VAL | CA-CB | -6.10 | 1.46 | 1.54 |
| 1 | 0 | 110 | HIS | ND1-CE1 | 6.10 | 1.38 | 1.32 |
| 1 | 0 | 893 | ILE | CA-CB | 6.10 | 1.62 | 1.54 |
| 2 | 1 | 656 | HIS | CA-CB | 6.10 | 1.61 | 1.53 |
| 4 | D | 673 | GLY | CA-C | -6.10 | 1.45 | 1.52 |
| 7 | M | 1148 | LEU | CA-CB | 6.10 | 1.62 | 1.53 |
| 8 | N | 987 | SER | CA-CB | 6.10 | 1.63 | 1.53 |
| 9 | Q | 338 | PHE | CA-C | -6.10 | 1.44 | 1.52 |
| 14 | a | 754 | GLU | CA-C | 6.10 | 1.58 | 1.52 |
| 19 | m | 617 | ILE | C-N | 6.10 | 1.41 | 1.33 |
| 21 | r | 20 | LEU | CA-C | -6.10 | 1.45 | 1.52 |
| 8 | N | 748 | HIS | CA-C | -6.09 | 1.44 | 1.52 |
| 2 | Z | 1247 | ASN | N-CA | -6.09 | 1.39 | 1.46 |
| 12 | v | 320 | ASP | CA-CB | 6.09 | 1.64 | 1.53 |
| 19 | m | 684 | ILE | CA-C | -6.09 | 1.46 | 1.53 |
| 1 | 0 | 163 | GLU | C-N | 6.09 | 1.42 | 1.33 |
| 2 | 1 | 245 | ASN | C-N | 6.09 | 1.41 | 1.33 |
| 5 | E | 528 | GLU | C-N | 6.09 | 1.42 | 1.34 |
| 7 | O | 123 | CYS | C-N | 6.09 | 1.42 | 1.33 |
| 2 | Z | 1085 | LYS | N-CA | -6.09 | 1.39 | 1.46 |
| 13 | w | 1386 | ALA | C-N | 6.09 | 1.42 | 1.33 |
| 16 | j | 297 | TYR | N-CA | -6.09 | 1.38 | 1.46 |
| 21 | o | 36 | GLN | CA-CB | 6.09 | 1.62 | 1.54 |
| 18 | e | 239 | ARG | CD-NE | 6.09 | 1.54 | 1.46 |
| 2 | Z | 173 | TRP | NE1-CE2 | 6.09 | 1.44 | 1.37 |
| 2 | Z | 489 | SER | CA-C | -6.09 | 1.45 | 1.52 |
| 4 | G | 682 | ASP | CA-CB | 6.09 | 1.62 | 1.53 |
| 7 | M | 742 | GLN | CA-C | -6.09 | 1.45 | 1.52 |
| 7 | O | 454 | LYS | CA-CB | 6.09 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 16 | j | 585 | ASN | CA-C | -6.09 | 1.46 | 1.52 |
| 14 | a | 229 | PHE | C-N | 6.09 | 1.42 | 1.33 |
| 4 | G | 813 | SER | CA-C | -6.09 | 1.44 | 1.52 |
| 8 | N | 1048 | LYS | CA-CB | 6.09 | 1.59 | 1.53 |
| 8 | P | 369 | LEU | CA-CB | 6.09 | 1.63 | 1.53 |
| 8 | P | 1551 | THR | CA-C | -6.08 | 1.44 | 1.52 |
| 9 | Q | 292 | LYS | N-CA | -6.08 | 1.38 | 1.46 |
| 14 | h | 690 | VAL | CA-C | 6.08 | 1.60 | 1.52 |
| 9 | R | 273 | VAL | C-N | 6.08 | 1.41 | 1.33 |
| 15 | i | 700 | ASP | N-CA | -6.08 | 1.38 | 1.46 |
| 19 | m | 180 | PHE | N-CA | -6.08 | 1.38 | 1.46 |
| 15 | b | 122 | ARG | CD-NE | 6.08 | 1.54 | 1.46 |
| 14 | a | 68 | ILE | CA-C | 6.08 | 1.59 | 1.52 |
| 7 | O | 1378 | ASP | CA-CB | 6.08 | 1.62 | 1.53 |
| 8 | P | 188 | ILE | CA-C | -6.08 | 1.45 | 1.52 |
| 9 | T | 72 | LEU | CA-C | -6.08 | 1.44 | 1.52 |
| 15 | i | 219 | PRO | CA-CB | 6.08 | 1.64 | 1.53 |
| 8 | P | 1638 | LYS | CA-CB | 6.08 | 1.62 | 1.53 |
| 19 | f | 625 | LYS | CA-C | -6.08 | 1.44 | 1.52 |
| 14 | a | 380 | GLU | N-CA | -6.08 | 1.39 | 1.46 |
| 7 | O | 1444 | ASP | C-N | 6.08 | 1.41 | 1.33 |
| 9 | T | 47 | ASN | CA-C | -6.08 | 1.45 | 1.52 |
| 1 | Y | 1106 | ASP | N-CA | -6.08 | 1.38 | 1.46 |
| 12 | u | 346 | ASN | CA-C | -6.08 | 1.45 | 1.52 |
| 20 | n | 516 | LEU | CA-CB | 6.08 | 1.61 | 1.53 |
| 11 | V | 298 | PHE | CA-CB | 6.08 | 1.60 | 1.54 |
| 2 | Z | 997 | PHE | C-O | -6.08 | 1.17 | 1.24 |
| 12 | u | 342 | TYR | N-CA | -6.08 | 1.38 | 1.46 |
| 15 | i | 544 | ASN | C-N | 6.08 | 1.41 | 1.33 |
| 7 | M | 1026 | PHE | CA-C | -6.08 | 1.45 | 1.52 |
| 8 | N | 1534 | TYR | C-N | 6.07 | 1.42 | 1.33 |
| 7 | O | 1404 | ASP | N-CA | -6.07 | 1.38 | 1.46 |
| 12 | u | 413 | LYS | C-N | 6.07 | 1.41 | 1.33 |
| 12 | v | 422 | ARG | NE-CZ | 6.07 | 1.39 | 1.33 |
| 15 | b | 728 | LEU | CA-C | -6.07 | 1.45 | 1.53 |
| 14 | h | 640 | PHE | C-N | 6.07 | 1.41 | 1.33 |
| 19 | m | 143 | LYS | C-N | 6.07 | 1.42 | 1.33 |
| 21 | o | 71 | HIS | CB-CG | 6.07 | 1.58 | 1.50 |
| 7 | O | 134 | LEU | C-N | 6.07 | 1.40 | 1.34 |
| 14 | a | 560 | ASN | CA-CB | 6.07 | 1.62 | 1.53 |
| 1 | 0 | 257 | PHE | C-O | 6.07 | 1.30 | 1.23 |
| 8 | N | 866 | ARG | CD-NE | 6.07 | 1.54 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | f | 387 | ARG | N-CA | -6.07 | 1.38 | 1.46 |
| 12 | u | 70 | HIS | C-N | 6.07 | 1.41 | 1.33 |
| 14 | h | 619 | LEU | N-CA | -6.07 | 1.39 | 1.46 |
| 8 | P | 1420 | VAL | CA-CB | -6.06 | 1.46 | 1.54 |
| 4 | A | 815 | GLU | N-CA | -6.06 | 1.38 | 1.46 |
| 6 | I | 287 | GLN | CA-CB | 6.06 | 1.62 | 1.53 |
| 8 | N | 755 | ASN | N-CA | -6.06 | 1.39 | 1.46 |
| 19 | f | 388 | ILE | CA-CB | -6.06 | 1.47 | 1.54 |
| 2 | Z | 391 | LEU | N-CA | -6.06 | 1.38 | 1.46 |
| 16 | c | 133 | ASP | C-N | 6.06 | 1.41 | 1.33 |
| 19 | f | 301 | TYR | N-CA | 6.06 | 1.53 | 1.46 |
| 5 | E | 404 | ARG | CA-C | -6.06 | 1.45 | 1.52 |
| 7 | M | 479 | GLU | N-CA | -6.06 | 1.39 | 1.46 |
| 8 | P | 26 | ALA | N-CA | -6.06 | 1.37 | 1.46 |
| 9 | S | 587 | THR | C-O | 6.06 | 1.28 | 1.23 |
| 9 | S | 743 | ASP | CA-C | -6.06 | 1.45 | 1.53 |
| 16 | c | 193 | GLU | C-N | 6.06 | 1.41 | 1.33 |
| 20 | g | 1107 | ASN | CA-C | -6.06 | 1.44 | 1.52 |
| 14 | a | 438 | GLU | CA-CB | 6.06 | 1.63 | 1.53 |
| 7 | M | 1453 | ARG | NE-CZ | 6.06 | 1.39 | 1.33 |
| 8 | N | 1432 | ARG | NE-CZ | 6.06 | 1.39 | 1.33 |
| 14 | a | 132 | GLN | CA-C | -6.06 | 1.45 | 1.52 |
| 14 | a | 146 | ASN | CA-C | -6.06 | 1.45 | 1.52 |
| 1 | 0 | 1011 | ARG | CD-NE | 6.06 | 1.54 | 1.46 |
| 7 | M | 1517 | ALA | C-N | 6.06 | 1.41 | 1.33 |
| 7 | M | 193 | LEU | C-N | 6.05 | 1.41 | 1.33 |
| 9 | T | 467 | ILE | CA-CB | -6.05 | 1.46 | 1.54 |
| 1 | Y | 589 | HIS | CA-C | -6.05 | 1.44 | 1.52 |
| 18 | l | 41 | ASP | N-CA | -6.05 | 1.40 | 1.46 |
| 14 | a | 620 | HIS | ND1-CE1 | 6.05 | 1.38 | 1.32 |
| 21 | q | 38 | GLU | C-O | -6.05 | 1.17 | 1.24 |
| 6 | I | 382 | LYS | N-CA | -6.05 | 1.40 | 1.46 |
| 7 | O | 1012 | ASN | CA-CB | 6.05 | 1.61 | 1.53 |
| 8 | P | 807 | LEU | CA-C | -6.05 | 1.44 | 1.52 |
| 9 | R | 19 | ASN | CA-CB | 6.05 | 1.62 | 1.53 |
| 9 | S | 410 | ALA | N-CA | -6.05 | 1.37 | 1.45 |
| 2 | Z | 228 | PHE | C-N | 6.05 | 1.41 | 1.33 |
| 2 | Z | 654 | SER | C-N | 6.05 | 1.42 | 1.33 |
| 12 | v | 49 | LEU | CA-CB | 6.05 | 1.61 | 1.53 |
| 15 | i | 49 | VAL | CA-CB | -6.05 | 1.49 | 1.54 |
| 19 | f | 429 | ILE | CA-CB | 6.05 | 1.61 | 1.54 |
| 7 | M | 288 | TRP | CA-C | -6.05 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 16 | j | 346 | GLY | CA-C | -6.05 | 1.43 | 1.51 |
| 18 | e | 139 | ALA | N-CA | -6.05 | 1.39 | 1.46 |
| 14 | a | 901 | ARG | CZ-NH1 | 6.05 | 1.41 | 1.32 |
| 4 | D | 644 | TRP | C-N | 6.05 | 1.41 | 1.33 |
| 4 | J | 718 | THR | CA-C | -6.05 | 1.45 | 1.52 |
| 8 | P | 324 | SER | CA-CB | 6.05 | 1.63 | 1.53 |
| 12 | v | 589 | ASP | CA-C | -6.05 | 1.45 | 1.52 |
| 8 | N | 442 | LEU | N-CA | -6.05 | 1.38 | 1.46 |
| 8 | N | 504 | LEU | C-N | 6.05 | 1.41 | 1.33 |
| 14 | h | 382 | VAL | CA-CB | -6.05 | 1.47 | 1.54 |
| 7 | M | 111 | GLN | CA-C | -6.04 | 1.45 | 1.52 |
| 11 | X | 384 | CYS | CA-C | -6.04 | 1.45 | 1.52 |
| 6 | I | 272 | GLN | CA-C | -6.04 | 1.45 | 1.52 |
| 8 | P | 1538 | ASP | CA-C | -6.04 | 1.44 | 1.52 |
| 21 | q | 71 | HIS | CG-CD2 | 6.04 | 1.42 | 1.35 |
| 2 | 1 | 712 | SER | N-CA | -6.04 | 1.39 | 1.46 |
| 7 | M | 431 | PHE | CA-C | -6.04 | 1.45 | 1.52 |
| 9 | R | 787 | HIS | ND1-CE1 | 6.04 | 1.38 | 1.32 |
| 9 | S | 464 | ASN | N-CA | -6.04 | 1.39 | 1.46 |
| 1 | Y | 461 | ARG | N-CA | -6.04 | 1.39 | 1.45 |
| 1 | Y | 665 | ASN | CA-C | -6.04 | 1.46 | 1.52 |
| 2 | Z | 1126 | LYS | N-CA | -6.04 | 1.38 | 1.46 |
| 15 | i | 145 | ASN | C-N | 6.04 | 1.42 | 1.33 |
| 7 | O | 886 | LEU | CA-C | -6.04 | 1.44 | 1.52 |
| 2 | Z | 183 | TRP | CA-CB | 6.04 | 1.63 | 1.53 |
| 15 | i | 121 | ASP | CA-C | -6.04 | 1.45 | 1.52 |
| 7 | M | 1253 | ARG | CD-NE | 6.04 | 1.54 | 1.46 |
| 12 | u | 660 | SER | C-N | 6.04 | 1.41 | 1.33 |
| 6 | I | 282 | GLN | CA-C | 6.04 | 1.61 | 1.52 |
| 7 | O | 668 | ARG | CA-CB | 6.04 | 1.64 | 1.53 |
| 9 | T | 217 | ARG | CA-C | -6.04 | 1.45 | 1.52 |
| 14 | h | 734 | HIS | ND1-CE1 | 6.04 | 1.38 | 1.32 |
| 19 | m | 539 | LEU | CA-C | -6.04 | 1.44 | 1.52 |
| 1 | 0 | 262 | SER | CA-C | -6.04 | 1.45 | 1.52 |
| 1 | 0 | 1212 | GLU | CA-C | 6.03 | 1.60 | 1.52 |
| 5 | B | 528 | GLU | N-CA | -6.03 | 1.39 | 1.46 |
| 4 | y | 806 | SER | C-N | 6.03 | 1.41 | 1.33 |
| 21 | q | 62 | GLY | CA-C | -6.03 | 1.45 | 1.51 |
| 20 | g | 634 | VAL | N-CA | -6.03 | 1.39 | 1.46 |
| 18 | l | 97 | ARG | CA-C | -6.03 | 1.44 | 1.52 |
| 5 | K | 309 | ARG | N-CA | -6.03 | 1.38 | 1.46 |
| 1 | Y | 989 | GLN | C-N | 6.03 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | i | 103 | GLU | C-N | 6.03 | 1.41 | 1.33 |
| 17 | d | 19 | TYR | CA-C | -6.03 | 1.45 | 1.52 |
| 10 | W | 338 | THR | CB-OG1 | -6.03 | 1.34 | 1.43 |
| 20 | g | 1001 | ASP | C-N | 6.03 | 1.42 | 1.34 |
| 1 | 0 | 1351 | PHE | N-CA | -6.03 | 1.39 | 1.46 |
| 2 | 1 | 817 | GLU | C-N | 6.03 | 1.40 | 1.33 |
| 7 | M | 1240 | HIS | ND1-CE1 | 6.03 | 1.38 | 1.32 |
| 8 | P | 1623 | GLU | N-CA | 6.03 | 1.53 | 1.46 |
| 9 | Q | 607 | ARG | CD-NE | 6.03 | 1.54 | 1.46 |
| 9 | T | 503 | ALA | C-N | 6.03 | 1.41 | 1.33 |
| 1 | Y | 966 | ILE | C-N | 6.03 | 1.42 | 1.33 |
| 12 | v | 188 | SER | CA-CB | 6.03 | 1.63 | 1.53 |
| 14 | h | 686 | PHE | C-N | 6.03 | 1.39 | 1.33 |
| 1 | 0 | 620 | LYS | C-N | -6.03 | 1.26 | 1.34 |
| 1 | 0 | 1027 | HIS | CA-C | -6.03 | 1.45 | 1.52 |
| 5 | K | 395 | ALA | N-CA | -6.03 | 1.39 | 1.46 |
| 8 | N | 522 | LYS | CA-C | -6.03 | 1.44 | 1.53 |
| 9 | Q | 612 | HIS | ND1-CE1 | 6.03 | 1.38 | 1.32 |
| 9 | T | 258 | LYS | CA-C | 6.03 | 1.60 | 1.52 |
| 1 | Y | 392 | SER | CA-CB | 6.03 | 1.63 | 1.53 |
| 2 | Z | 1369 | LEU | CA-CB | 6.03 | 1.62 | 1.53 |
| 16 | c | 765 | GLU | C-N | 6.03 | 1.42 | 1.33 |
| 20 | g | 747 | LYS | CA-C | -6.03 | 1.44 | 1.52 |
| 8 | N | 1093 | ASN | N-CA | -6.02 | 1.38 | 1.46 |
| 7 | O | 96 | ASP | CA-C | -6.02 | 1.45 | 1.52 |
| 9 | S | 343 | ALA | C-N | 6.02 | 1.41 | 1.33 |
| 2 | Z | 880 | SER | CA-C | -6.02 | 1.46 | 1.52 |
| 17 | k | 129 | GLU | N-CA | -6.02 | 1.38 | 1.46 |
| 18 | e | 183 | LEU | CA-C | -6.02 | 1.45 | 1.52 |
| 14 | a | 901 | ARG | CD-NE | 6.02 | 1.54 | 1.46 |
| 2 | 1 | 192 | HIS | ND1-CE1 | 6.02 | 1.38 | 1.32 |
| 5 | B | 471 | LYS | C-N | 6.02 | 1.41 | 1.33 |
| 4 | J | 655 | PHE | CA-C | 6.02 | 1.60 | 1.52 |
| 8 | N | 264 | LEU | CA-CB | 6.02 | 1.62 | 1.53 |
| 7 | O | 256 | HIS | ND1-CE1 | 6.02 | 1.38 | 1.32 |
| 9 | Q | 218 | ILE | C-N | 6.02 | 1.41 | 1.33 |
| 9 | S | 236 | ASN | CA-C | 6.02 | 1.60 | 1.52 |
| 8 | N | 793 | LEU | N-CA | -6.02 | 1.34 | 1.46 |
| 10 | W | 305 | TYR | CA-C | 6.02 | 1.60 | 1.52 |
| 13 | x | 1438 | GLU | C-N | 6.02 | 1.41 | 1.33 |
| 7 | O | 110 | ARG | CD-NE | 6.02 | 1.54 | 1.46 |
| 9 | R | 322 | ILE | N-CA | 6.02 | 1.54 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 14 | h | 404 | VAL | CA-CB | -6.02 | 1.46 | 1.54 |
| 14 | h | 1016 | GLN | N-CA | -6.02 | 1.38 | 1.46 |
| 14 | a | 600 | ASP | C-N | 6.02 | 1.41 | 1.33 |
| 21 | s | 87 | LEU | N-CA | -6.02 | 1.38 | 1.46 |
| 6 | I | 301 | HIS | N-CA | 6.02 | 1.53 | 1.46 |
| 9 | R | 712 | GLU | CA-C | -6.02 | 1.45 | 1.52 |
| 12 | u | 340 | ASP | CA-C | -6.02 | 1.45 | 1.52 |
| 18 | l | 241 | ARG | CZ-NH2 | 6.02 | 1.41 | 1.33 |
| 5 | E | 457 | ASN | CA-CB | 6.01 | 1.63 | 1.53 |
| 5 | K | 329 | HIS | C-N | 6.01 | 1.41 | 1.33 |
| 7 | M | 777 | GLN | CA-C | -6.01 | 1.44 | 1.52 |
| 8 | P | 1613 | ASN | C-N | 6.01 | 1.41 | 1.33 |
| 9 | Q | 357 | LYS | CA-CB | 6.01 | 1.62 | 1.53 |
| 9 | T | 329 | ASN | CA-CB | 6.01 | 1.62 | 1.53 |
| 20 | n | 373 | ASN | CA-C | -6.01 | 1.44 | 1.52 |
| 7 | M | 1353 | LEU | CA-CB | 6.01 | 1.62 | 1.53 |
| 7 | M | 693 | ARG | NE-CZ | 6.01 | 1.39 | 1.33 |
| 1 | Y | 1286 | ASP | CA-CB | 6.01 | 1.63 | 1.53 |
| 17 | d | 264 | LEU | CA-C | 6.01 | 1.60 | 1.52 |
| 14 | a | 956 | GLY | N-CA | 6.01 | 1.53 | 1.45 |
| 2 | 1 | 771 | PRO | N-CA | 6.01 | 1.55 | 1.47 |
| 6 | F | 437 | ALA | CA-C | -6.01 | 1.44 | 1.52 |
| 7 | M | 417 | SER | N-CA | 6.01 | 1.57 | 1.46 |
| 9 | S | 500 | GLU | CA-CB | 6.01 | 1.63 | 1.53 |
| 15 | i | 198 | GLU | N-CA | -6.01 | 1.38 | 1.46 |
| 16 | c | 397 | TYR | N-CA | 6.01 | 1.53 | 1.45 |
| 19 | f | 458 | ARG | CZ-NH1 | 6.01 | 1.41 | 1.32 |
| 5 | H | 343 | PRO | CA-C | -6.01 | 1.43 | 1.52 |
| 12 | u | 160 | GLN | C-N | 6.01 | 1.41 | 1.33 |
| 14 | a | 69 | CYS | C-N | 6.01 | 1.41 | 1.33 |
| 14 | a | 999 | CYS | CA-CB | 6.01 | 1.64 | 1.53 |
| 1 | 0 | 519 | THR | CA-C | -6.01 | 1.45 | 1.52 |
| 13 | x | 1221 | VAL | CA-CB | -6.01 | 1.47 | 1.54 |
| 14 | h | 847 | LYS | CA-C | -6.01 | 1.44 | 1.52 |
| 21 | p | 41 | ILE | C-N | 6.01 | 1.41 | 1.33 |
| 14 | a | 763 | THR | N-CA | -6.01 | 1.39 | 1.46 |
| 7 | M | 1500 | ASN | CA-CB | 6.00 | 1.63 | 1.53 |
| 8 | P | 278 | SER | C-N | 6.00 | 1.41 | 1.33 |
| 14 | h | 614 | ILE | CA-C | -6.00 | 1.44 | 1.52 |
| 20 | n | 795 | VAL | C-N | 6.00 | 1.41 | 1.33 |
| 17 | d | 148 | VAL | N-CA | -6.00 | 1.38 | 1.46 |
| 19 | f | 542 | ARG | CA-CB | 6.00 | 1.63 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 14 | h | 740 | PHE | C-N | 6.00 | 1.42 | 1.33 |
| 16 | j | 607 | ARG | NE-CZ | 6.00 | 1.39 | 1.33 |
| 20 | g | 494 | VAL | C-O | -6.00 | 1.16 | 1.23 |
| 5 | E | 460 | TRP | N-CA | 6.00 | 1.53 | 1.46 |
| 9 | R | 652 | ILE | CA-CB | -6.00 | 1.46 | 1.54 |
| 11 | X | 282 | ASN | CA-CB | 6.00 | 1.63 | 1.53 |
| 2 | Z | 536 | HIS | CG-ND1 | 6.00 | 1.44 | 1.38 |
| 12 | u | 178 | ARG | CZ-NH1 | 6.00 | 1.41 | 1.32 |
| 12 | v | 682 | GLU | C-N | 6.00 | 1.41 | 1.33 |
| 18 | e | 227 | TRP | CA-CB | 6.00 | 1.63 | 1.54 |
| 14 | a | 697 | GLN | N-CA | -6.00 | 1.39 | 1.46 |
| 8 | N | 1546 | SER | CA-C | -6.00 | 1.45 | 1.52 |
| 7 | O | 225 | SER | N-CA | -6.00 | 1.39 | 1.46 |
| 7 | O | 507 | ALA | C-N | 6.00 | 1.41 | 1.33 |
| 11 | X | 354 | SER | N-CA | -6.00 | 1.38 | 1.46 |
| 16 | j | 191 | ASP | CA-CB | 6.00 | 1.63 | 1.53 |
| 1 | 0 | 1011 | ARG | CZ-NH2 | 6.00 | 1.41 | 1.33 |
| 6 | F | 449 | LEU | CA-C | -6.00 | 1.44 | 1.52 |
| 15 | i | 630 | LEU | N-CA | -6.00 | 1.38 | 1.46 |
| 1 | 0 | 359 | LEU | C-N | 5.99 | 1.41 | 1.33 |
| 7 | O | 891 | LYS | CA-CB | 5.99 | 1.63 | 1.53 |
| 9 | R | 541 | TYR | C-O | -5.99 | 1.17 | 1.24 |
| 21 | p | 67 | SER | CA-C | -5.99 | 1.45 | 1.52 |
| 20 | g | 778 | ASN | C-N | 5.99 | 1.42 | 1.33 |
| 8 | N | 971 | PHE | N-CA | -5.99 | 1.38 | 1.46 |
| 10 | U | 345 | TYR | CA-CB | 5.99 | 1.63 | 1.53 |
| 14 | h | 175 | VAL | C-N | 5.99 | 1.41 | 1.33 |
| 16 | j | 185 | PHE | CA-CB | 5.99 | 1.61 | 1.52 |
| 2 | Z | 1344 | VAL | N-CA | -5.99 | 1.39 | 1.46 |
| 15 | i | 331 | TYR | C-N | 5.99 | 1.41 | 1.33 |
| 18 | e | 1 | MET | N-CA | 5.99 | 1.57 | 1.46 |
| 1 | 0 | 284 | PHE | CA-C | -5.99 | 1.45 | 1.52 |
| 7 | O | 214 | LEU | CA-CB | 5.99 | 1.62 | 1.53 |
| 15 | i | 337 | LEU | N-CA | -5.99 | 1.38 | 1.46 |
| 20 | n | 1002 | LEU | CA-C | -5.99 | 1.45 | 1.52 |
| 15 | b | 330 | ASP | CA-CB | 5.99 | 1.63 | 1.53 |
| 17 | k | 289 | TRP | N-CA | -5.99 | 1.38 | 1.46 |
| 14 | a | 866 | GLU | N-CA | -5.99 | 1.39 | 1.46 |
| 4 | J | 651 | SER | C-N | 5.99 | 1.41 | 1.33 |
| 7 | O | 779 | PRO | CA-CB | -5.99 | 1.45 | 1.53 |
| 7 | O | 836 | ILE | C-N | 5.99 | 1.42 | 1.34 |
| 7 | O | 969 | PHE | CA-CB | 5.99 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1284 | SER | CA-CB | 5.99 | 1.62 | 1.53 |
| 7 | O | 1440 | ILE | C-N | 5.99 | 1.41 | 1.33 |
| 8 | P | 1248 | THR | N-CA | -5.99 | 1.38 | 1.46 |
| 10 | U | 283 | ILE | CB-CG1 | 5.99 | 1.65 | 1.53 |
| 15 | i | 300 | SER | C-N | 5.99 | 1.41 | 1.33 |
| 20 | g | 721 | CYS | C-N | 5.99 | 1.41 | 1.33 |
| 20 | g | 1054 | GLY | C-N | 5.99 | 1.42 | 1.33 |
| 2 | 1 | 799 | ILE | CA-CB | -5.98 | 1.46 | 1.54 |
| 8 | N | 584 | ASP | CA-CB | 5.98 | 1.65 | 1.53 |
| 9 | Q | 295 | ASN | CA-C | -5.98 | 1.45 | 1.53 |
| 9 | Q | 624 | THR | C-O | -5.98 | 1.17 | 1.24 |
| 18 | e | 320 | SER | N-CA | -5.98 | 1.38 | 1.45 |
| 14 | a | 666 | ASN | N-CA | -5.98 | 1.38 | 1.46 |
| 6 | I | 310 | ARG | C-N | 5.98 | 1.42 | 1.33 |
| 4 | J | 715 | GLU | N-CA | -5.98 | 1.38 | 1.46 |
| 7 | M | 174 | LEU | CA-CB | 5.98 | 1.62 | 1.53 |
| 7 | O | 619 | VAL | N-CA | -5.98 | 1.38 | 1.46 |
| 8 | P | 297 | THR | C-N | 5.98 | 1.41 | 1.33 |
| 18 | l | 239 | ARG | NE-CZ | 5.98 | 1.39 | 1.33 |
| 1 | Y | 1429 | ILE | N-CA | -5.98 | 1.39 | 1.46 |
| 16 | j | 530 | LEU | CA-CB | 5.98 | 1.63 | 1.53 |
| 17 | k | 124 | LYS | N-CA | 5.98 | 1.53 | 1.45 |
| 19 | m | 189 | LEU | CA-C | -5.98 | 1.45 | 1.52 |
| 20 | n | 917 | LEU | CA-C | -5.98 | 1.45 | 1.52 |
| 15 | b | 645 | ALA | CA-C | -5.98 | 1.44 | 1.52 |
| 1 | 0 | 298 | TYR | N-CA | 5.98 | 1.53 | 1.46 |
| 5 | B | 390 | HIS | CA-C | -5.98 | 1.44 | 1.52 |
| 7 | M | 998 | LEU | CA-C | -5.98 | 1.44 | 1.52 |
| 9 | R | 614 | ARG | NE-CZ | 5.98 | 1.39 | 1.33 |
| 9 | T | 618 | GLU | N-CA | -5.98 | 1.39 | 1.46 |
| 6 | C | 281 | ASP | C-N | 5.98 | 1.42 | 1.33 |
| 7 | O | 360 | LEU | N-CA | -5.98 | 1.39 | 1.46 |
| 8 | P | 955 | PHE | CA-CB | 5.98 | 1.62 | 1.53 |
| 15 | i | 661 | HIS | CA-C | -5.98 | 1.44 | 1.52 |
| 20 | n | 102 | HIS | N-CA | -5.98 | 1.39 | 1.46 |
| 20 | n | 436 | SER | CA-C | -5.98 | 1.45 | 1.53 |
| 14 | a | 936 | TYR | CA-C | -5.98 | 1.45 | 1.52 |
| 8 | P | 1401 | SER | CA-C | -5.98 | 1.45 | 1.52 |
| 14 | a | 439 | ASP | C-N | 5.98 | 1.41 | 1.33 |
| 2 | 1 | 1332 | SER | CA-C | -5.97 | 1.45 | 1.52 |
| 4 | G | 698 | GLN | CA-C | 5.97 | 1.60 | 1.52 |
| 8 | N | 664 | LEU | CA-CB | 5.97 | 1.63 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | N | 1004 | LEU | CA-C | -5.97 | 1.45 | 1.53 |
| 9 | Q | 599 | ARG | CD-NE | 5.97 | 1.54 | 1.46 |
| 14 | a | 772 | GLN | N-CA | 5.97 | 1.53 | 1.46 |
| 1 | Y | 942 | LYS | N-CA | -5.97 | 1.38 | 1.46 |
| 17 | k | 83 | LYS | CA-C | -5.97 | 1.45 | 1.52 |
| 2 | 1 | 825 | LEU | N-CA | -5.97 | 1.38 | 1.46 |
| 8 | N | 1433 | ILE | CA-C | -5.97 | 1.45 | 1.52 |
| 16 | c | 514 | GLU | C-N | 5.97 | 1.41 | 1.33 |
| 5 | H | 438 | SER | N-CA | -5.97 | 1.39 | 1.46 |
| 8 | N | 1020 | ILE | C-N | 5.97 | 1.42 | 1.34 |
| 15 | i | 71 | LEU | C-N | 5.97 | 1.42 | 1.33 |
| 20 | g | 451 | ASN | C-N | 5.97 | 1.42 | 1.33 |
| 2 | Z | 727 | ARG | NE-CZ | 5.97 | 1.39 | 1.33 |
| 19 | m | 248 | TYR | CA-CB | 5.97 | 1.63 | 1.53 |
| 20 | g | 918 | SER | CA-C | -5.97 | 1.44 | 1.52 |
| 6 | F | 274 | ARG | NE-CZ | 5.97 | 1.39 | 1.33 |
| 8 | N | 655 | VAL | N-CA | -5.97 | 1.38 | 1.46 |
| 9 | R | 563 | ASN | CA-C | -5.97 | 1.45 | 1.52 |
| 9 | S | 812 | GLN | CA-CB | 5.97 | 1.63 | 1.53 |
| 1 | Y | 896 | MET | N-CA | -5.97 | 1.39 | 1.46 |
| 16 | j | 446 | ASP | N-CA | -5.97 | 1.38 | 1.46 |
| 16 | c | 305 | ARG | C-N | 5.97 | 1.41 | 1.33 |
| 20 | g | 615 | GLU | CA-CB | 5.97 | 1.63 | 1.53 |
| 1 | 0 | 1107 | LEU | N-CA | -5.96 | 1.38 | 1.46 |
| 8 | P | 1473 | PRO | CA-C | 5.96 | 1.62 | 1.52 |
| 8 | P | 1502 | ILE | N-CA | -5.96 | 1.39 | 1.46 |
| 16 | j | 347 | GLY | N-CA | -5.96 | 1.36 | 1.45 |
| 20 | n | 1116 | GLU | C-N | 5.96 | 1.41 | 1.33 |
| 20 | g | 1071 | PRO | N-CA | -5.96 | 1.39 | 1.47 |
| 1 | 0 | 658 | ILE | N-CA | -5.96 | 1.39 | 1.46 |
| 8 | N | 893 | TYR | CA-CB | 5.96 | 1.66 | 1.54 |
| 7 | O | 719 | ILE | CA-CB | -5.96 | 1.47 | 1.54 |
| 9 | Q | 432 | ILE | CA-CB | -5.96 | 1.45 | 1.54 |
| 9 | T | 707 | HIS | CD2-NE2 | -5.96 | 1.31 | 1.37 |
| 19 | f | 558 | ILE | CA-C | -5.96 | 1.46 | 1.52 |
| 6 | I | 321 | ALA | CA-C | -5.96 | 1.44 | 1.52 |
| 1 | Y | 1009 | HIS | CA-CB | 5.96 | 1.63 | 1.53 |
| 20 | n | 162 | GLY | C-N | 5.96 | 1.39 | 1.32 |
| 20 | n | 224 | ASN | CA-C | -5.96 | 1.46 | 1.53 |
| 17 | d | 206 | TRP | C-N | 5.96 | 1.41 | 1.33 |
| 19 | f | 472 | ALA | CA-C | 5.96 | 1.60 | 1.52 |
| 8 | N | 920 | LEU | CA-C | -5.96 | 1.44 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1408 | LEU | CA-CB | 5.96 | 1.62 | 1.53 |
| 8 | P | 1074 | LEU | N-CA | -5.96 | 1.39 | 1.46 |
| 2 | Z | 144 | THR | CA-C | -5.96 | 1.44 | 1.53 |
| 12 | v | 28 | SER | CA-C | -5.96 | 1.45 | 1.52 |
| 18 | e | 317 | THR | CA-C | -5.96 | 1.44 | 1.52 |
| 2 | 1 | 345 | LEU | N-CA | -5.96 | 1.38 | 1.46 |
| 8 | P | 1613 | ASN | N-CA | -5.96 | 1.39 | 1.46 |
| 1 | Y | 124 | ARG | CD-NE | 5.96 | 1.54 | 1.46 |
| 2 | Z | 914 | GLN | CA-CB | 5.96 | 1.61 | 1.53 |
| 12 | u | 176 | ASP | N-CA | -5.96 | 1.38 | 1.46 |
| 15 | i | 158 | PHE | CA-CB | 5.96 | 1.63 | 1.53 |
| 19 | f | 50 | ALA | N-CA | -5.96 | 1.38 | 1.46 |
| 14 | a | 141 | SER | CA-CB | 5.96 | 1.63 | 1.53 |
| 5 | B | 330 | VAL | CA-CB | -5.96 | 1.49 | 1.55 |
| 1 | 0 | 139 | LYS | CA-C | -5.95 | 1.44 | 1.52 |
| 5 | H | 346 | GLN | C-N | 5.95 | 1.42 | 1.33 |
| 8 | N | 32 | VAL | CA-C | 5.95 | 1.60 | 1.52 |
| 7 | O | 817 | ASN | CA-CB | 5.95 | 1.63 | 1.53 |
| 12 | u | 413 | LYS | CA-CB | 5.95 | 1.61 | 1.53 |
| 19 | m | 235 | GLN | C-N | 5.95 | 1.40 | 1.32 |
| 20 | g | 159 | ASP | CA-CB | 5.95 | 1.63 | 1.53 |
| 9 | Q | 754 | ARG | C-N | 5.95 | 1.41 | 1.33 |
| 1 | Y | 660 | GLU | C-N | 5.95 | 1.41 | 1.33 |
| 1 | Y | 1115 | VAL | CA-C | -5.95 | 1.45 | 1.52 |
| 4 | z | 802 | ASP | N-CA | -5.95 | 1.39 | 1.46 |
| 15 | i | 149 | GLU | N-CA | 5.95 | 1.53 | 1.46 |
| 1 | 0 | 1359 | ASP | N-CA | -5.95 | 1.39 | 1.46 |
| 7 | M | 1532 | ARG | N-CA | -5.95 | 1.39 | 1.46 |
| 1 | Y | 850 | ASN | C-N | 5.95 | 1.41 | 1.33 |
| 2 | Z | 125 | PHE | C-N | 5.95 | 1.40 | 1.33 |
| 16 | j | 335 | LEU | CA-C | -5.95 | 1.45 | 1.52 |
| 21 | o | 25 | LEU | CA-C | -5.95 | 1.45 | 1.52 |
| 21 | t | 73 | LYS | C-N | 5.95 | 1.42 | 1.33 |
| 16 | c | 377 | SER | CA-C | -5.95 | 1.44 | 1.52 |
| 6 | L | 326 | LEU | CA-C | -5.95 | 1.45 | 1.52 |
| 1 | Y | 580 | VAL | N-CA | -5.95 | 1.40 | 1.46 |
| 2 | Z | 180 | LEU | C-N | 5.95 | 1.41 | 1.33 |
| 20 | g | 920 | CYS | CA-CB | 5.95 | 1.62 | 1.53 |
| 2 | 1 | 1124 | ASP | C-N | 5.95 | 1.41 | 1.33 |
| 4 | D | 668 | VAL | N-CA | -5.95 | 1.38 | 1.46 |
| 8 | P | 1560 | MET | CA-C | -5.95 | 1.45 | 1.52 |
| 9 | T | 696 | TYR | N-CA | -5.95 | 1.38 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 14 | h | 55 | GLU | CA-CB | 5.95 | 1.63 | 1.53 |
| 15 | i | 467 | ASN | C-N | 5.95 | 1.42 | 1.33 |
| 15 | b | 411 | SER | N-CA | -5.95 | 1.38 | 1.46 |
| 16 | c | 225 | GLU | C-N | 5.95 | 1.42 | 1.33 |
| 20 | g | 275 | ILE | C-N | 5.95 | 1.41 | 1.33 |
| 7 | O | 2 | LYS | CA-C | -5.94 | 1.44 | 1.52 |
| 20 | g | 757 | LYS | CA-CB | 5.94 | 1.62 | 1.53 |
| 7 | M | 840 | ILE | C-O | 5.94 | 1.29 | 1.24 |
| 7 | O | 109 | ARG | CD-NE | 5.94 | 1.54 | 1.46 |
| 9 | Q | 783 | SER | N-CA | -5.94 | 1.38 | 1.46 |
| 1 | Y | 708 | PRO | CA-C | -5.94 | 1.44 | 1.52 |
| 2 | Z | 1138 | ASN | C-N | 5.94 | 1.41 | 1.33 |
| 12 | v | 389 | TRP | C-N | 5.94 | 1.41 | 1.33 |
| 12 | v | 539 | ILE | N-CA | -5.94 | 1.39 | 1.46 |
| 14 | h | 225 | SER | CA-C | -5.94 | 1.45 | 1.52 |
| 18 | e | 179 | SER | CA-CB | 5.94 | 1.61 | 1.53 |
| 13 | x | 1401 | LEU | C-O | -5.94 | 1.17 | 1.24 |
| 16 | c | 404 | GLN | CA-CB | 5.94 | 1.63 | 1.53 |
| 7 | M | 1538 | LEU | CA-CB | 5.94 | 1.62 | 1.53 |
| 2 | 1 | 511 | VAL | CA-CB | -5.94 | 1.47 | 1.54 |
| 4 | A | 647 | GLN | CA-C | -5.94 | 1.44 | 1.52 |
| 9 | R | 690 | ARG | CA-C | -5.94 | 1.45 | 1.52 |
| 14 | a | 227 | LYS | CA-C | 5.94 | 1.59 | 1.52 |
| 7 | O | 6 | ILE | CA-C | 5.94 | 1.59 | 1.52 |
| 7 | O | 145 | LEU | CA-CB | 5.94 | 1.62 | 1.53 |
| 20 | n | 415 | SER | N-CA | -5.94 | 1.41 | 1.46 |
| 18 | e | 47 | LEU | N-CA | -5.94 | 1.38 | 1.46 |
| 8 | N | 604 | PRO | N-CA | -5.93 | 1.39 | 1.47 |
| 19 | m | 105 | PHE | C-N | 5.93 | 1.41 | 1.33 |
| 20 | n | 232 | THR | CA-C | -5.93 | 1.45 | 1.52 |
| 20 | g | 295 | TRP | CA-C | -5.93 | 1.45 | 1.52 |
| 1 | 0 | 661 | ASP | CA-C | -5.93 | 1.45 | 1.52 |
| 5 | K | 404 | ARG | CD-NE | 5.93 | 1.54 | 1.46 |
| 8 | N | 1468 | VAL | C-O | 5.93 | 1.31 | 1.24 |
| 7 | O | 644 | LYS | CA-C | -5.93 | 1.45 | 1.52 |
| 9 | T | 308 | PHE | CA-C | -5.93 | 1.45 | 1.52 |
| 1 | Y | 899 | MET | CA-C | -5.93 | 1.45 | 1.52 |
| 8 | N | 203 | LYS | C-N | 5.93 | 1.38 | 1.32 |
| 9 | Q | 644 | TYR | CA-C | -5.93 | 1.44 | 1.52 |
| 13 | w | 1346 | ARG | CA-C | -5.93 | 1.44 | 1.52 |
| 5 | E | 315 | LYS | C-N | 5.93 | 1.41 | 1.33 |
| 5 | E | 513 | LEU | CA-CB | 5.93 | 1.63 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 764 | VAL | CA-CB | -5.93 | 1.46 | 1.54 |
| 7 | O | 1385 | PHE | CA-C | -5.93 | 1.45 | 1.52 |
| 9 | Q | 475 | SER | CA-C | 5.93 | 1.59 | 1.52 |
| 9 | Q | 624 | THR | CA-C | -5.93 | 1.45 | 1.52 |
| 16 | j | 298 | LEU | C-N | 5.93 | 1.42 | 1.33 |
| 19 | m | 320 | HIS | C-N | 5.93 | 1.42 | 1.33 |
| 8 | N | 1439 | LEU | C-N | 5.93 | 1.41 | 1.33 |
| 9 | Q | 421 | SER | N-CA | -5.93 | 1.38 | 1.46 |
| 9 | S | 217 | ARG | NE-CZ | 5.93 | 1.39 | 1.33 |
| 19 | m | 253 | GLN | C-N | 5.93 | 1.41 | 1.33 |
| 7 | M | 1486 | LEU | CA-C | -5.93 | 1.45 | 1.52 |
| 8 | N | 106 | ARG | CA-C | -5.93 | 1.45 | 1.52 |
| 14 | h | 975 | ARG | CA-C | -5.93 | 1.44 | 1.52 |
| 15 | b | 356 | SER | N-CA | -5.93 | 1.38 | 1.46 |
| 5 | B | 409 | GLU | CA-C | -5.92 | 1.44 | 1.52 |
| 8 | N | 335 | LEU | N-CA | -5.92 | 1.38 | 1.46 |
| 11 | V | 364 | SER | CA-CB | 5.92 | 1.62 | 1.53 |
| 18 | l | 88 | PRO | N-CA | 5.92 | 1.53 | 1.47 |
| 20 | n | 553 | LEU | CA-CB | 5.92 | 1.62 | 1.53 |
| 9 | R | 811 | ARG | CZ-NH2 | 5.92 | 1.41 | 1.33 |
| 6 | I | 346 | ASP | C-O | -5.92 | 1.17 | 1.24 |
| 9 | Q | 706 | ILE | CA-CB | -5.92 | 1.47 | 1.54 |
| 2 | Z | 721 | SER | CA-C | 5.92 | 1.60 | 1.52 |
| 2 | Z | 1228 | PHE | CA-CB | 5.92 | 1.62 | 1.53 |
| 20 | n | 1110 | ARG | CZ-NH1 | 5.92 | 1.41 | 1.32 |
| 8 | P | 981 | LYS | CA-CB | 5.92 | 1.61 | 1.53 |
| 1 | Y | 436 | LEU | CA-C | -5.92 | 1.45 | 1.52 |
| 12 | v | 57 | LEU | CA-CB | 5.92 | 1.63 | 1.53 |
| 14 | h | 209 | THR | CA-C | 5.92 | 1.61 | 1.53 |
| 15 | i | 648 | LEU | N-CA | -5.92 | 1.38 | 1.46 |
| 15 | b | 589 | PRO | N-CD | -5.92 | 1.39 | 1.47 |
| 9 | T | 236 | ASN | CA-CB | 5.92 | 1.62 | 1.53 |
| 12 | u | 39 | GLN | C-N | 5.92 | 1.42 | 1.33 |
| 16 | j | 240 | LEU | N-CA | -5.92 | 1.38 | 1.46 |
| 20 | n | 673 | ILE | N-CA | -5.92 | 1.39 | 1.46 |
| 19 | f | 223 | ILE | N-CA | 5.92 | 1.52 | 1.46 |
| 19 | f | 311 | ASP | N-CA | -5.92 | 1.39 | 1.46 |
| 1 | 0 | 1215 | GLU | N-CA | 5.92 | 1.52 | 1.46 |
| 8 | P | 398 | ARG | C-N | 5.92 | 1.41 | 1.33 |
| 8 | P | 1219 | THR | C-N | 5.92 | 1.39 | 1.33 |
| 9 | S | 674 | LEU | CB-CG | 5.92 | 1.65 | 1.53 |
| 15 | b | 500 | LYS | C-N | 5.92 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | f | 427 | GLU | CA-C | -5.92 | 1.45 | 1.52 |
| 19 | f | 717 | LEU | CA-CB | 5.92 | 1.63 | 1.53 |
| 1 | 0 | 142 | LEU | CB-CG | 5.91 | 1.65 | 1.53 |
| 2 | 1 | 399 | LEU | C-N | 5.91 | 1.42 | 1.33 |
| 5 | E | 445 | GLN | CA-C | -5.91 | 1.45 | 1.52 |
| 8 | P | 747 | ILE | CA-CB | -5.91 | 1.46 | 1.54 |
| 8 | P | 1190 | ALA | C-N | 5.91 | 1.41 | 1.33 |
| 14 | h | 158 | PHE | N-CA | -5.91 | 1.39 | 1.46 |
| 14 | h | 499 | SER | CA-C | -5.91 | 1.44 | 1.52 |
| 15 | i | 529 | TRP | CA-C | -5.91 | 1.45 | 1.52 |
| 20 | n | 832 | TYR | N-CA | -5.91 | 1.39 | 1.46 |
| 1 | Y | 129 | SER | C-N | 5.91 | 1.41 | 1.32 |
| 2 | Z | 806 | LYS | CA-CB | 5.91 | 1.63 | 1.53 |
| 14 | h | 995 | ARG | N-CA | -5.91 | 1.39 | 1.46 |
| 14 | h | 1034 | LEU | CA-CB | 5.91 | 1.63 | 1.53 |
| 6 | I | 403 | THR | CA-CB | -5.91 | 1.42 | 1.53 |
| 2 | Z | 347 | VAL | N-CA | -5.91 | 1.39 | 1.46 |
| 15 | i | 704 | GLU | CA-C | -5.91 | 1.45 | 1.53 |
| 20 | g | 1089 | LEU | CA-CB | 5.91 | 1.62 | 1.53 |
| 14 | a | 818 | PRO | C-N | 5.91 | 1.41 | 1.33 |
| 2 | 1 | 866 | ILE | C-N | 5.91 | 1.42 | 1.33 |
| 7 | O | 907 | HIS | ND1-CE1 | 5.91 | 1.38 | 1.32 |
| 9 | Q | 646 | LEU | CA-CB | 5.91 | 1.61 | 1.53 |
| 2 | Z | 253 | VAL | CA-C | -5.91 | 1.45 | 1.52 |
| 12 | v | 586 | LYS | CA-C | -5.91 | 1.45 | 1.52 |
| 18 | l | 92 | GLU | CA-C | -5.91 | 1.45 | 1.52 |
| 16 | c | 396 | GLU | CA-C | -5.91 | 1.45 | 1.52 |
| 14 | h | 314 | THR | C-N | 5.91 | 1.41 | 1.33 |
| 16 | j | 480 | GLN | CA-CB | 5.91 | 1.62 | 1.53 |
| 20 | n | 887 | TRP | NE1-CE2 | 5.91 | 1.44 | 1.37 |
| 7 | M | 1147 | PHE | C-N | 5.91 | 1.41 | 1.33 |
| 8 | N | 62 | VAL | CA-CB | -5.91 | 1.46 | 1.54 |
| 9 | S | 323 | SER | CA-CB | 5.91 | 1.63 | 1.53 |
| 1 | Y | 1307 | LEU | CA-C | -5.91 | 1.45 | 1.52 |
| 12 | u | 61 | ARG | CD-NE | 5.91 | 1.54 | 1.46 |
| 15 | b | 559 | PHE | C-N | 5.91 | 1.42 | 1.34 |
| 17 | d | 15 | ALA | CA-C | -5.91 | 1.47 | 1.53 |
| 20 | g | 1126 | ASP | C-N | 5.91 | 1.42 | 1.33 |
| 8 | N | 869 | LYS | CA-CB | 5.90 | 1.61 | 1.53 |
| 1 | Y | 272 | ASP | CA-CB | 5.90 | 1.63 | 1.53 |
| 14 | h | 285 | ASN | C-N | 5.90 | 1.41 | 1.33 |
| 18 | l | 16 | VAL | CA-C | -5.90 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 14 | a | 118 | LEU | N-CA | -5.90 | 1.39 | 1.46 |
| 1 | 0 | 889 | GLU | CA-C | -5.90 | 1.45 | 1.52 |
| 2 | 1 | 508 | PHE | C-O | -5.90 | 1.16 | 1.23 |
| 5 | E | 522 | TYR | C-N | 5.90 | 1.41 | 1.33 |
| 4 | G | 702 | ARG | CZ-NH1 | 5.90 | 1.41 | 1.32 |
| 5 | H | 287 | GLN | N-CA | 5.90 | 1.57 | 1.46 |
| 8 | P | 1500 | LEU | N-CA | -5.90 | 1.38 | 1.46 |
| 2 | Z | 165 | ILE | CA-C | -5.90 | 1.46 | 1.52 |
| 19 | m | 76 | HIS | CA-C | -5.90 | 1.45 | 1.52 |
| 16 | c | 284 | ILE | CB-CG1 | 5.90 | 1.65 | 1.53 |
| 7 | O | 643 | THR | C-N | 5.90 | 1.41 | 1.33 |
| 7 | O | 1584 | ASN | C-N | 5.90 | 1.42 | 1.34 |
| 12 | u | 208 | PHE | CA-C | 5.90 | 1.59 | 1.52 |
| 12 | v | 569 | LYS | C-N | 5.90 | 1.41 | 1.33 |
| 7 | M | 1621 | ALA | CA-C | -5.90 | 1.44 | 1.52 |
| 14 | h | 447 | GLU | C-N | 5.90 | 1.42 | 1.33 |
| 20 | n | 1002 | LEU | C-N | 5.90 | 1.41 | 1.33 |
| 9 | R | 132 | ALA | C-N | 5.90 | 1.41 | 1.33 |
| 9 | S | 576 | LEU | CA-CB | 5.90 | 1.62 | 1.53 |
| 2 | Z | 1211 | ASP | C-N | 5.90 | 1.38 | 1.33 |
| 20 | n | 507 | ILE | CA-C | -5.90 | 1.45 | 1.53 |
| 21 | q | 39 | ARG | N-CA | -5.90 | 1.39 | 1.46 |
| 20 | g | 669 | VAL | CA-CB | -5.90 | 1.47 | 1.54 |
| 5 | K | 397 | ARG | CA-C | -5.89 | 1.44 | 1.52 |
| 7 | M | 198 | TYR | CA-C | -5.89 | 1.44 | 1.52 |
| 7 | M | 1529 | ALA | N-CA | -5.89 | 1.39 | 1.46 |
| 8 | P | 767 | ILE | CA-C | -5.89 | 1.45 | 1.52 |
| 9 | Q | 211 | LYS | CA-C | -5.89 | 1.44 | 1.52 |
| 13 | w | 1288 | ILE | CA-C | -5.89 | 1.45 | 1.52 |
| 14 | h | 264 | ASP | CA-C | -5.89 | 1.44 | 1.53 |
| 14 | h | 430 | ASN | CA-C | -5.89 | 1.44 | 1.52 |
| 17 | k | 13 | HIS | ND1-CE1 | 5.89 | 1.38 | 1.32 |
| 17 | k | 230 | THR | C-N | 5.89 | 1.41 | 1.33 |
| 20 | n | 839 | PHE | C-N | 5.89 | 1.41 | 1.33 |
| 15 | b | 661 | HIS | CB-CG | 5.89 | 1.58 | 1.50 |
| 18 | e | 84 | TRP | C-N | 5.89 | 1.41 | 1.33 |
| 14 | a | 376 | TYR | C-N | 5.89 | 1.41 | 1.33 |
| 8 | N | 1391 | LEU | N-CA | 5.89 | 1.53 | 1.46 |
| 8 | P | 691 | SER | CA-C | -5.89 | 1.44 | 1.52 |
| 14 | h | 720 | PHE | CA-C | 5.89 | 1.61 | 1.53 |
| 20 | n | 348 | LEU | CA-CB | 5.89 | 1.60 | 1.52 |
| 14 | a | 304 | LEU | C-N | 5.89 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 12 | u | 93 | VAL | N-CA | -5.89 | 1.41 | 1.47 |
| 15 | i | 75 | SER | CA-CB | 5.89 | 1.63 | 1.53 |
| 18 | l | 241 | ARG | NE-CZ | 5.89 | 1.39 | 1.33 |
| 6 | L | 458 | ALA | C-N | 5.89 | 1.41 | 1.33 |
| 8 | P | 980 | LYS | N-CA | -5.89 | 1.38 | 1.46 |
| 4 | y | 681 | SER | N-CA | -5.89 | 1.39 | 1.46 |
| 14 | h | 639 | LEU | CA-C | -5.89 | 1.44 | 1.52 |
| 17 | k | 219 | ARG | CA-C | -5.89 | 1.44 | 1.52 |
| 18 | l | 318 | ILE | C-N | 5.89 | 1.41 | 1.33 |
| 20 | n | 519 | GLU | C-N | 5.89 | 1.40 | 1.34 |
| 1 | 0 | 1413 | VAL | N-CA | -5.89 | 1.40 | 1.46 |
| 7 | M | 1651 | ASP | N-CA | 5.89 | 1.53 | 1.46 |
| 8 | N | 777 | ASP | CA-CB | 5.89 | 1.61 | 1.53 |
| 8 | P | 1119 | ASN | CA-CB | 5.89 | 1.65 | 1.53 |
| 9 | T | 668 | SER | C-N | 5.89 | 1.41 | 1.33 |
| 10 | U | 309 | THR | CA-C | -5.89 | 1.45 | 1.52 |
| 4 | G | 790 | ASN | C-N | 5.89 | 1.41 | 1.33 |
| 7 | M | 662 | PRO | N-CA | -5.89 | 1.40 | 1.47 |
| 7 | M | 1508 | ILE | C-N | 5.89 | 1.40 | 1.33 |
| 9 | S | 656 | LEU | N-CA | -5.89 | 1.38 | 1.46 |
| 12 | u | 55 | HIS | ND1-CE1 | 5.89 | 1.38 | 1.32 |
| 12 | u | 138 | ARG | CA-C | -5.89 | 1.44 | 1.52 |
| 17 | k | 175 | THR | C-N | 5.89 | 1.42 | 1.33 |
| 20 | g | 912 | LYS | N-CA | -5.89 | 1.37 | 1.46 |
| 7 | M | 1553 | LEU | N-CA | -5.88 | 1.37 | 1.45 |
| 8 | N | 879 | ILE | N-CA | -5.88 | 1.38 | 1.46 |
| 19 | m | 528 | HIS | CD2-NE2 | -5.88 | 1.31 | 1.37 |
| 18 | e | 105 | ASN | CA-C | -5.88 | 1.45 | 1.52 |
| 19 | f | 458 | ARG | NE-CZ | 5.88 | 1.39 | 1.33 |
| 4 | A | 759 | SER | CA-CB | 5.88 | 1.64 | 1.54 |
| 7 | O | 682 | ASP | CA-CB | 5.88 | 1.63 | 1.53 |
| 2 | Z | 949 | ARG | CZ-NH1 | 5.88 | 1.41 | 1.32 |
| 4 | A | 820 | SER | CA-C | -5.88 | 1.44 | 1.52 |
| 7 | O | 707 | LEU | CA-CB | 5.88 | 1.63 | 1.53 |
| 9 | S | 456 | ARG | NE-CZ | 5.88 | 1.39 | 1.33 |
| 1 | Y | 859 | SER | N-CA | -5.88 | 1.38 | 1.46 |
| 12 | v | 63 | LEU | CA-C | -5.88 | 1.45 | 1.52 |
| 5 | H | 370 | ALA | C-N | 5.88 | 1.41 | 1.33 |
| 7 | M | 318 | ALA | N-CA | -5.88 | 1.38 | 1.46 |
| 8 | N | 1441 | GLN | C-N | 5.88 | 1.40 | 1.33 |
| 7 | O | 1098 | SER | C-N | 5.88 | 1.41 | 1.33 |
| 9 | R | 249 | ARG | CA-C | -5.88 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 381 | VAL | CA-CB | 5.88 | 1.61 | 1.54 |
| 15 | i | 137 | ALA | CA-CB | 5.88 | 1.62 | 1.54 |
| 4 | A | 684 | VAL | CA-C | -5.88 | 1.45 | 1.52 |
| 5 | K | 521 | THR | N-CA | -5.88 | 1.39 | 1.46 |
| 7 | M | 286 | ILE | C-N | 5.88 | 1.42 | 1.33 |
| 8 | N | 1388 | LEU | CA-CB | 5.88 | 1.62 | 1.53 |
| 9 | Q | 692 | MET | C-N | 5.88 | 1.42 | 1.33 |
| 9 | R | 159 | PHE | N-CA | 5.88 | 1.53 | 1.46 |
| 9 | R | 551 | ARG | CD-NE | 5.88 | 1.54 | 1.46 |
| 4 | y | 644 | TRP | CA-CB | 5.88 | 1.62 | 1.53 |
| 14 | h | 234 | LEU | N-CA | -5.88 | 1.39 | 1.46 |
| 14 | h | 979 | GLU | N-CA | -5.88 | 1.39 | 1.46 |
| 16 | c | 501 | LYS | N-CA | -5.88 | 1.39 | 1.46 |
| 7 | M | 52 | GLU | CA-CB | 5.88 | 1.62 | 1.53 |
| 8 | P | 1637 | VAL | C-N | 5.88 | 1.41 | 1.33 |
| 12 | u | 204 | ASP | C-N | 5.88 | 1.41 | 1.33 |
| 1 | 0 | 713 | ILE | N-CA | 5.87 | 1.52 | 1.46 |
| 1 | 0 | 1021 | TYR | N-CA | -5.87 | 1.35 | 1.46 |
| 6 | C | 319 | GLU | CA-C | -5.87 | 1.44 | 1.52 |
| 5 | E | 410 | LYS | C-N | 5.87 | 1.42 | 1.33 |
| 5 | H | 288 | ILE | CA-C | -5.87 | 1.47 | 1.52 |
| 9 | S | 479 | LEU | CA-C | 5.87 | 1.60 | 1.52 |
| 15 | b | 349 | TYR | CA-C | -5.87 | 1.45 | 1.52 |
| 14 | a | 610 | PHE | N-CA | -5.87 | 1.38 | 1.46 |
| 7 | M | 251 | ASP | C-N | 5.87 | 1.41 | 1.33 |
| 7 | O | 917 | PHE | CA-C | -5.87 | 1.44 | 1.52 |
| 9 | Q | 777 | ILE | C-N | 5.87 | 1.41 | 1.33 |
| 14 | a | 255 | GLN | N-CA | -5.87 | 1.38 | 1.46 |
| 12 | u | 220 | GLU | C-N | 5.87 | 1.41 | 1.33 |
| 19 | f | 166 | THR | N-CA | -5.87 | 1.38 | 1.46 |
| 2 | 1 | 193 | CYS | N-CA | -5.87 | 1.38 | 1.46 |
| 5 | H | 391 | GLU | N-CA | -5.87 | 1.39 | 1.46 |
| 9 | T | 745 | LEU | C-O | -5.87 | 1.19 | 1.24 |
| 12 | v | 306 | LEU | C-N | 5.87 | 1.41 | 1.33 |
| 14 | h | 297 | LEU | CA-CB | 5.87 | 1.63 | 1.53 |
| 15 | i | 200 | ASN | N-CA | 5.87 | 1.54 | 1.46 |
| 12 | v | 112 | PHE | CA-CB | 5.87 | 1.63 | 1.53 |
| 15 | b | 250 | ASN | C-O | 5.87 | 1.31 | 1.23 |
| 19 | f | 73 | ARG | CA-C | 5.87 | 1.60 | 1.52 |
| 2 | 1 | 1184 | ASP | CA-C | -5.87 | 1.45 | 1.52 |
| 6 | L | 374 | GLN | C-N | 5.87 | 1.42 | 1.33 |
| 8 | N | 1163 | LEU | C-N | 5.87 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | O | 118 | SER | C-N | 5.87 | 1.40 | 1.33 |
| 7 | O | 246 | VAL | CA-C | -5.87 | 1.44 | 1.52 |
| 10 | U | 269 | HIS | CE1-NE2 | -5.87 | 1.26 | 1.32 |
| 4 | y | 675 | GLN | C-N | 5.87 | 1.41 | 1.33 |
| 20 | n | 645 | ILE | CA-CB | -5.87 | 1.46 | 1.54 |
| 6 | I | 314 | TYR | CA-C | -5.86 | 1.44 | 1.52 |
| 9 | T | 156 | MET | C-O | -5.86 | 1.17 | 1.24 |
| 12 | u | 630 | TRP | C-N | 5.86 | 1.42 | 1.33 |
| 13 | x | 1355 | LYS | CA-C | 5.86 | 1.60 | 1.52 |
| 20 | n | 237 | MET | C-N | 5.86 | 1.42 | 1.33 |
| 20 | n | 751 | TYR | CA-CB | 5.86 | 1.62 | 1.53 |
| 2 | 1 | 723 | ILE | N-CA | -5.86 | 1.38 | 1.46 |
| 5 | E | 517 | GLN | CA-C | -5.86 | 1.44 | 1.52 |
| 2 | Z | 824 | SER | CA-CB | 5.86 | 1.62 | 1.53 |
| 4 | y | 722 | LEU | C-N | 5.86 | 1.41 | 1.33 |
| 15 | i | 196 | ASP | CA-CB | 5.86 | 1.61 | 1.53 |
| 14 | a | 996 | LYS | CA-C | -5.86 | 1.45 | 1.52 |
| 4 | A | 638 | ASP | CA-CB | 5.86 | 1.65 | 1.53 |
| 4 | J | 804 | LEU | CA-C | -5.86 | 1.45 | 1.52 |
| 7 | M | 1150 | PHE | N-CA | -5.86 | 1.39 | 1.46 |
| 9 | S | 622 | THR | N-CA | -5.86 | 1.38 | 1.46 |
| 11 | X | 278 | GLU | CA-CB | 5.86 | 1.60 | 1.52 |
| 15 | i | 158 | PHE | CG-CD1 | 5.86 | 1.51 | 1.38 |
| 8 | P | 1602 | LEU | CA-CB | 5.86 | 1.62 | 1.53 |
| 9 | S | 240 | SER | C-N | 5.86 | 1.41 | 1.33 |
| 21 | q | 23 | ASP | CA-CB | 5.86 | 1.62 | 1.53 |
| 20 | g | 317 | LEU | CA-C | -5.86 | 1.45 | 1.52 |
| 6 | C | 462 | GLN | CA-C | -5.86 | 1.44 | 1.52 |
| 5 | E | 442 | THR | CA-C | 5.86 | 1.60 | 1.52 |
| 8 | P | 208 | ILE | C-N | -5.86 | 1.26 | 1.33 |
| 1 | Y | 362 | ASP | C-N | 5.86 | 1.42 | 1.33 |
| 16 | c | 271 | TRP | CA-CB | 5.86 | 1.62 | 1.53 |
| 16 | c | 408 | ASP | CA-C | -5.86 | 1.45 | 1.52 |
| 14 | a | 59 | CYS | CA-C | -5.86 | 1.45 | 1.53 |
| 14 | a | 645 | GLU | C-N | 5.86 | 1.40 | 1.33 |
| 4 | G | 772 | VAL | CA-CB | -5.86 | 1.46 | 1.54 |
| 7 | O | 771 | ARG | CA-CB | 5.86 | 1.62 | 1.53 |
| 7 | O | 943 | ARG | CD-NE | 5.86 | 1.54 | 1.46 |
| 14 | a | 583 | LEU | N-CA | -5.86 | 1.38 | 1.46 |
| 6 | F | 278 | GLU | N-CA | -5.85 | 1.39 | 1.46 |
| 20 | n | 968 | GLU | CA-C | -5.85 | 1.45 | 1.52 |
| 16 | c | 236 | LEU | C-N | 5.85 | 1.41 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | f | 467 | PHE | N-CA | -5.85 | 1.38 | 1.46 |
| 9 | Q | 25 | LEU | N-CA | -5.85 | 1.39 | 1.46 |
| 20 | g | 443 | TRP | CA-CB | 5.85 | 1.61 | 1.52 |
| 14 | a | 477 | GLN | N-CA | -5.85 | 1.37 | 1.46 |
| 14 | a | 846 | SER | C-N | 5.85 | 1.41 | 1.33 |
| 14 | a | 949 | LEU | C-N | 5.85 | 1.41 | 1.33 |
| 1 | 0 | 1405 | GLU | CA-CB | 5.85 | 1.63 | 1.53 |
| 9 | T | 614 | ARG | CA-C | 5.85 | 1.60 | 1.52 |
| 1 | 0 | 671 | LEU | N-CA | -5.85 | 1.39 | 1.46 |
| 7 | M | 616 | VAL | CA-CB | -5.85 | 1.46 | 1.54 |
| 8 | N | 1466 | TYR | CA-C | -5.85 | 1.45 | 1.52 |
| 7 | O | 488 | PHE | C-N | 5.85 | 1.42 | 1.34 |
| 8 | P | 1488 | SER | CA-CB | 5.85 | 1.62 | 1.53 |
| 2 | Z | 1210 | ALA | CA-C | -5.85 | 1.45 | 1.52 |
| 20 | g | 207 | LYS | N-CA | -5.85 | 1.39 | 1.46 |
| 2 | 1 | 1258 | GLN | CA-C | -5.85 | 1.45 | 1.52 |
| 9 | R | 358 | ALA | CA-C | -5.85 | 1.45 | 1.52 |
| 9 | T | 456 | ARG | CZ-NH1 | 5.85 | 1.41 | 1.32 |
| 1 | Y | 137 | ARG | CA-CB | 5.85 | 1.62 | 1.53 |
| 1 | Y | 171 | THR | C-N | 5.85 | 1.41 | 1.33 |
| 2 | Z | 947 | LEU | C-O | -5.85 | 1.17 | 1.24 |
| 4 | z | 669 | LEU | CA-C | 5.85 | 1.60 | 1.52 |
| 18 | l | 8 | HIS | CG-CD2 | 5.85 | 1.42 | 1.35 |
| 20 | n | 1044 | ARG | NE-CZ | 5.85 | 1.39 | 1.33 |
| 20 | g | 898 | ASP | CA-CB | 5.85 | 1.62 | 1.53 |
| 14 | a | 841 | ALA | N-CA | -5.85 | 1.39 | 1.46 |
| 7 | O | 541 | LEU | C-N | 5.85 | 1.41 | 1.33 |
| 1 | Y | 1316 | SER | N-CA | -5.85 | 1.38 | 1.46 |
| 14 | h | 11 | LEU | C-O | 5.85 | 1.32 | 1.24 |
| 5 | E | 314 | ASN | CA-C | 5.84 | 1.60 | 1.52 |
| 8 | N | 1486 | GLU | C-N | 5.84 | 1.41 | 1.33 |
| 8 | P | 1413 | ASN | C-O | -5.84 | 1.17 | 1.24 |
| 9 | R | 217 | ARG | NE-CZ | 5.84 | 1.39 | 1.33 |
| 1 | Y | 1015 | GLU | N-CA | -5.84 | 1.39 | 1.46 |
| 2 | Z | 751 | GLN | C-N | 5.84 | 1.41 | 1.33 |
| 15 | b | 172 | PHE | N-CA | 5.84 | 1.53 | 1.46 |
| 16 | c | 142 | ARG | CZ-NH2 | 5.84 | 1.41 | 1.33 |
| 20 | g | 140 | LEU | N-CA | -5.84 | 1.39 | 1.46 |
| 7 | O | 1372 | THR | N-CA | -5.84 | 1.38 | 1.46 |
| 9 | Q | 91 | GLN | CA-C | -5.84 | 1.45 | 1.52 |
| 9 | T | 281 | GLN | CA-CB | 5.84 | 1.62 | 1.53 |
| 1 | Y | 1454 | GLU | CA-CB | 5.84 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | i | 479 | LYS | N-CA | -5.84 | 1.39 | 1.46 |
| 17 | d | 23 | ARG | CD-NE | 5.84 | 1.54 | 1.46 |
| 14 | a | 631 | LEU | N-CA | 5.84 | 1.53 | 1.46 |
| 1 | 0 | 294 | TRP | NE1-CE2 | 5.84 | 1.43 | 1.37 |
| 2 | 1 | 229 | ASP | C-O | -5.84 | 1.17 | 1.24 |
| 7 | M | 571 | ASN | C-N | 5.84 | 1.41 | 1.33 |
| 8 | P | 947 | ASN | N-CA | -5.84 | 1.38 | 1.45 |
| 9 | Q | 536 | ASN | CA-C | -5.84 | 1.45 | 1.52 |
| 9 | S | 673 | PRO | N-CA | 5.84 | 1.53 | 1.47 |
| 1 | Y | 1158 | HIS | CA-CB | 5.84 | 1.62 | 1.53 |
| 20 | n | 679 | ASP | CA-C | 5.84 | 1.60 | 1.52 |
| 17 | d | 110 | HIS | CE1-NE2 | -5.84 | 1.26 | 1.32 |
| 8 | N | 756 | TRP | CA-CB | 5.84 | 1.65 | 1.54 |
| 8 | P | 839 | ILE | CA-C | -5.84 | 1.45 | 1.52 |
| 1 | Y | 1316 | SER | CA-C | -5.84 | 1.46 | 1.53 |
| 15 | i | 83 | THR | N-CA | -5.84 | 1.39 | 1.46 |
| 20 | n | 437 | TYR | N-CA | -5.84 | 1.38 | 1.46 |
| 20 | n | 646 | PHE | C-N | 5.84 | 1.41 | 1.34 |
| 19 | f | 674 | ALA | C-N | 5.84 | 1.41 | 1.33 |
| 1 | 0 | 1338 | ALA | CA-CB | 5.84 | 1.60 | 1.52 |
| 5 | H | 351 | GLN | CA-CB | 5.84 | 1.63 | 1.53 |
| 7 | M | 1490 | ARG | NE-CZ | 5.84 | 1.39 | 1.33 |
| 7 | O | 1169 | SER | CA-C | -5.84 | 1.44 | 1.52 |
| 2 | Z | 1162 | GLU | CA-C | -5.84 | 1.45 | 1.52 |
| 9 | Q | 590 | LEU | C-N | 5.84 | 1.42 | 1.33 |
| 16 | c | 440 | GLN | N-CA | -5.84 | 1.38 | 1.46 |
| 20 | g | 659 | PRO | CA-CB | 5.84 | 1.61 | 1.53 |
| 4 | A | 720 | ALA | CA-C | -5.83 | 1.44 | 1.52 |
| 9 | R | 234 | ILE | CA-CB | -5.83 | 1.48 | 1.54 |
| 9 | S | 543 | LYS | N-CA | -5.83 | 1.38 | 1.46 |
| 1 | Y | 438 | ALA | CA-C | -5.83 | 1.45 | 1.52 |
| 2 | Z | 967 | LEU | N-CA | -5.83 | 1.38 | 1.46 |
| 20 | n | 451 | ASN | CA-CB | 5.83 | 1.63 | 1.53 |
| 1 | 0 | 1148 | ALA | CA-CB | 5.83 | 1.62 | 1.53 |
| 12 | u | 531 | ILE | N-CA | -5.83 | 1.39 | 1.46 |
| 20 | n | 321 | GLN | CA-C | -5.83 | 1.44 | 1.52 |
| 14 | a | 400 | LYS | CA-CB | 5.83 | 1.61 | 1.53 |
| 2 | 1 | 1245 | MET | CA-CB | 5.83 | 1.63 | 1.53 |
| 7 | M | 1201 | LEU | C-N | 5.83 | 1.42 | 1.33 |
| 8 | P | 693 | MET | CA-CB | 5.83 | 1.62 | 1.53 |
| 8 | P | 1052 | LYS | CA-C | -5.83 | 1.45 | 1.52 |
| 9 | Q | 494 | TYR | CA-CB | 5.83 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | K | 533 | ILE | N-CA | -5.83 | 1.38 | 1.46 |
| 14 | h | 208 | LEU | N-CA | -5.83 | 1.38 | 1.45 |
| 20 | n | 668 | ASN | C-O | 5.83 | 1.30 | 1.24 |
| 20 | g | 1127 | ASN | CA-CB | 5.83 | 1.62 | 1.53 |
| 1 | 0 | 613 | GLY | CA-C | -5.83 | 1.43 | 1.52 |
| 2 | 1 | 591 | ALA | N-CA | -5.83 | 1.39 | 1.46 |
| 5 | B | 305 | LYS | CA-C | -5.83 | 1.44 | 1.53 |
| 7 | M | 79 | ASP | C-N | 5.83 | 1.41 | 1.33 |
| 8 | N | 962 | SER | CA-C | -5.83 | 1.45 | 1.52 |
| 10 | U | 318 | TYR | N-CA | -5.83 | 1.37 | 1.46 |
| 1 | Y | 626 | ASN | CA-C | -5.83 | 1.45 | 1.52 |
| 2 | Z | 1327 | ARG | CD-NE | 5.83 | 1.54 | 1.46 |
| 12 | u | 241 | THR | CA-C | -5.83 | 1.45 | 1.52 |
| 19 | f | 627 | THR | C-N | 5.83 | 1.41 | 1.33 |
| 1 | 0 | 128 | ASN | CA-CB | 5.83 | 1.62 | 1.53 |
| 2 | 1 | 1267 | ASN | CA-CB | 5.83 | 1.62 | 1.54 |
| 8 | P | 734 | SER | CA-CB | 5.83 | 1.62 | 1.53 |
| 16 | c | 309 | LEU | CA-CB | 5.83 | 1.63 | 1.53 |
| 14 | a | 58 | ASN | C-N | 5.83 | 1.40 | 1.33 |
| 1 | 0 | 1468 | TYR | C-N | 5.83 | 1.40 | 1.33 |
| 9 | R | 283 | LEU | CA-CB | 5.83 | 1.62 | 1.53 |
| 12 | u | 139 | ASP | C-N | 5.83 | 1.41 | 1.33 |
| 12 | v | 322 | GLY | C-N | 5.83 | 1.41 | 1.33 |
| 16 | j | 497 | LEU | C-N | 5.83 | 1.41 | 1.33 |
| 17 | k | 102 | VAL | C-N | 5.83 | 1.43 | 1.33 |
| 18 | l | 55 | ASP | CA-CB | 5.83 | 1.61 | 1.53 |
| 18 | e | 292 | LEU | CA-C | -5.83 | 1.45 | 1.52 |
| 7 | O | 897 | ASP | CA-C | -5.82 | 1.45 | 1.52 |
| 9 | T | 429 | THR | C-N | 5.82 | 1.41 | 1.33 |
| 14 | h | 939 | THR | CA-C | 5.82 | 1.59 | 1.53 |
| 9 | R | 823 | ARG | NE-CZ | 5.82 | 1.39 | 1.33 |
| 1 | 0 | 989 | GLN | N-CA | -5.82 | 1.38 | 1.46 |
| 8 | N | 817 | PRO | CA-C | 5.82 | 1.60 | 1.52 |
| 8 | P | 966 | GLY | CA-C | -5.82 | 1.43 | 1.51 |
| 18 | l | 130 | ASN | N-CA | -5.82 | 1.39 | 1.46 |
| 19 | m | 264 | TYR | C-N | 5.82 | 1.41 | 1.33 |
| 15 | b | 106 | ALA | C-N | 5.82 | 1.41 | 1.33 |
| 16 | c | 617 | PHE | CA-CB | 5.82 | 1.62 | 1.53 |
| 20 | g | 531 | LEU | CA-CB | 5.82 | 1.63 | 1.53 |
| 14 | a | 66 | GLU | CA-C | -5.82 | 1.45 | 1.52 |
| 9 | T | 508 | ILE | C-N | 5.82 | 1.41 | 1.33 |
| 1 | Y | 1270 | GLY | C-N | 5.82 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 1375 | GLY | CA-C | -5.82 | 1.44 | 1.51 |
| 19 | m | 148 | ILE | C-N | 5.82 | 1.42 | 1.33 |
| 6 | L | 460 | LEU | CA-CB | 5.82 | 1.62 | 1.53 |
| 8 | N | 664 | LEU | C-O | -5.82 | 1.16 | 1.24 |
| 7 | O | 243 | SER | CA-CB | 5.82 | 1.61 | 1.53 |
| 8 | P | 859 | ILE | CA-C | 5.82 | 1.60 | 1.52 |
| 1 | Y | 1259 | ALA | C-N | 5.82 | 1.41 | 1.33 |
| 12 | u | 125 | SER | CA-C | -5.82 | 1.45 | 1.52 |
| 20 | n | 240 | PRO | CA-CB | 5.82 | 1.61 | 1.53 |
| 16 | c | 463 | ARG | C-O | -5.82 | 1.17 | 1.24 |
| 20 | g | 1147 | THR | CA-CB | 5.82 | 1.63 | 1.53 |
| 18 | l | 15 | VAL | C-N | 5.82 | 1.41 | 1.33 |
| 20 | n | 412 | GLU | N-CA | -5.82 | 1.41 | 1.46 |
| 15 | b | 312 | LYS | CA-CB | 5.82 | 1.63 | 1.53 |
| 4 | J | 660 | LYS | CA-CB | 5.81 | 1.62 | 1.53 |
| 7 | O | 624 | ASP | CA-C | 5.81 | 1.59 | 1.52 |
| 7 | M | 758 | ASN | CA-CB | 5.81 | 1.63 | 1.53 |
| 9 | Q | 573 | HIS | CA-C | -5.81 | 1.44 | 1.52 |
| 13 | w | 1116 | ASN | C-N | 5.81 | 1.41 | 1.33 |
| 20 | n | 1025 | ASP | C-N | 5.81 | 1.42 | 1.33 |
| 19 | f | 186 | GLU | CA-CB | 5.81 | 1.62 | 1.53 |
| 20 | g | 277 | GLY | C-N | 5.81 | 1.41 | 1.33 |
| 20 | g | 565 | GLN | CA-CB | 5.81 | 1.62 | 1.53 |
| 14 | a | 989 | ALA | CA-C | -5.81 | 1.45 | 1.52 |
| 19 | m | 535 | ARG | CA-C | -5.81 | 1.44 | 1.52 |
| 16 | c | 232 | ASN | C-N | 5.81 | 1.41 | 1.33 |
| 1 | 0 | 442 | GLY | C-N | 5.81 | 1.40 | 1.33 |
| 7 | M | 1247 | ARG | NE-CZ | 5.81 | 1.39 | 1.33 |
| 8 | N | 985 | GLU | CA-C | -5.81 | 1.45 | 1.52 |
| 9 | T | 157 | LYS | CA-C | -5.81 | 1.45 | 1.52 |
| 10 | U | 308 | TYR | CA-CB | 5.81 | 1.61 | 1.53 |
| 19 | m | 472 | ALA | CA-C | -5.81 | 1.45 | 1.52 |
| 20 | n | 577 | TYR | CA-CB | 5.81 | 1.63 | 1.53 |
| 19 | f | 137 | LYS | C-N | 5.81 | 1.40 | 1.33 |
| 19 | f | 383 | PRO | C-N | 5.81 | 1.41 | 1.33 |
| 19 | f | 600 | TRP | NE1-CE2 | 5.81 | 1.43 | 1.37 |
| 4 | A | 664 | SER | CA-CB | 5.81 | 1.62 | 1.53 |
| 4 | G | 760 | SER | N-CA | -5.81 | 1.39 | 1.46 |
| 5 | H | 348 | ILE | CA-CB | 5.81 | 1.59 | 1.53 |
| 7 | M | 891 | LYS | N-CA | -5.81 | 1.38 | 1.46 |
| 8 | N | 1229 | LEU | N-CA | -5.81 | 1.38 | 1.46 |
| 9 | T | 412 | TYR | CA-CB | 5.81 | 1.63 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | n | 347 | PHE | C-N | 5.81 | 1.41 | 1.33 |
| 20 | g | 719 | ASN | CA-CB | 5.81 | 1.62 | 1.53 |
| 20 | g | 950 | ASN | N-CA | -5.81 | 1.38 | 1.46 |
| 7 | M | 19 | GLU | CA-CB | 5.81 | 1.61 | 1.53 |
| 19 | m | 620 | LEU | CA-CB | 5.81 | 1.62 | 1.53 |
| 1 | 0 | 1179 | THR | CA-C | 5.80 | 1.59 | 1.52 |
| 7 | O | 1300 | LEU | C-N | 5.80 | 1.41 | 1.33 |
| 9 | Q | 264 | LYS | C-N | 5.80 | 1.42 | 1.33 |
| 10 | W | 339 | LEU | CA-C | -5.80 | 1.45 | 1.52 |
| 16 | j | 657 | CYS | C-N | 5.80 | 1.41 | 1.33 |
| 17 | k | 72 | SER | C-N | 5.80 | 1.41 | 1.33 |
| 17 | d | 201 | GLU | C-N | 5.80 | 1.42 | 1.33 |
| 14 | a | 189 | VAL | N-CA | -5.80 | 1.39 | 1.46 |
| 20 | g | 935 | GLU | C-N | 5.80 | 1.41 | 1.33 |
| 7 | O | 1303 | LEU | CA-C | -5.80 | 1.45 | 1.52 |
| 8 | P | 982 | ILE | C-N | 5.80 | 1.40 | 1.33 |
| 9 | Q | 130 | ASN | CA-C | -5.80 | 1.45 | 1.52 |
| 11 | X | 275 | GLY | N-CA | -5.80 | 1.36 | 1.45 |
| 17 | d | 91 | GLN | CA-CB | 5.80 | 1.60 | 1.52 |
| 14 | a | 511 | ARG | C-N | 5.80 | 1.41 | 1.33 |
| 8 | N | 470 | LEU | C-N | 5.80 | 1.41 | 1.33 |
| 9 | Q | 503 | ALA | C-N | 5.80 | 1.40 | 1.33 |
| 1 | Y | 1010 | LEU | N-CA | -5.80 | 1.39 | 1.46 |
| 2 | Z | 346 | GLU | CA-CB | 5.80 | 1.61 | 1.52 |
| 21 | p | 19 | LYS | CA-CB | 5.80 | 1.62 | 1.53 |
| 1 | 0 | 833 | SER | CA-C | 5.80 | 1.60 | 1.52 |
| 9 | T | 781 | CYS | N-CA | 5.80 | 1.53 | 1.46 |
| 16 | j | 564 | SER | N-CA | -5.80 | 1.42 | 1.47 |
| 7 | M | 58 | LEU | C-N | 5.80 | 1.42 | 1.33 |
| 9 | R | 493 | ASP | CA-CB | 5.80 | 1.62 | 1.53 |
| 14 | h | 811 | LEU | N-CA | -5.80 | 1.38 | 1.46 |
| 19 | m | 173 | ASP | CA-C | -5.80 | 1.44 | 1.52 |
| 7 | O | 10 | THR | C-N | 5.79 | 1.41 | 1.33 |
| 7 | O | 1343 | ILE | C-N | 5.79 | 1.42 | 1.33 |
| 1 | Y | 377 | ILE | N-CA | -5.79 | 1.39 | 1.46 |
| 12 | u | 261 | GLU | CA-C | -5.79 | 1.45 | 1.52 |
| 8 | N | 1560 | MET | N-CA | -5.79 | 1.38 | 1.46 |
| 7 | O | 167 | ILE | N-CA | -5.79 | 1.38 | 1.46 |
| 8 | P | 468 | SER | CA-C | -5.79 | 1.45 | 1.53 |
| 2 | Z | 185 | ILE | C-N | 5.79 | 1.41 | 1.33 |
| 12 | v | 418 | ALA | N-CA | -5.79 | 1.38 | 1.45 |
| 14 | h | 850 | GLU | N-CA | -5.79 | 1.38 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | t | 73 | LYS | CA-CB | 5.79 | 1.61 | 1.53 |
| 16 | c | 265 | HIS | C-O | -5.79 | 1.16 | 1.24 |
| 4 | G | 789 | GLU | CA-C | -5.79 | 1.45 | 1.52 |
| 8 | P | 106 | ARG | CD-NE | 5.79 | 1.54 | 1.46 |
| 9 | T | 713 | ILE | CA-C | -5.79 | 1.45 | 1.52 |
| 2 | Z | 847 | LEU | CA-C | 5.79 | 1.60 | 1.52 |
| 19 | f | 438 | GLU | CA-C | -5.79 | 1.45 | 1.52 |
| 8 | N | 1532 | THR | C-N | 5.79 | 1.40 | 1.33 |
| 9 | Q | 603 | VAL | C-N | 5.79 | 1.41 | 1.33 |
| 19 | m | 163 | ARG | CZ-NH2 | 5.79 | 1.41 | 1.33 |
| 5 | B | 363 | GLN | CA-C | -5.79 | 1.45 | 1.52 |
| 9 | Q | 249 | ARG | CD-NE | 5.79 | 1.54 | 1.46 |
| 9 | R | 372 | LYS | C-N | 5.79 | 1.41 | 1.33 |
| 2 | Z | 946 | GLU | CA-CB | 5.79 | 1.66 | 1.54 |
| 14 | h | 277 | GLY | C-N | 5.79 | 1.41 | 1.33 |
| 19 | m | 264 | TYR | CA-CB | 5.79 | 1.63 | 1.53 |
| 15 | i | 238 | LYS | C-N | 5.79 | 1.40 | 1.33 |
| 21 | o | 67 | SER | C-N | 5.79 | 1.41 | 1.33 |
| 7 | O | 1566 | ASP | CA-C | -5.79 | 1.45 | 1.52 |
| 15 | i | 675 | PHE | C-N | 5.79 | 1.41 | 1.33 |
| 19 | f | 690 | PHE | CA-CB | 5.79 | 1.61 | 1.53 |
| 5 | K | 315 | LYS | CA-CB | 5.78 | 1.62 | 1.53 |
| 5 | K | 410 | LYS | C-N | 5.78 | 1.42 | 1.34 |
| 7 | M | 251 | ASP | CA-C | -5.78 | 1.45 | 1.52 |
| 8 | P | 1090 | THR | CA-C | -5.78 | 1.45 | 1.52 |
| 17 | k | 289 | TRP | CA-CB | -5.78 | 1.45 | 1.53 |
| 7 | M | 1412 | TYR | N-CA | 5.78 | 1.53 | 1.46 |
| 16 | j | 465 | PHE | C-N | 5.78 | 1.41 | 1.33 |
| 19 | m | 376 | SER | C-N | 5.78 | 1.40 | 1.33 |
| 20 | g | 75 | ASP | CA-CB | 5.78 | 1.62 | 1.53 |
| 1 | 0 | 841 | TYR | C-N | 5.78 | 1.41 | 1.33 |
| 2 | 1 | 97 | PHE | C-N | 5.78 | 1.41 | 1.33 |
| 4 | J | 719 | GLU | C-N | 5.78 | 1.42 | 1.33 |
| 7 | M | 647 | THR | CA-CB | -5.78 | 1.45 | 1.54 |
| 7 | M | 1106 | PHE | C-O | -5.78 | 1.17 | 1.24 |
| 7 | O | 1119 | PHE | N-CA | -5.78 | 1.38 | 1.46 |
| 8 | P | 212 | TRP | NE1-CE2 | -5.78 | 1.31 | 1.37 |
| 12 | u | 153 | MET | C-N | 5.78 | 1.42 | 1.33 |
| 15 | i | 215 | SER | CA-CB | 5.78 | 1.62 | 1.53 |
| 20 | n | 251 | PRO | N-CD | 5.78 | 1.55 | 1.47 |
| 16 | c | 429 | GLU | C-N | 5.78 | 1.41 | 1.33 |
| 18 | e | 21 | GLY | N-CA | -5.78 | 1.37 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | P | 520 | ILE | CA-C | -5.78 | 1.46 | 1.52 |
| 9 | S | 543 | LYS | C-N | 5.78 | 1.41 | 1.33 |
| 1 | Y | 634 | SER | CA-C | -5.78 | 1.45 | 1.52 |
| 16 | j | 207 | TYR | CA-C | 5.78 | 1.60 | 1.53 |
| 14 | a | 861 | LEU | C-N | 5.78 | 1.41 | 1.33 |
| 6 | F | 334 | SER | CA-CB | 5.78 | 1.62 | 1.53 |
| 7 | M | 493 | PRO | C-N | 5.78 | 1.41 | 1.33 |
| 14 | h | 335 | VAL | CA-CB | -5.78 | 1.47 | 1.54 |
| 17 | d | 41 | GLU | CA-CB | 5.78 | 1.62 | 1.53 |
| 20 | g | 180 | SER | CA-CB | 5.78 | 1.61 | 1.53 |
| 2 | 1 | 244 | LEU | CA-CB | 5.78 | 1.62 | 1.53 |
| 5 | E | 469 | ARG | CD-NE | 5.78 | 1.54 | 1.46 |
| 7 | O | 443 | ILE | C-N | 5.78 | 1.42 | 1.33 |
| 7 | O | 618 | SER | C-N | 5.78 | 1.41 | 1.33 |
| 7 | O | 1496 | ASP | CA-C | -5.78 | 1.45 | 1.52 |
| 18 | l | 96 | ARG | NE-CZ | 5.78 | 1.39 | 1.33 |
| 16 | c | 321 | LEU | C-N | 5.78 | 1.40 | 1.33 |
| 19 | f | 694 | VAL | CA-C | -5.78 | 1.45 | 1.52 |
| 20 | g | 311 | ASN | C-N | 5.78 | 1.42 | 1.33 |
| 6 | C | 273 | ILE | CA-CB | -5.77 | 1.47 | 1.54 |
| 7 | O | 1171 | SER | N-CA | -5.77 | 1.38 | 1.46 |
| 8 | P | 1210 | LEU | CA-C | -5.77 | 1.45 | 1.52 |
| 9 | S | 729 | ASN | CA-CB | 5.77 | 1.62 | 1.53 |
| 13 | w | 1436 | VAL | C-N | 5.77 | 1.41 | 1.33 |
| 14 | h | 407 | GLY | C-N | 5.77 | 1.41 | 1.33 |
| 15 | i | 661 | HIS | N-CA | 5.77 | 1.53 | 1.46 |
| 20 | n | 509 | ALA | CA-C | -5.77 | 1.45 | 1.52 |
| 20 | g | 213 | ASN | CA-CB | 5.77 | 1.62 | 1.53 |
| 17 | d | 8 | HIS | ND1-CE1 | 5.77 | 1.38 | 1.32 |
| 5 | K | 300 | ASP | N-CA | -5.77 | 1.38 | 1.45 |
| 5 | K | 332 | GLN | N-CA | 5.77 | 1.53 | 1.46 |
| 9 | R | 689 | ALA | N-CA | -5.77 | 1.39 | 1.46 |
| 9 | T | 125 | ILE | CA-C | -5.77 | 1.45 | 1.52 |
| 18 | l | 322 | ALA | CA-C | -5.77 | 1.45 | 1.52 |
| 2 | 1 | 1353 | SER | C-N | 5.77 | 1.40 | 1.33 |
| 4 | A | 695 | GLN | CA-C | -5.77 | 1.45 | 1.52 |
| 8 | N | 1072 | TYR | CA-CB | 5.77 | 1.62 | 1.53 |
| 7 | O | 447 | ALA | CA-C | -5.77 | 1.44 | 1.52 |
| 1 | Y | 313 | CYS | N-CA | 5.77 | 1.57 | 1.46 |
| 16 | c | 591 | GLU | N-CA | -5.77 | 1.39 | 1.46 |
| 14 | a | 928 | ALA | C-N | 5.77 | 1.41 | 1.33 |
| 1 | 0 | 514 | SER | CA-C | -5.77 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 1260 | SER | CA-C | -5.77 | 1.45 | 1.52 |
| 9 | S | 722 | SER | C-N | 5.76 | 1.41 | 1.33 |
| 2 | Z | 1366 | ILE | CA-C | -5.76 | 1.45 | 1.52 |
| 19 | m | 528 | HIS | CG-CD2 | 5.76 | 1.42 | 1.35 |
| 16 | c | 182 | LYS | CA-C | -5.76 | 1.44 | 1.52 |
| 1 | 0 | 782 | ARG | CD-NE | 5.76 | 1.54 | 1.46 |
| 8 | N | 1233 | PHE | CA-C | -5.76 | 1.45 | 1.52 |
| 9 | S | 554 | VAL | CA-C | 5.76 | 1.61 | 1.52 |
| 12 | v | 699 | GLU | C-N | 5.76 | 1.41 | 1.33 |
| 8 | P | 1254 | ARG | C-N | 5.76 | 1.41 | 1.33 |
| 9 | Q | 224 | ASN | CA-CB | 5.76 | 1.62 | 1.53 |
| 21 | o | 23 | ASP | CA-C | 5.76 | 1.60 | 1.52 |
| 19 | f | 335 | HIS | CE1-NE2 | -5.76 | 1.26 | 1.32 |
| 1 | 0 | 1065 | GLU | CA-CB | 5.76 | 1.62 | 1.53 |
| 8 | P | 340 | SER | CA-CB | 5.76 | 1.63 | 1.53 |
| 12 | v | 70 | HIS | CA-C | -5.76 | 1.45 | 1.52 |
| 14 | h | 482 | SER | C-N | 5.76 | 1.41 | 1.33 |
| 21 | o | 32 | LEU | CA-CB | 5.76 | 1.62 | 1.53 |
| 21 | t | 36 | GLN | N-CA | -5.76 | 1.37 | 1.45 |
| 15 | b | 524 | SER | N-CA | 5.76 | 1.53 | 1.46 |
| 20 | g | 293 | GLN | CA-C | -5.76 | 1.45 | 1.52 |
| 20 | g | 657 | LEU | CA-C | -5.76 | 1.45 | 1.52 |
| 7 | M | 1157 | TRP | CA-C | -5.76 | 1.45 | 1.52 |
| 9 | S | 722 | SER | CA-C | 5.76 | 1.60 | 1.52 |
| 2 | Z | 624 | LEU | CA-C | -5.76 | 1.46 | 1.52 |
| 8 | N | 1213 | THR | N-CA | -5.76 | 1.38 | 1.46 |
| 8 | P | 273 | LEU | C-N | 5.76 | 1.40 | 1.34 |
| 9 | Q | 221 | GLN | N-CA | 5.76 | 1.53 | 1.46 |
| 9 | R | 270 | ILE | N-CA | -5.76 | 1.38 | 1.46 |
| 12 | v | 447 | PHE | N-CA | -5.76 | 1.39 | 1.46 |
| 14 | h | 139 | PHE | CA-C | -5.76 | 1.45 | 1.52 |
| 14 | a | 731 | ASN | CA-C | -5.76 | 1.47 | 1.53 |
| 9 | Q | 617 | LYS | N-CA | -5.75 | 1.39 | 1.46 |
| 12 | v | 70 | HIS | CB-CG | 5.75 | 1.58 | 1.50 |
| 15 | i | 607 | ILE | C-N | 5.75 | 1.40 | 1.34 |
| 20 | g | 821 | LEU | CA-CB | 5.75 | 1.63 | 1.54 |
| 2 | 1 | 906 | ALA | CA-C | -5.75 | 1.45 | 1.52 |
| 5 | K | 411 | ARG | CD-NE | 5.75 | 1.54 | 1.46 |
| 7 | M | 662 | PRO | C-N | 5.75 | 1.40 | 1.33 |
| 7 | M | 818 | TYR | CA-CB | 5.75 | 1.62 | 1.53 |
| 7 | M | 1085 | LYS | C-N | 5.75 | 1.41 | 1.33 |
| 9 | Q | 608 | GLN | CA-C | -5.75 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 176 | PHE | CA-CB | 5.75 | 1.61 | 1.53 |
| 2 | Z | 956 | LYS | CA-CB | 5.75 | 1.62 | 1.53 |
| 12 | u | 659 | LYS | C-N | 5.75 | 1.42 | 1.33 |
| 19 | m | 295 | GLN | C-N | 5.75 | 1.41 | 1.33 |
| 19 | m | 447 | PHE | CA-CB | 5.75 | 1.62 | 1.54 |
| 15 | b | 613 | ASP | CA-CB | 5.75 | 1.63 | 1.53 |
| 7 | O | 324 | ILE | C-N | 5.75 | 1.42 | 1.33 |
| 7 | O | 1574 | LYS | CA-C | -5.75 | 1.45 | 1.52 |
| 8 | P | 1186 | GLU | CG-CD | 5.75 | 1.66 | 1.52 |
| 9 | Q | 814 | MET | CA-C | -5.75 | 1.45 | 1.52 |
| 10 | W | 356 | LEU | CA-C | -5.75 | 1.45 | 1.52 |
| 2 | Z | 97 | PHE | CG-CD2 | 5.75 | 1.50 | 1.38 |
| 16 | j | 548 | TYR | N-CA | 5.75 | 1.53 | 1.45 |
| 18 | e | 89 | ASP | CA-CB | 5.75 | 1.63 | 1.53 |
| 7 | O | 1565 | PHE | CA-C | -5.75 | 1.46 | 1.53 |
| 14 | h | 602 | ILE | N-CA | -5.75 | 1.39 | 1.46 |
| 20 | n | 1121 | GLU | C-N | 5.75 | 1.41 | 1.33 |
| 1 | 0 | 706 | GLY | N-CA | 5.75 | 1.49 | 1.44 |
| 1 | Y | 1303 | SER | CA-C | 5.75 | 1.60 | 1.52 |
| 14 | h | 1003 | VAL | CA-CB | 5.75 | 1.62 | 1.54 |
| 20 | n | 369 | ASP | CA-C | -5.75 | 1.46 | 1.53 |
| 21 | p | 42 | ALA | C-O | -5.75 | 1.17 | 1.24 |
| 15 | b | 497 | ARG | CD-NE | 5.75 | 1.54 | 1.46 |
| 14 | a | 841 | ALA | CA-C | -5.75 | 1.45 | 1.52 |
| 2 | 1 | 431 | ARG | CD-NE | 5.75 | 1.54 | 1.46 |
| 8 | P | 346 | ILE | CA-C | -5.75 | 1.44 | 1.52 |
| 8 | P | 393 | THR | C-N | 5.75 | 1.43 | 1.33 |
| 10 | U | 343 | VAL | C-N | 5.75 | 1.41 | 1.33 |
| 12 | u | 214 | SER | CA-CB | 5.75 | 1.62 | 1.53 |
| 20 | g | 430 | ASN | CA-C | -5.75 | 1.45 | 1.52 |
| 12 | v | 634 | ILE | N-CA | -5.75 | 1.39 | 1.46 |
| 18 | l | 183 | LEU | N-CA | -5.75 | 1.39 | 1.46 |
| 16 | c | 394 | ILE | C-N | 5.75 | 1.42 | 1.33 |
| 7 | M | 188 | ARG | CA-C | -5.74 | 1.45 | 1.52 |
| 17 | k | 62 | ALA | CA-C | -5.74 | 1.45 | 1.53 |
| 21 | p | 49 | LEU | C-N | 5.74 | 1.41 | 1.33 |
| 20 | g | 210 | LEU | CA-C | -5.74 | 1.45 | 1.52 |
| 8 | N | 1392 | PHE | CA-CB | 5.74 | 1.62 | 1.53 |
| 1 | Y | 894 | ASN | N-CA | -5.74 | 1.39 | 1.46 |
| 1 | 0 | 1229 | LEU | CA-C | -5.74 | 1.44 | 1.52 |
| 5 | E | 377 | ASN | CA-CB | 5.74 | 1.62 | 1.53 |
| 4 | G | 811 | SER | C-N | 5.74 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 682 | ALA | C-N | 5.74 | 1.41 | 1.33 |
| 7 | M | 72 | PHE | CA-C | -5.74 | 1.44 | 1.52 |
| 17 | k | 31 | LYS | CA-CB | 5.74 | 1.61 | 1.53 |
| 2 | 1 | 230 | ILE | CA-C | -5.74 | 1.47 | 1.53 |
| 9 | R | 807 | LYS | CA-C | -5.74 | 1.44 | 1.52 |
| 16 | j | 532 | ILE | CA-C | -5.74 | 1.46 | 1.52 |
| 18 | l | 298 | SER | CA-C | -5.74 | 1.45 | 1.52 |
| 5 | B | 467 | LYS | C-N | 5.74 | 1.41 | 1.33 |
| 7 | M | 458 | GLU | CA-CB | 5.74 | 1.61 | 1.53 |
| 8 | N | 780 | HIS | ND1-CE1 | 5.74 | 1.38 | 1.32 |
| 8 | P | 574 | HIS | CB-CG | 5.74 | 1.58 | 1.50 |
| 11 | V | 391 | ALA | C-N | 5.74 | 1.41 | 1.33 |
| 14 | h | 203 | SER | CA-CB | 5.74 | 1.59 | 1.53 |
| 14 | a | 444 | ALA | C-N | 5.74 | 1.41 | 1.33 |
| 2 | 1 | 875 | ILE | CA-CB | -5.73 | 1.48 | 1.54 |
| 6 | L | 291 | SER | C-N | 5.73 | 1.41 | 1.33 |
| 9 | Q | 422 | ARG | CA-C | -5.73 | 1.45 | 1.52 |
| 15 | b | 255 | ARG | CA-C | -5.73 | 1.48 | 1.52 |
| 16 | c | 150 | PHE | CA-CB | 5.73 | 1.64 | 1.53 |
| 1 | 0 | 1171 | GLU | CA-C | 5.73 | 1.60 | 1.52 |
| 4 | A | 810 | ASN | C-N | 5.73 | 1.41 | 1.33 |
| 7 | M | 681 | LYS | CA-CB | 5.73 | 1.61 | 1.53 |
| 7 | M | 767 | ILE | CA-C | -5.73 | 1.45 | 1.52 |
| 8 | P | 1233 | PHE | CA-CB | 5.73 | 1.62 | 1.53 |
| 9 | T | 778 | THR | CB-OG1 | -5.73 | 1.34 | 1.43 |
| 13 | x | 1122 | ILE | CA-C | -5.73 | 1.46 | 1.52 |
| 4 | A | 773 | SER | CA-CB | -5.73 | 1.44 | 1.53 |
| 7 | M | 1118 | ARG | N-CA | -5.73 | 1.39 | 1.46 |
| 8 | N | 968 | SER | CA-C | -5.73 | 1.45 | 1.52 |
| 8 | P | 1615 | ARG | CD-NE | 5.73 | 1.54 | 1.46 |
| 9 | T | 743 | ASP | CA-C | -5.73 | 1.45 | 1.52 |
| 20 | n | 564 | PHE | N-CA | -5.73 | 1.39 | 1.46 |
| 7 | M | 1388 | CYS | CA-CB | 5.73 | 1.62 | 1.53 |
| 21 | q | 75 | HIS | CB-CG | 5.73 | 1.58 | 1.50 |
| 19 | f | 537 | PHE | N-CA | 5.73 | 1.53 | 1.46 |
| 7 | M | 1481 | LYS | CA-CB | 5.73 | 1.62 | 1.53 |
| 12 | u | 180 | ASN | CA-C | -5.73 | 1.45 | 1.52 |
| 13 | w | 1268 | ILE | N-CA | 5.73 | 1.57 | 1.46 |
| 4 | z | 689 | SER | C-O | 5.73 | 1.30 | 1.24 |
| 19 | m | 622 | GLY | C-N | 5.73 | 1.41 | 1.33 |
| 1 | 0 | 1479 | ILE | CA-C | -5.73 | 1.45 | 1.52 |
| 2 | 1 | 364 | ARG | N-CA | -5.73 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | A | 645 | THR | N-CA | -5.73 | 1.39 | 1.46 |
| 9 | Q | 95 | PHE | C-N | 5.73 | 1.41 | 1.33 |
| 12 | u | 448 | GLN | CA-CB | 5.73 | 1.63 | 1.53 |
| 2 | 1 | 650 | LYS | CA-C | -5.72 | 1.45 | 1.52 |
| 7 | M | 135 | ILE | CA-C | 5.72 | 1.58 | 1.52 |
| 7 | O | 1211 | GLU | CA-C | -5.72 | 1.45 | 1.52 |
| 9 | T | 25 | LEU | C-O | 5.72 | 1.30 | 1.24 |
| 13 | w | 1310 | VAL | CA-CB | -5.72 | 1.47 | 1.54 |
| 20 | n | 1025 | ASP | N-CA | -5.72 | 1.39 | 1.46 |
| 20 | n | 1028 | LEU | CA-C | 5.72 | 1.60 | 1.52 |
| 20 | g | 889 | GLN | N-CA | 5.72 | 1.53 | 1.46 |
| 2 | 1 | 1110 | GLU | CA-C | -5.72 | 1.45 | 1.52 |
| 8 | N | 1519 | CYS | C-N | 5.72 | 1.41 | 1.33 |
| 7 | O | 120 | ILE | CA-C | -5.72 | 1.46 | 1.52 |
| 8 | P | 459 | ASP | C-N | 5.72 | 1.41 | 1.33 |
| 8 | P | 668 | TYR | C-N | 5.72 | 1.41 | 1.33 |
| 15 | i | 732 | ARG | CD-NE | 5.72 | 1.54 | 1.46 |
| 7 | M | 351 | HIS | C-N | 5.72 | 1.37 | 1.33 |
| 7 | M | 1211 | GLU | CA-CB | 5.72 | 1.64 | 1.53 |
| 15 | b | 102 | LYS | CA-CB | 5.72 | 1.63 | 1.54 |
| 16 | c | 143 | ARG | CD-NE | 5.72 | 1.54 | 1.46 |
| 20 | g | 177 | ASP | CA-C | -5.72 | 1.45 | 1.52 |
| 2 | 1 | 284 | TRP | N-CA | -5.72 | 1.39 | 1.46 |
| 7 | M | 1507 | ASN | N-CA | 5.72 | 1.53 | 1.46 |
| 9 | T | 431 | SER | N-CA | -5.72 | 1.39 | 1.45 |
| 15 | i | 501 | LYS | N-CA | -5.72 | 1.38 | 1.46 |
| 16 | j | 144 | PHE | CA-CB | 5.72 | 1.61 | 1.53 |
| 20 | g | 479 | VAL | CA-CB | -5.72 | 1.47 | 1.54 |
| 9 | S | 774 | LEU | CA-CB | 5.72 | 1.63 | 1.53 |
| 12 | u | 408 | LEU | C-N | 5.72 | 1.40 | 1.33 |
| 14 | h | 191 | GLY | C-N | 5.72 | 1.41 | 1.33 |
| 15 | b | 314 | SER | N-CA | -5.72 | 1.39 | 1.46 |
| 7 | M | 1611 | VAL | CA-CB | 5.72 | 1.62 | 1.54 |
| 7 | O | 963 | ASN | CA-CB | 5.72 | 1.63 | 1.53 |
| 4 | y | 710 | PHE | CA-C | -5.72 | 1.45 | 1.52 |
| 16 | j | 211 | SER | N-CA | -5.72 | 1.39 | 1.46 |
| 7 | M | 544 | TYR | C-N | 5.71 | 1.41 | 1.33 |
| 8 | P | 973 | THR | CA-C | -5.71 | 1.48 | 1.53 |
| 9 | R | 545 | PHE | CA-C | -5.71 | 1.45 | 1.52 |
| 2 | Z | 883 | TYR | C-N | 5.71 | 1.41 | 1.33 |
| 12 | u | 244 | ILE | C-N | 5.71 | 1.41 | 1.33 |
| 12 | u | 326 | LEU | C-N | 5.71 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 12 | v | 386 | PHE | C-N | 5.71 | 1.41 | 1.33 |
| 14 | h | 58 | ASN | CA-CB | 5.71 | 1.62 | 1.53 |
| 15 | i | 525 | ILE | C-O | -5.71 | 1.18 | 1.24 |
| 14 | a | 152 | LEU | N-CA | -5.71 | 1.39 | 1.46 |
| 14 | a | 434 | MET | CA-C | -5.71 | 1.45 | 1.52 |
| 1 | 0 | 1109 | PHE | C-N | 5.71 | 1.41 | 1.33 |
| 7 | O | 893 | HIS | CE1-NE2 | -5.71 | 1.26 | 1.32 |
| 14 | h | 936 | TYR | N-CA | -5.71 | 1.38 | 1.45 |
| 20 | g | 1024 | VAL | C-N | 5.71 | 1.41 | 1.33 |
| 2 | 1 | 1212 | PRO | N-CD | 5.71 | 1.55 | 1.47 |
| 4 | J | 687 | GLU | N-CA | -5.71 | 1.39 | 1.46 |
| 1 | Y | 617 | ALA | C-O | -5.71 | 1.17 | 1.24 |
| 2 | Z | 623 | SER | N-CA | -5.71 | 1.38 | 1.46 |
| 12 | v | 181 | ASP | C-N | 5.71 | 1.41 | 1.33 |
| 14 | h | 451 | ARG | CD-NE | 5.71 | 1.54 | 1.46 |
| 16 | j | 490 | SER | CA-C | 5.71 | 1.60 | 1.52 |
| 21 | t | 26 | THR | N-CA | -5.71 | 1.39 | 1.46 |
| 19 | f | 459 | LYS | CA-CB | 5.71 | 1.62 | 1.53 |
| 9 | Q | 96 | LEU | N-CA | -5.71 | 1.39 | 1.46 |
| 9 | Q | 771 | ILE | CA-CB | -5.71 | 1.50 | 1.53 |
| 20 | n | 316 | ILE | N-CA | -5.71 | 1.39 | 1.46 |
| 20 | n | 349 | SER | C-N | 5.71 | 1.41 | 1.33 |
| 21 | p | 29 | LYS | C-N | 5.71 | 1.41 | 1.33 |
| 6 | C | 284 | ILE | C-N | 5.71 | 1.41 | 1.33 |
| 9 | Q | 293 | ASN | CA-C | -5.71 | 1.45 | 1.52 |
| 14 | h | 1004 | ILE | CA-C | -5.71 | 1.45 | 1.52 |
| 20 | n | 1046 | VAL | CA-CB | -5.71 | 1.47 | 1.54 |
| 2 | 1 | 1063 | LEU | CA-CB | 5.71 | 1.62 | 1.53 |
| 6 | C | 437 | ALA | CA-C | -5.71 | 1.45 | 1.52 |
| 5 | E | 313 | TYR | CA-CB | 5.71 | 1.60 | 1.52 |
| 8 | P | 988 | ILE | C-N | 5.71 | 1.41 | 1.33 |
| 9 | Q | 595 | ARG | C-N | 5.71 | 1.42 | 1.33 |
| 9 | R | 92 | THR | N-CA | -5.71 | 1.39 | 1.46 |
| 2 | Z | 811 | LEU | CA-CB | 5.71 | 1.62 | 1.53 |
| 21 | r | 41 | ILE | N-CA | -5.71 | 1.39 | 1.46 |
| 15 | b | 653 | ILE | C-N | 5.71 | 1.40 | 1.33 |
| 20 | g | 297 | LEU | C-N | -5.71 | 1.25 | 1.33 |
| 20 | g | 604 | ILE | CA-C | -5.71 | 1.46 | 1.52 |
| 8 | P | 87 | PRO | C-N | 5.71 | 1.41 | 1.33 |
| 12 | v | 26 | ILE | CA-C | -5.71 | 1.45 | 1.52 |
| 18 | e | 97 | ARG | CD-NE | 5.71 | 1.54 | 1.46 |
| 1 | 0 | 240 | LEU | CA-C | -5.70 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 789 | ASP | CA-C | -5.70 | 1.45 | 1.52 |
| 5 | B | 467 | LYS | N-CA | -5.70 | 1.39 | 1.46 |
| 4 | G | 810 | ASN | C-N | 5.70 | 1.41 | 1.33 |
| 7 | O | 1026 | PHE | CA-C | -5.70 | 1.45 | 1.52 |
| 9 | Q | 690 | ARG | CA-CB | 5.70 | 1.62 | 1.53 |
| 1 | Y | 1348 | ARG | CZ-NH2 | 5.70 | 1.40 | 1.33 |
| 2 | Z | 1178 | ARG | NE-CZ | 5.70 | 1.39 | 1.33 |
| 12 | u | 87 | GLU | N-CA | -5.70 | 1.38 | 1.46 |
| 14 | h | 117 | LEU | N-CA | 5.70 | 1.53 | 1.46 |
| 15 | i | 259 | SER | CA-CB | 5.70 | 1.62 | 1.54 |
| 20 | g | 260 | ILE | C-N | 5.70 | 1.41 | 1.33 |
| 20 | g | 296 | GLN | C-N | 5.70 | 1.41 | 1.33 |
| 20 | g | 831 | LEU | CA-CB | 5.70 | 1.60 | 1.53 |
| 8 | N | 811 | ASP | CA-C | -5.70 | 1.45 | 1.52 |
| 7 | O | 1532 | ARG | C-N | 5.70 | 1.41 | 1.33 |
| 1 | 0 | 580 | VAL | C-O | 5.70 | 1.28 | 1.23 |
| 4 | J | 803 | ALA | N-CA | -5.70 | 1.39 | 1.46 |
| 8 | N | 1255 | ILE | C-N | 5.70 | 1.41 | 1.33 |
| 9 | R | 577 | ARG | NE-CZ | 5.70 | 1.39 | 1.33 |
| 20 | n | 1067 | ASP | CA-CB | 5.70 | 1.63 | 1.53 |
| 16 | c | 170 | VAL | C-N | 5.70 | 1.40 | 1.33 |
| 7 | O | 1655 | SER | CA-C | -5.70 | 1.45 | 1.52 |
| 9 | T | 583 | THR | CA-CB | 5.70 | 1.61 | 1.53 |
| 1 | Y | 914 | TYR | CA-C | -5.70 | 1.45 | 1.52 |
| 1 | Y | 1048 | LYS | C-N | 5.70 | 1.41 | 1.33 |
| 14 | h | 913 | ILE | CA-CB | 5.70 | 1.60 | 1.54 |
| 19 | m | 449 | LEU | CA-CB | 5.70 | 1.62 | 1.53 |
| 20 | g | 944 | LEU | N-CA | -5.70 | 1.38 | 1.46 |
| 1 | 0 | 1299 | GLY | C-N | 5.70 | 1.41 | 1.33 |
| 8 | P | 784 | THR | CA-C | -5.70 | 1.45 | 1.52 |
| 2 | 1 | 708 | ARG | CA-C | -5.70 | 1.45 | 1.52 |
| 4 | A | 649 | THR | CA-C | 5.70 | 1.60 | 1.52 |
| 6 | C | 286 | LYS | CA-CB | 5.70 | 1.62 | 1.53 |
| 5 | E | 511 | GLU | CA-CB | 5.70 | 1.62 | 1.53 |
| 8 | P | 1251 | TYR | CA-CB | 5.70 | 1.61 | 1.53 |
| 4 | y | 701 | GLU | CA-C | -5.70 | 1.45 | 1.52 |
| 14 | h | 1008 | SER | CA-CB | 5.70 | 1.63 | 1.53 |
| 19 | m | 506 | ILE | C-N | 5.70 | 1.41 | 1.33 |
| 21 | s | 69 | VAL | C-O | -5.70 | 1.16 | 1.23 |
| 19 | f | 314 | ILE | CA-CB | -5.70 | 1.46 | 1.54 |
| 20 | g | 281 | ARG | C-N | 5.70 | 1.41 | 1.33 |
| 12 | v | 373 | LEU | C-N | 5.69 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 14 | h | 597 | TRP | CA-CB | 5.69 | 1.62 | 1.54 |
| 12 | u | 358 | ARG | CZ-NH2 | 5.69 | 1.40 | 1.33 |
| 19 | m | 410 | SER | N-CA | -5.69 | 1.39 | 1.46 |
| 20 | n | 102 | HIS | ND1-CE1 | 5.69 | 1.38 | 1.32 |
| 4 | J | 685 | MET | C-O | -5.69 | 1.17 | 1.24 |
| 7 | O | 728 | TYR | N-CA | 5.69 | 1.52 | 1.46 |
| 8 | P | 648 | ARG | NE-CZ | 5.69 | 1.39 | 1.33 |
| 14 | h | 916 | ARG | CA-C | -5.69 | 1.46 | 1.52 |
| 14 | a | 854 | LYS | N-CA | -5.69 | 1.39 | 1.46 |
| 8 | P | 1482 | ASP | CA-CB | 5.69 | 1.63 | 1.53 |
| 1 | Y | 1052 | SER | CA-C | -5.69 | 1.45 | 1.52 |
| 2 | Z | 1221 | ARG | NE-CZ | 5.69 | 1.39 | 1.33 |
| 20 | n | 138 | CYS | CA-CB | 5.69 | 1.61 | 1.53 |
| 4 | G | 747 | THR | C-N | 5.69 | 1.41 | 1.33 |
| 7 | M | 1390 | GLN | C-N | 5.69 | 1.41 | 1.33 |
| 8 | N | 680 | ASP | N-CA | -5.69 | 1.39 | 1.46 |
| 2 | Z | 240 | ARG | CZ-NH2 | 5.69 | 1.40 | 1.33 |
| 12 | u | 277 | ARG | NE-CZ | 5.69 | 1.39 | 1.33 |
| 19 | m | 625 | LYS | C-O | -5.69 | 1.17 | 1.24 |
| 21 | o | 17 | THR | N-CA | -5.69 | 1.38 | 1.45 |
| 1 | 0 | 577 | PHE | N-CA | -5.69 | 1.39 | 1.46 |
| 9 | S | 675 | VAL | CA-CB | 5.69 | 1.62 | 1.54 |
| 12 | v | 133 | HIS | CA-C | -5.69 | 1.45 | 1.52 |
| 15 | i | 529 | TRP | N-CA | -5.69 | 1.38 | 1.45 |
| 19 | f | 663 | LEU | CA-CB | 5.69 | 1.62 | 1.53 |
| 20 | g | 167 | ILE | CA-CB | 5.69 | 1.61 | 1.54 |
| 1 | 0 | 426 | VAL | C-N | 5.68 | 1.42 | 1.33 |
| 2 | 1 | 354 | LEU | CA-C | -5.68 | 1.45 | 1.52 |
| 2 | 1 | 545 | TYR | CA-C | -5.68 | 1.45 | 1.52 |
| 7 | M | 1289 | ILE | CA-C | -5.68 | 1.45 | 1.52 |
| 7 | O | 1335 | ILE | CA-C | -5.68 | 1.46 | 1.52 |
| 15 | b | 679 | ASP | N-CA | -5.68 | 1.42 | 1.46 |
| 16 | c | 181 | ARG | N-CA | -5.68 | 1.38 | 1.45 |
| 6 | I | 358 | LEU | CA-CB | 5.68 | 1.62 | 1.53 |
| 7 | O | 227 | ASP | CA-C | -5.68 | 1.50 | 1.53 |
| 7 | O | 1484 | ARG | CZ-NH2 | 5.68 | 1.40 | 1.33 |
| 9 | T | 799 | LYS | C-N | 5.68 | 1.42 | 1.33 |
| 18 | l | 209 | PRO | C-N | 5.68 | 1.40 | 1.33 |
| 14 | a | 620 | HIS | CB-CG | 5.68 | 1.58 | 1.50 |
| 5 | K | 464 | ALA | C-N | 5.68 | 1.41 | 1.33 |
| 9 | T | 766 | ASN | C-N | 5.68 | 1.39 | 1.33 |
| 12 | v | 601 | ARG | N-CA | -5.68 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | i | 57 | PRO | CA-CB | 5.68 | 1.61 | 1.53 |
| 19 | m | 357 | SER | C-O | -5.68 | 1.17 | 1.24 |
| 20 | n | 201 | ASN | C-N | 5.68 | 1.41 | 1.33 |
| 16 | c | 644 | PHE | C-N | 5.68 | 1.41 | 1.33 |
| 14 | a | 426 | ILE | CA-CB | 5.68 | 1.60 | 1.54 |
| 8 | P | 224 | CYS | CA-C | 5.68 | 1.64 | 1.52 |
| 9 | Q | 408 | ARG | CD-NE | 5.68 | 1.54 | 1.46 |
| 11 | V | 287 | HIS | ND1-CE1 | 5.68 | 1.38 | 1.32 |
| 14 | a | 300 | MET | CA-C | -5.68 | 1.45 | 1.52 |
| 6 | F | 446 | GLU | CA-C | -5.68 | 1.45 | 1.52 |
| 8 | P | 923 | LEU | N-CA | -5.68 | 1.39 | 1.45 |
| 9 | S | 681 | SER | CA-C | -5.68 | 1.45 | 1.52 |
| 16 | j | 317 | HIS | C-N | 5.68 | 1.42 | 1.33 |
| 7 | O | 1141 | SER | CA-CB | 5.68 | 1.63 | 1.53 |
| 9 | Q | 45 | SER | N-CA | -5.68 | 1.38 | 1.46 |
| 14 | h | 174 | SER | CA-C | -5.68 | 1.45 | 1.53 |
| 14 | h | 700 | ALA | N-CA | -5.68 | 1.39 | 1.46 |
| 20 | n | 761 | ASN | CB-CG | 5.68 | 1.66 | 1.52 |
| 20 | g | 658 | PHE | CA-C | 5.68 | 1.59 | 1.52 |
| 2 | 1 | 724 | TRP | NE1-CE2 | -5.67 | 1.31 | 1.37 |
| 4 | A | 657 | GLN | C-N | 5.67 | 1.41 | 1.34 |
| 5 | E | 383 | SER | N-CA | -5.67 | 1.39 | 1.46 |
| 7 | M | 1414 | SER | CA-C | -5.67 | 1.45 | 1.52 |
| 9 | S | 302 | VAL | N-CA | 5.67 | 1.54 | 1.46 |
| 9 | T | 138 | ASN | CA-C | -5.67 | 1.45 | 1.52 |
| 1 | Y | 438 | ALA | N-CA | -5.67 | 1.39 | 1.46 |
| 1 | Y | 691 | LYS | CA-C | -5.67 | 1.46 | 1.52 |
| 2 | Z | 1076 | ASP | N-CA | -5.67 | 1.38 | 1.45 |
| 2 | Z | 1230 | ASP | CA-C | -5.67 | 1.45 | 1.52 |
| 12 | v | 51 | ASP | CA-CB | 5.67 | 1.63 | 1.53 |
| 14 | h | 599 | LYS | CA-C | -5.67 | 1.48 | 1.52 |
| 20 | n | 718 | ILE | CA-CB | 5.67 | 1.61 | 1.54 |
| 16 | c | 653 | GLU | CA-C | 5.67 | 1.60 | 1.52 |
| 20 | g | 219 | ILE | C-N | 5.67 | 1.39 | 1.33 |
| 14 | a | 156 | TYR | CA-C | -5.67 | 1.45 | 1.52 |
| 2 | Z | 989 | ASN | CA-CB | 5.67 | 1.61 | 1.53 |
| 16 | c | 521 | SER | N-CA | -5.67 | 1.39 | 1.46 |
| 1 | 0 | 911 | ASN | CA-C | -5.67 | 1.45 | 1.52 |
| 1 | 0 | 955 | PRO | N-CA | -5.67 | 1.41 | 1.47 |
| 2 | 1 | 196 | GLU | CA-C | -5.67 | 1.44 | 1.52 |
| 6 | I | 328 | GLN | CA-C | -5.67 | 1.45 | 1.52 |
| 10 | W | 267 | ILE | C-N | 5.67 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 525 | ILE | CA-C | -5.67 | 1.45 | 1.52 |
| 12 | u | 543 | GLN | C-N | 5.67 | 1.41 | 1.33 |
| 12 | u | 606 | SER | C-N | 5.67 | 1.41 | 1.33 |
| 19 | f | 552 | ARG | C-N | 5.67 | 1.41 | 1.33 |
| 6 | F | 378 | HIS | ND1-CE1 | 5.67 | 1.38 | 1.32 |
| 7 | M | 1334 | THR | C-N | 5.67 | 1.41 | 1.33 |
| 1 | Y | 1473 | HIS | CG-CD2 | -5.67 | 1.29 | 1.35 |
| 18 | e | 22 | ARG | NE-CZ | 5.67 | 1.39 | 1.33 |
| 1 | 0 | 1479 | ILE | C-N | 5.67 | 1.41 | 1.33 |
| 6 | F | 342 | GLU | N-CA | -5.67 | 1.38 | 1.46 |
| 5 | K | 308 | LEU | CA-C | -5.67 | 1.43 | 1.52 |
| 7 | M | 254 | LEU | C-O | -5.67 | 1.17 | 1.24 |
| 7 | M | 1193 | ARG | CA-CB | 5.67 | 1.63 | 1.53 |
| 7 | O | 977 | ARG | CA-C | -5.67 | 1.45 | 1.52 |
| 4 | y | 817 | GLN | CA-C | -5.67 | 1.45 | 1.52 |
| 20 | n | 350 | SER | N-CA | -5.67 | 1.39 | 1.46 |
| 1 | 0 | 1473 | HIS | CG-CD2 | 5.67 | 1.42 | 1.35 |
| 1 | Y | 898 | LYS | C-O | 5.67 | 1.31 | 1.24 |
| 1 | Y | 1384 | ILE | N-CA | -5.67 | 1.39 | 1.46 |
| 1 | Y | 1409 | SER | CA-C | 5.67 | 1.60 | 1.52 |
| 2 | Z | 1212 | PRO | CA-C | 5.67 | 1.57 | 1.52 |
| 16 | j | 588 | GLN | CA-CB | 5.67 | 1.62 | 1.53 |
| 19 | f | 376 | SER | C-N | 5.67 | 1.43 | 1.33 |
| 8 | N | 589 | GLU | CA-CB | 5.67 | 1.62 | 1.53 |
| 7 | M | 1469 | ARG | CD-NE | 5.66 | 1.54 | 1.46 |
| 8 | N | 1073 | LYS | C-O | -5.66 | 1.17 | 1.24 |
| 7 | O | 1088 | ARG | NE-CZ | 5.66 | 1.39 | 1.33 |
| 9 | R | 227 | GLN | CA-C | -5.66 | 1.45 | 1.52 |
| 2 | Z | 988 | CYS | CA-C | -5.66 | 1.45 | 1.52 |
| 12 | v | 34 | ARG | CZ-NH1 | 5.66 | 1.40 | 1.32 |
| 19 | m | 527 | VAL | CA-CB | 5.66 | 1.62 | 1.54 |
| 20 | n | 414 | THR | CA-CB | 5.66 | 1.62 | 1.53 |
| 14 | a | 28 | VAL | CA-C | -5.66 | 1.45 | 1.52 |
| 1 | Y | 975 | ILE | CA-C | -5.66 | 1.46 | 1.52 |
| 13 | x | 1122 | ILE | CA-CB | 5.66 | 1.63 | 1.55 |
| 14 | h | 516 | PHE | CA-CB | 5.66 | 1.62 | 1.53 |
| 15 | i | 337 | LEU | C-N | 5.66 | 1.41 | 1.33 |
| 20 | n | 340 | GLN | CA-C | -5.66 | 1.45 | 1.52 |
| 17 | d | 250 | GLU | C-N | 5.66 | 1.41 | 1.33 |
| 19 | f | 517 | LEU | CA-C | -5.66 | 1.45 | 1.52 |
| 14 | a | 254 | ILE | C-N | 5.66 | 1.41 | 1.33 |
| 8 | P | 1011 | GLU | C-N | 5.66 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 14 | h | 534 | ASP | CA-C | -5.66 | 1.45 | 1.52 |
| 20 | n | 879 | ALA | CA-C | -5.66 | 1.46 | 1.52 |
| 16 | c | 312 | GLU | CA-C | -5.66 | 1.44 | 1.52 |
| 20 | g | 1077 | PRO | CA-C | -5.66 | 1.47 | 1.52 |
| 6 | C | 454 | ALA | C-N | 5.66 | 1.41 | 1.33 |
| 7 | M | 1395 | PRO | CA-CB | 5.66 | 1.61 | 1.53 |
| 9 | R | 704 | ARG | NE-CZ | 5.66 | 1.39 | 1.33 |
| 2 | Z | 1381 | ASP | CA-C | -5.66 | 1.45 | 1.52 |
| 14 | a | 522 | ASN | N-CA | 5.66 | 1.53 | 1.46 |
| 6 | I | 298 | THR | N-CA | 5.66 | 1.53 | 1.46 |
| 8 | P | 1413 | ASN | C-N | 5.66 | 1.41 | 1.33 |
| 9 | S | 611 | LEU | CA-C | 5.66 | 1.59 | 1.52 |
| 9 | T | 301 | ASN | C-N | 5.66 | 1.40 | 1.33 |
| 18 | e | 167 | SER | N-CA | -5.66 | 1.39 | 1.46 |
| 2 | 1 | 402 | ARG | CD-NE | 5.66 | 1.54 | 1.46 |
| 7 | M | 1609 | SER | C-N | 5.66 | 1.40 | 1.33 |
| 8 | N | 494 | PRO | N-CA | -5.66 | 1.40 | 1.47 |
| 9 | T | 745 | LEU | CA-CB | -5.66 | 1.47 | 1.54 |
| 21 | t | 46 | LYS | N-CA | -5.66 | 1.39 | 1.46 |
| 20 | g | 647 | LYS | CA-CB | 5.66 | 1.62 | 1.53 |
| 14 | a | 751 | ARG | CZ-NH1 | 5.66 | 1.40 | 1.32 |
| 2 | 1 | 882 | ASP | N-CA | -5.65 | 1.39 | 1.46 |
| 5 | K | 439 | GLN | CA-C | -5.65 | 1.45 | 1.52 |
| 8 | P | 1289 | LYS | C-N | 5.65 | 1.40 | 1.33 |
| 9 | S | 63 | SER | N-CA | -5.65 | 1.38 | 1.45 |
| 9 | T | 102 | LYS | N-CA | 5.65 | 1.53 | 1.46 |
| 14 | a | 982 | TYR | N-CA | -5.65 | 1.39 | 1.46 |
| 2 | 1 | 765 | PHE | N-CA | 5.65 | 1.53 | 1.46 |
| 5 | K | 358 | LEU | C-N | 5.65 | 1.41 | 1.34 |
| 8 | N | 1313 | ARG | CD-NE | 5.65 | 1.54 | 1.46 |
| 7 | O | 291 | GLU | CA-CB | 5.65 | 1.62 | 1.54 |
| 8 | P | 1062 | ARG | CZ-NH2 | 5.65 | 1.40 | 1.33 |
| 11 | X | 292 | GLY | C-N | 5.65 | 1.41 | 1.33 |
| 12 | v | 242 | ASP | C-N | 5.65 | 1.41 | 1.33 |
| 14 | h | 779 | LEU | N-CA | -5.65 | 1.40 | 1.46 |
| 18 | e | 321 | SER | CA-C | -5.65 | 1.47 | 1.53 |
| 19 | f | 212 | LEU | C-O | -5.65 | 1.17 | 1.24 |
| 2 | 1 | 486 | GLN | C-N | 5.65 | 1.41 | 1.33 |
| 2 | 1 | 575 | ARG | CD-NE | 5.65 | 1.54 | 1.46 |
| 6 | F | 326 | LEU | C-N | 5.65 | 1.41 | 1.33 |
| 7 | M | 86 | ILE | CA-C | -5.65 | 1.46 | 1.52 |
| 7 | M | 212 | PHE | CA-C | 5.65 | 1.60 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 12 | v | 175 | LEU | CA-C | -5.65 | 1.45 | 1.52 |
| 14 | h | 507 | PHE | C-O | -5.65 | 1.17 | 1.24 |
| 17 | d | 187 | TYR | N-CA | 5.65 | 1.53 | 1.46 |
| 20 | g | 754 | ASN | CA-CB | 5.65 | 1.61 | 1.53 |
| 14 | h | 739 | PHE | CA-CB | 5.65 | 1.61 | 1.53 |
| 16 | c | 381 | TRP | N-CA | -5.65 | 1.39 | 1.46 |
| 5 | E | 290 | GLU | CA-C | -5.65 | 1.44 | 1.52 |
| 8 | P | 865 | ASN | N-CA | -5.65 | 1.39 | 1.46 |
| 10 | W | 254 | ILE | CA-C | -5.65 | 1.46 | 1.52 |
| 18 | l | 64 | ALA | CA-CB | 5.65 | 1.62 | 1.53 |
| 15 | b | 66 | PRO | CA-CB | -5.65 | 1.49 | 1.53 |
| 16 | c | 531 | LYS | C-N | 5.65 | 1.39 | 1.33 |
| 20 | g | 466 | TYR | C-N | 5.65 | 1.40 | 1.33 |
| 9 | Q | 541 | TYR | N-CA | 5.65 | 1.53 | 1.46 |
| 18 | e | 184 | ALA | CA-C | -5.65 | 1.45 | 1.52 |
| 1 | 0 | 1311 | PHE | CA-CB | 5.64 | 1.62 | 1.53 |
| 7 | M | 934 | ASP | C-N | 5.64 | 1.40 | 1.33 |
| 8 | N | 1554 | LEU | N-CA | -5.64 | 1.39 | 1.46 |
| 1 | Y | 1367 | LEU | CA-C | -5.64 | 1.45 | 1.52 |
| 12 | u | 364 | ILE | CA-C | 5.64 | 1.59 | 1.52 |
| 4 | z | 801 | PHE | N-CA | -5.64 | 1.39 | 1.46 |
| 14 | h | 150 | PHE | C-N | 5.64 | 1.40 | 1.33 |
| 14 | h | 206 | LYS | N-CA | -5.64 | 1.39 | 1.46 |
| 15 | i | 561 | ARG | CZ-NH1 | 5.64 | 1.40 | 1.32 |
| 18 | l | 213 | SER | N-CA | -5.64 | 1.39 | 1.45 |
| 2 | 1 | 572 | PRO | CA-C | 5.64 | 1.59 | 1.52 |
| 7 | M | 1667 | VAL | CA-C | -5.64 | 1.45 | 1.52 |
| 7 | O | 977 | ARG | CA-CB | 5.64 | 1.62 | 1.53 |
| 9 | Q | 241 | ILE | CA-CB | -5.64 | 1.46 | 1.54 |
| 12 | v | 416 | ASP | N-CA | -5.64 | 1.39 | 1.46 |
| 4 | z | 675 | GLN | N-CA | -5.64 | 1.39 | 1.46 |
| 17 | k | 65 | LYS | C-N | 5.64 | 1.41 | 1.33 |
| 4 | J | 715 | GLU | C-N | 5.64 | 1.41 | 1.33 |
| 8 | N | 570 | GLN | C-N | 5.64 | 1.41 | 1.33 |
| 5 | K | 344 | SER | CA-CB | 5.64 | 1.62 | 1.53 |
| 7 | M | 611 | SER | C-N | 5.64 | 1.42 | 1.33 |
| 8 | N | 1518 | THR | CB-OG1 | 5.64 | 1.52 | 1.43 |
| 7 | O | 557 | ASN | CA-CB | 5.64 | 1.63 | 1.53 |
| 9 | Q | 574 | GLU | CA-C | -5.64 | 1.45 | 1.52 |
| 9 | T | 492 | ILE | CA-CB | 5.64 | 1.61 | 1.54 |
| 14 | h | 226 | CYS | C-N | 5.64 | 1.41 | 1.33 |
| 19 | m | 429 | ILE | C-N | 5.64 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | b | 466 | LEU | CA-CB | 5.64 | 1.62 | 1.53 |
| 14 | a | 230 | HIS | CE1-NE2 | -5.64 | 1.26 | 1.32 |
| 14 | a | 851 | TYR | CA-C | -5.64 | 1.45 | 1.53 |
| 9 | R | 484 | LEU | CA-C | -5.64 | 1.45 | 1.52 |
| 12 | v | 84 | ASN | CA-CB | 5.64 | 1.62 | 1.53 |
| 14 | a | 64 | ASN | CA-C | -5.64 | 1.45 | 1.52 |
| 14 | a | 653 | THR | CB-OG1 | -5.64 | 1.34 | 1.43 |
| 7 | M | 475 | LYS | CA-C | 5.64 | 1.60 | 1.52 |
| 8 | N | 1261 | ILE | N-CA | -5.64 | 1.40 | 1.46 |
| 7 | O | 428 | GLN | C-N | 5.64 | 1.41 | 1.33 |
| 7 | O | 918 | PHE | N-CA | -5.64 | 1.39 | 1.46 |
| 8 | P | 326 | SER | C-O | -5.64 | 1.17 | 1.23 |
| 9 | Q | 227 | GLN | CA-CB | 5.64 | 1.62 | 1.53 |
| 1 | Y | 293 | ILE | CA-CB | -5.64 | 1.46 | 1.54 |
| 2 | Z | 609 | LEU | CB-CG | 5.64 | 1.64 | 1.53 |
| 15 | i | 313 | LEU | C-N | 5.64 | 1.42 | 1.33 |
| 1 | 0 | 1028 | LEU | N-CA | -5.63 | 1.39 | 1.46 |
| 7 | M | 714 | HIS | CE1-NE2 | -5.63 | 1.26 | 1.32 |
| 7 | O | 4 | SER | CA-C | -5.63 | 1.45 | 1.52 |
| 7 | O | 1122 | TRP | NE1-CE2 | -5.63 | 1.31 | 1.37 |
| 9 | R | 342 | ARG | CZ-NH2 | 5.63 | 1.40 | 1.33 |
| 9 | R | 476 | ASN | CA-C | -5.63 | 1.45 | 1.52 |
| 11 | X | 393 | GLU | N-CA | -5.63 | 1.39 | 1.46 |
| 12 | u | 331 | LEU | CA-C | -5.63 | 1.46 | 1.52 |
| 15 | i | 122 | ARG | NE-CZ | 5.63 | 1.39 | 1.33 |
| 15 | i | 161 | ARG | N-CA | 5.63 | 1.52 | 1.46 |
| 19 | f | 299 | GLU | CA-CB | 5.63 | 1.62 | 1.53 |
| 20 | g | 777 | ILE | C-N | 5.63 | 1.41 | 1.33 |
| 8 | N | 811 | ASP | CA-CB | 5.63 | 1.61 | 1.53 |
| 9 | R | 533 | ARG | CZ-NH2 | 5.63 | 1.40 | 1.33 |
| 15 | i | 484 | VAL | N-CA | -5.63 | 1.39 | 1.46 |
| 18 | l | 49 | ASP | C-N | 5.63 | 1.40 | 1.33 |
| 14 | a | 912 | ASP | CA-CB | 5.63 | 1.62 | 1.53 |
| 7 | O | 692 | TYR | C-N | 5.63 | 1.41 | 1.33 |
| 9 | R | 355 | GLU | CA-C | -5.63 | 1.45 | 1.52 |
| 14 | h | 990 | ASP | CA-C | -5.63 | 1.45 | 1.52 |
| 17 | k | 277 | LYS | CA-C | -5.63 | 1.45 | 1.52 |
| 19 | f | 137 | LYS | CA-C | -5.63 | 1.45 | 1.52 |
| 2 | 1 | 844 | PHE | CA-CB | 5.63 | 1.62 | 1.53 |
| 7 | O | 1332 | PHE | N-CA | -5.63 | 1.39 | 1.46 |
| 8 | P | 952 | LEU | C-N | 5.63 | 1.40 | 1.33 |
| 9 | S | 648 | GLU | CA-CB | 5.63 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 12 | u | 526 | GLU | C-N | 5.63 | 1.41 | 1.33 |
| 20 | g | 252 | PHE | CA-CB | 5.63 | 1.60 | 1.53 |
| 4 | J | 810 | ASN | N-CA | -5.63 | 1.39 | 1.46 |
| 8 | N | 114 | TYR | CA-CB | 5.63 | 1.62 | 1.53 |
| 9 | S | 705 | GLN | CA-CB | 5.63 | 1.62 | 1.53 |
| 9 | T | 16 | LYS | C-N | -5.63 | 1.26 | 1.33 |
| 12 | u | 169 | PRO | C-N | 5.63 | 1.41 | 1.33 |
| 18 | l | 329 | ARG | CA-CB | 5.63 | 1.61 | 1.53 |
| 19 | f | 317 | LEU | CA-CB | 5.63 | 1.62 | 1.53 |
| 14 | a | 914 | TYR | CZ-OH | 5.63 | 1.49 | 1.38 |
| 5 | K | 288 | ILE | N-CA | 5.63 | 1.53 | 1.46 |
| 12 | u | 281 | VAL | C-N | 5.63 | 1.41 | 1.33 |
| 14 | h | 454 | LYS | CA-C | -5.63 | 1.45 | 1.52 |
| 18 | l | 316 | GLY | CA-C | -5.63 | 1.44 | 1.51 |
| 4 | J | 801 | PHE | CA-CB | 5.62 | 1.62 | 1.53 |
| 7 | O | 1563 | LEU | N-CA | -5.62 | 1.39 | 1.46 |
| 9 | T | 612 | HIS | CB-CG | 5.62 | 1.58 | 1.50 |
| 12 | u | 188 | SER | CA-CB | 5.62 | 1.62 | 1.53 |
| 12 | u | 707 | GLU | C-N | 5.62 | 1.41 | 1.33 |
| 12 | v | 566 | SER | C-N | 5.62 | 1.41 | 1.33 |
| 21 | o | 15 | ASP | N-CA | -5.62 | 1.39 | 1.47 |
| 15 | b | 362 | LEU | CA-CB | 5.62 | 1.62 | 1.53 |
| 14 | a | 27 | TYR | CA-C | -5.62 | 1.46 | 1.52 |
| 2 | 1 | 1335 | ASN | CA-CB | 5.62 | 1.62 | 1.53 |
| 7 | M | 1101 | ILE | N-CA | -5.62 | 1.40 | 1.46 |
| 1 | Y | 600 | GLU | C-N | 5.62 | 1.41 | 1.33 |
| 1 | Y | 642 | LEU | N-CA | -5.62 | 1.39 | 1.46 |
| 2 | Z | 974 | ILE | CA-CB | -5.62 | 1.48 | 1.54 |
| 17 | d | 255 | ASP | CA-C | -5.62 | 1.45 | 1.52 |
| 20 | g | 632 | LYS | C-N | 5.62 | 1.41 | 1.33 |
| 2 | 1 | 1015 | VAL | CA-C | -5.62 | 1.45 | 1.52 |
| 8 | N | 422 | GLU | C-N | 5.62 | 1.41 | 1.33 |
| 16 | j | 135 | ALA | C-N | 5.62 | 1.41 | 1.33 |
| 7 | O | 200 | LEU | CA-CB | 5.62 | 1.62 | 1.53 |
| 9 | R | 294 | MET | C-N | 5.62 | 1.41 | 1.33 |
| 1 | Y | 1431 | LYS | C-N | 5.62 | 1.41 | 1.33 |
| 4 | z | 664 | SER | C-N | 5.62 | 1.41 | 1.33 |
| 14 | h | 70 | TYR | N-CA | -5.62 | 1.39 | 1.46 |
| 15 | i | 94 | ARG | CD-NE | 5.62 | 1.54 | 1.46 |
| 20 | n | 805 | ALA | CA-C | -5.62 | 1.45 | 1.52 |
| 6 | I | 391 | LEU | C-N | 5.62 | 1.41 | 1.33 |
| 8 | N | 1434 | ASN | C-N | 5.62 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | g | 577 | TYR | CZ-OH | 5.62 | 1.49 | 1.38 |
| 1 | 0 | 784 | ILE | CA-C | 5.62 | 1.59 | 1.52 |
| 2 | 1 | 242 | HIS | CE1-NE2 | -5.62 | 1.26 | 1.32 |
| 7 | O | 635 | PHE | CA-CB | 5.62 | 1.61 | 1.53 |
| 7 | O | 1010 | LEU | C-N | 5.62 | 1.41 | 1.34 |
| 7 | O | 1158 | THR | N-CA | -5.62 | 1.39 | 1.46 |
| 8 | P | 894 | VAL | CA-C | -5.62 | 1.45 | 1.52 |
| 9 | R | 792 | SER | CA-C | -5.62 | 1.45 | 1.52 |
| 1 | Y | 249 | LYS | CA-CB | 5.62 | 1.61 | 1.53 |
| 12 | v | 442 | ASN | C-N | 5.62 | 1.42 | 1.33 |
| 20 | n | 649 | PHE | CA-CB | 5.62 | 1.63 | 1.53 |
| 14 | a | 139 | PHE | C-N | 5.62 | 1.41 | 1.33 |
| 1 | 0 | 149 | GLU | CA-CB | 5.61 | 1.63 | 1.53 |
| 2 | 1 | 1272 | ILE | CA-C | -5.61 | 1.44 | 1.52 |
| 6 | I | 443 | VAL | CA-CB | -5.61 | 1.46 | 1.54 |
| 7 | M | 218 | HIS | C-N | 5.61 | 1.41 | 1.33 |
| 7 | M | 886 | LEU | CA-C | -5.61 | 1.45 | 1.52 |
| 7 | M | 1581 | THR | CA-C | -5.61 | 1.45 | 1.52 |
| 8 | P | 78 | LEU | CA-CB | 5.61 | 1.62 | 1.53 |
| 14 | h | 18 | PRO | C-N | 5.61 | 1.39 | 1.33 |
| 18 | l | 196 | ARG | CZ-NH1 | 5.61 | 1.40 | 1.32 |
| 17 | d | 215 | THR | CA-C | -5.61 | 1.46 | 1.52 |
| 2 | 1 | 996 | VAL | CA-C | -5.61 | 1.45 | 1.52 |
| 8 | P | 1624 | GLN | CA-CB | 5.61 | 1.62 | 1.53 |
| 11 | X | 399 | LYS | CA-C | -5.61 | 1.45 | 1.52 |
| 14 | h | 16 | GLU | CA-CB | 5.61 | 1.61 | 1.53 |
| 1 | 0 | 531 | PHE | CA-C | -5.61 | 1.45 | 1.52 |
| 1 | 0 | 614 | LEU | CA-C | -5.61 | 1.45 | 1.53 |
| 7 | M | 752 | TYR | CA-C | -5.61 | 1.45 | 1.52 |
| 7 | O | 1336 | ILE | CA-CB | -5.61 | 1.50 | 1.53 |
| 12 | v | 542 | ALA | C-N | 5.61 | 1.41 | 1.33 |
| 14 | h | 796 | ASP | C-N | 5.61 | 1.41 | 1.33 |
| 18 | e | 129 | GLY | C-N | 5.61 | 1.41 | 1.33 |
| 2 | 1 | 232 | ILE | CA-C | -5.61 | 1.47 | 1.53 |
| 7 | O | 427 | THR | N-CA | -5.61 | 1.39 | 1.46 |
| 8 | P | 1627 | LEU | C-N | 5.61 | 1.41 | 1.33 |
| 9 | Q | 439 | HIS | CA-CB | 5.61 | 1.60 | 1.53 |
| 14 | h | 863 | ASP | CA-CB | 5.61 | 1.60 | 1.53 |
| 19 | m | 644 | ALA | CA-C | -5.61 | 1.45 | 1.52 |
| 20 | g | 609 | VAL | N-CA | -5.61 | 1.38 | 1.46 |
| 9 | Q | 323 | SER | CA-C | -5.61 | 1.45 | 1.52 |
| 2 | Z | 611 | ILE | CA-C | -5.61 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | m | 668 | HIS | CB-CG | 5.61 | 1.58 | 1.50 |
| 21 | t | 39 | ARG | C-O | -5.61 | 1.17 | 1.24 |
| 15 | b | 413 | ASP | C-N | 5.61 | 1.41 | 1.33 |
| 20 | g | 1043 | ARG | CD-NE | 5.61 | 1.54 | 1.46 |
| 14 | a | 920 | SER | CA-C | 5.61 | 1.60 | 1.52 |
| 4 | J | 714 | PHE | C-N | 5.61 | 1.41 | 1.34 |
| 1 | Y | 1321 | ALA | CA-C | -5.61 | 1.45 | 1.52 |
| 2 | Z | 569 | GLU | CA-C | -5.61 | 1.45 | 1.52 |
| 12 | v | 270 | VAL | CA-C | -5.61 | 1.45 | 1.52 |
| 20 | n | 341 | ASP | N-CA | -5.61 | 1.39 | 1.46 |
| 14 | a | 1031 | ARG | CZ-NH1 | 5.61 | 1.40 | 1.32 |
| 7 | O | 236 | ALA | N-CA | -5.60 | 1.39 | 1.46 |
| 12 | u | 214 | SER | N-CA | -5.60 | 1.39 | 1.46 |
| 4 | y | 794 | ILE | CA-C | -5.60 | 1.46 | 1.52 |
| 14 | h | 475 | CYS | C-N | 5.60 | 1.41 | 1.34 |
| 16 | j | 305 | ARG | CD-NE | 5.60 | 1.54 | 1.46 |
| 2 | 1 | 716 | ILE | CA-CB | 5.60 | 1.61 | 1.54 |
| 7 | M | 745 | ARG | NE-CZ | 5.60 | 1.39 | 1.33 |
| 7 | M | 963 | ASN | C-N | 5.60 | 1.41 | 1.33 |
| 8 | N | 1350 | LEU | C-N | 5.60 | 1.40 | 1.33 |
| 8 | P | 599 | THR | CA-CB | -5.60 | 1.44 | 1.53 |
| 2 | Z | 981 | GLN | CA-CB | 5.60 | 1.62 | 1.53 |
| 14 | h | 807 | ILE | CA-CB | -5.60 | 1.48 | 1.54 |
| 15 | i | 119 | GLY | C-N | 5.60 | 1.41 | 1.33 |
| 15 | b | 219 | PRO | N-CD | -5.60 | 1.40 | 1.47 |
| 17 | d | 256 | VAL | CA-CB | -5.60 | 1.48 | 1.54 |
| 19 | f | 720 | ARG | NE-CZ | 5.60 | 1.39 | 1.33 |
| 13 | w | 1336 | THR | C-N | 5.60 | 1.41 | 1.33 |
| 20 | g | 572 | ALA | N-CA | -5.60 | 1.39 | 1.46 |
| 1 | 0 | 1339 | LYS | N-CA | -5.60 | 1.38 | 1.46 |
| 1 | 0 | 1396 | ASN | CA-CB | 5.60 | 1.62 | 1.53 |
| 5 | E | 373 | ARG | N-CA | -5.60 | 1.39 | 1.46 |
| 7 | M | 866 | GLN | N-CA | -5.60 | 1.39 | 1.46 |
| 8 | N | 455 | PHE | CA-C | -5.60 | 1.45 | 1.52 |
| 12 | u | 207 | ALA | CA-C | -5.60 | 1.45 | 1.52 |
| 12 | u | 532 | SER | C-N | 5.60 | 1.41 | 1.33 |
| 14 | h | 606 | LYS | CA-C | -5.60 | 1.45 | 1.52 |
| 15 | i | 140 | HIS | ND1-CE1 | 5.60 | 1.38 | 1.32 |
| 16 | j | 333 | ARG | NE-CZ | 5.60 | 1.39 | 1.33 |
| 20 | g | 516 | LEU | N-CA | -5.60 | 1.41 | 1.46 |
| 1 | 0 | 453 | GLY | C-N | 5.60 | 1.41 | 1.34 |
| 7 | O | 107 | PHE | C-N | 5.60 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1099 | TYR | C-N | 5.60 | 1.41 | 1.34 |
| 7 | O | 1292 | ARG | C-N | 5.60 | 1.41 | 1.33 |
| 8 | P | 872 | ASN | CA-C | -5.60 | 1.45 | 1.52 |
| 1 | Y | 297 | HIS | CE1-NE2 | 5.60 | 1.38 | 1.32 |
| 4 | z | 647 | GLN | C-N | 5.60 | 1.40 | 1.33 |
| 19 | f | 330 | ARG | C-N | 5.60 | 1.40 | 1.33 |
| 7 | M | 316 | LEU | CA-C | -5.59 | 1.45 | 1.52 |
| 8 | P | 997 | VAL | C-N | 5.59 | 1.41 | 1.33 |
| 12 | u | 388 | SER | CA-CB | 5.59 | 1.62 | 1.53 |
| 14 | h | 960 | CYS | CA-C | -5.59 | 1.45 | 1.52 |
| 18 | l | 108 | LYS | CA-C | -5.59 | 1.45 | 1.52 |
| 19 | m | 68 | TRP | C-N | 5.59 | 1.41 | 1.33 |
| 7 | M | 1250 | LYS | N-CA | 5.59 | 1.53 | 1.46 |
| 8 | N | 641 | ILE | CA-CB | 5.59 | 1.61 | 1.54 |
| 8 | N | 913 | ASN | CA-CB | 5.59 | 1.62 | 1.53 |
| 9 | S | 209 | ARG | NE-CZ | 5.59 | 1.39 | 1.33 |
| 19 | f | 609 | SER | CA-CB | 5.59 | 1.64 | 1.53 |
| 1 | 0 | 1084 | VAL | N-CA | -5.59 | 1.39 | 1.46 |
| 6 | I | 389 | ARG | NE-CZ | 5.59 | 1.39 | 1.33 |
| 7 | M | 248 | PRO | N-CA | -5.59 | 1.40 | 1.47 |
| 7 | M | 1508 | ILE | CA-C | -5.59 | 1.45 | 1.52 |
| 9 | R | 418 | CYS | C-N | 5.59 | 1.41 | 1.33 |
| 1 | Y | 591 | LYS | CA-CB | 5.59 | 1.63 | 1.53 |
| 17 | d | 194 | TYR | CA-C | -5.59 | 1.45 | 1.52 |
| 20 | g | 714 | TYR | CA-C | -5.59 | 1.45 | 1.52 |
| 4 | G | 665 | TRP | N-CA | -5.59 | 1.39 | 1.46 |
| 1 | Y | 1300 | LYS | CA-C | -5.59 | 1.46 | 1.52 |
| 12 | u | 374 | TYR | CA-C | -5.59 | 1.46 | 1.52 |
| 4 | z | 672 | GLY | C-N | 5.59 | 1.40 | 1.33 |
| 14 | h | 167 | PHE | N-CA | -5.59 | 1.40 | 1.46 |
| 14 | h | 629 | ILE | N-CA | -5.59 | 1.40 | 1.46 |
| 19 | f | 301 | TYR | CA-CB | 5.59 | 1.62 | 1.53 |
| 1 | 0 | 716 | VAL | N-CA | -5.59 | 1.39 | 1.46 |
| 7 | O | 650 | VAL | CA-CB | -5.59 | 1.46 | 1.54 |
| 9 | T | 64 | LYS | CA-C | 5.59 | 1.59 | 1.53 |
| 12 | u | 47 | ASN | C-N | 5.59 | 1.38 | 1.33 |
| 20 | n | 1104 | ILE | C-N | 5.59 | 1.41 | 1.33 |
| 2 | 1 | 482 | PRO | C-O | -5.59 | 1.17 | 1.24 |
| 2 | 1 | 726 | GLU | N-CA | -5.59 | 1.39 | 1.46 |
| 9 | Q | 770 | ASN | CA-CB | 5.59 | 1.62 | 1.53 |
| 15 | i | 48 | LEU | N-CA | -5.59 | 1.39 | 1.46 |
| 20 | n | 818 | LEU | CA-CB | 5.59 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | f | 139 | VAL | CA-C | -5.59 | 1.47 | 1.52 |
| 9 | Q | 424 | ASN | C-O | -5.58 | 1.17 | 1.23 |
| 10 | U | 337 | GLY | CA-C | -5.58 | 1.43 | 1.51 |
| 17 | k | 111 | GLU | CA-CB | 5.58 | 1.63 | 1.53 |
| 20 | g | 878 | SER | CA-C | -5.58 | 1.45 | 1.52 |
| 14 | a | 81 | PHE | CA-CB | 5.58 | 1.61 | 1.53 |
| 2 | 1 | 1288 | LEU | CA-C | -5.58 | 1.45 | 1.52 |
| 7 | M | 529 | MET | C-N | 5.58 | 1.40 | 1.34 |
| 7 | M | 668 | ARG | NE-CZ | 5.58 | 1.39 | 1.33 |
| 8 | N | 804 | GLN | CD-NE2 | 5.58 | 1.45 | 1.33 |
| 8 | N | 929 | MET | CA-C | -5.58 | 1.46 | 1.52 |
| 8 | N | 1445 | THR | CA-CB | -5.58 | 1.44 | 1.53 |
| 8 | P | 1286 | THR | CA-C | 5.58 | 1.60 | 1.52 |
| 14 | h | 923 | LEU | CA-C | 5.58 | 1.60 | 1.52 |
| 17 | k | 224 | SER | CA-CB | 5.58 | 1.60 | 1.52 |
| 19 | m | 336 | PRO | N-CA | -5.58 | 1.43 | 1.47 |
| 16 | c | 445 | LEU | CA-CB | 5.58 | 1.60 | 1.53 |
| 5 | H | 367 | GLU | N-CA | 5.58 | 1.53 | 1.46 |
| 7 | O | 731 | PHE | C-N | 5.58 | 1.40 | 1.33 |
| 9 | Q | 90 | LEU | CA-C | -5.58 | 1.45 | 1.52 |
| 2 | Z | 159 | ILE | C-N | 5.58 | 1.41 | 1.33 |
| 14 | h | 321 | THR | C-N | 5.58 | 1.40 | 1.33 |
| 20 | n | 92 | MET | CA-C | -5.58 | 1.45 | 1.52 |
| 20 | n | 977 | ASN | CA-C | -5.58 | 1.45 | 1.52 |
| 21 | o | 39 | ARG | CD-NE | 5.58 | 1.54 | 1.46 |
| 19 | f | 193 | ILE | CA-CB | 5.58 | 1.62 | 1.54 |
| 20 | g | 170 | SER | CA-C | -5.58 | 1.45 | 1.52 |
| 5 | E | 376 | LEU | CA-CB | 5.58 | 1.62 | 1.53 |
| 8 | N | 897 | LYS | N-CA | -5.58 | 1.39 | 1.46 |
| 9 | R | 300 | THR | C-N | 5.58 | 1.41 | 1.33 |
| 2 | 1 | 542 | ALA | C-N | 5.58 | 1.40 | 1.33 |
| 5 | H | 537 | TYR | C-N | 5.58 | 1.41 | 1.33 |
| 7 | M | 435 | PHE | C-N | 5.58 | 1.41 | 1.33 |
| 10 | W | 342 | CYS | N-CA | -5.58 | 1.39 | 1.46 |
| 1 | Y | 1427 | TYR | CA-C | -5.58 | 1.45 | 1.52 |
| 16 | j | 520 | ALA | N-CA | 5.58 | 1.53 | 1.46 |
| 17 | k | 138 | PRO | C-N | 5.58 | 1.40 | 1.33 |
| 18 | l | 4 | PHE | N-CA | -5.58 | 1.39 | 1.46 |
| 20 | n | 476 | GLN | C-N | 5.58 | 1.41 | 1.33 |
| 17 | d | 36 | PHE | CA-C | -5.58 | 1.45 | 1.53 |
| 18 | e | 8 | HIS | ND1-CE1 | 5.58 | 1.38 | 1.32 |
| 14 | a | 882 | PHE | CA-CB | 5.58 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | J | 808 | ASP | N-CA | 5.58 | 1.53 | 1.46 |
| 1 | Y | 122 | ASP | C-N | 5.58 | 1.40 | 1.33 |
| 15 | b | 246 | TRP | NE1-CE2 | -5.58 | 1.31 | 1.37 |
| 8 | N | 415 | PHE | CA-C | -5.58 | 1.45 | 1.52 |
| 8 | P | 1527 | LYS | C-N | 5.58 | 1.41 | 1.33 |
| 2 | Z | 1256 | VAL | C-N | 5.58 | 1.40 | 1.34 |
| 1 | 0 | 446 | LEU | C-N | 5.57 | 1.41 | 1.33 |
| 2 | 1 | 1112 | ALA | C-O | -5.57 | 1.17 | 1.24 |
| 4 | A | 686 | ALA | CA-CB | 5.57 | 1.61 | 1.53 |
| 7 | M | 1542 | ASN | CA-C | -5.57 | 1.46 | 1.53 |
| 9 | R | 441 | MET | N-CA | -5.57 | 1.39 | 1.46 |
| 9 | S | 472 | SER | CA-C | -5.57 | 1.45 | 1.52 |
| 11 | V | 346 | LYS | CA-CB | 5.57 | 1.64 | 1.53 |
| 11 | X | 293 | HIS | C-N | 5.57 | 1.40 | 1.33 |
| 14 | h | 146 | ASN | C-N | 5.57 | 1.40 | 1.33 |
| 14 | h | 271 | ARG | CA-C | -5.57 | 1.45 | 1.52 |
| 16 | j | 411 | SER | N-CA | -5.57 | 1.39 | 1.46 |
| 19 | m | 97 | HIS | CE1-NE2 | -5.57 | 1.26 | 1.32 |
| 20 | g | 777 | ILE | CA-C | -5.57 | 1.44 | 1.52 |
| 20 | g | 904 | LYS | CA-CB | 5.57 | 1.62 | 1.53 |
| 14 | a | 26 | LEU | CB-CG | 5.57 | 1.64 | 1.53 |
| 2 | 1 | 1065 | ALA | CA-CB | 5.57 | 1.62 | 1.53 |
| 7 | M | 126 | GLU | CA-C | -5.57 | 1.45 | 1.52 |
| 8 | P | 1320 | GLU | C-N | 5.57 | 1.41 | 1.33 |
| 9 | T | 549 | ASP | C-N | -5.57 | 1.27 | 1.34 |
| 1 | Y | 626 | ASN | C-O | -5.57 | 1.17 | 1.23 |
| 2 | Z | 947 | LEU | N-CA | -5.57 | 1.39 | 1.46 |
| 12 | u | 662 | LEU | C-N | 5.57 | 1.41 | 1.33 |
| 14 | h | 332 | VAL | CA-C | -5.57 | 1.44 | 1.52 |
| 14 | h | 649 | GLN | CA-CB | 5.57 | 1.62 | 1.53 |
| 14 | h | 787 | ASN | C-N | 5.57 | 1.41 | 1.33 |
| 16 | j | 664 | GLU | CA-CB | 5.57 | 1.62 | 1.53 |
| 20 | g | 290 | GLY | C-N | 5.57 | 1.39 | 1.33 |
| 5 | B | 512 | ILE | CA-C | -5.57 | 1.45 | 1.52 |
| 18 | l | 97 | ARG | CZ-NH2 | 5.57 | 1.40 | 1.33 |
| 19 | f | 718 | VAL | CA-C | 5.57 | 1.59 | 1.52 |
| 8 | N | 517 | LEU | CB-CG | 5.57 | 1.64 | 1.53 |
| 8 | N | 991 | LYS | C-N | 5.57 | 1.42 | 1.33 |
| 8 | N | 1120 | LYS | CA-C | -5.57 | 1.45 | 1.52 |
| 8 | P | 1435 | ASP | C-O | -5.57 | 1.17 | 1.24 |
| 9 | Q | 544 | SER | C-N | 5.57 | 1.41 | 1.33 |
| 1 | Y | 359 | LEU | N-CA | -5.57 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 18 | e | 231 | ILE | C-N | 5.57 | 1.40 | 1.33 |
| 19 | f | 74 | PHE | C-O | -5.57 | 1.17 | 1.24 |
| 1 | 0 | 1482 | ASP | CA-CB | 5.57 | 1.61 | 1.54 |
| 5 | H | 295 | CYS | C-O | 5.57 | 1.28 | 1.23 |
| 7 | M | 143 | ASN | C-O | 5.57 | 1.31 | 1.24 |
| 9 | S | 816 | TYR | C-O | -5.57 | 1.17 | 1.24 |
| 13 | x | 1370 | THR | N-CA | -5.57 | 1.38 | 1.46 |
| 14 | a | 931 | ASP | N-CA | 5.57 | 1.52 | 1.45 |
| 7 | M | 543 | VAL | CA-C | 5.56 | 1.59 | 1.52 |
| 9 | S | 621 | HIS | CA-CB | 5.56 | 1.61 | 1.53 |
| 2 | Z | 377 | VAL | C-N | -5.56 | 1.25 | 1.33 |
| 15 | i | 664 | VAL | CA-C | 5.56 | 1.60 | 1.52 |
| 4 | D | 687 | GLU | CA-C | -5.56 | 1.45 | 1.52 |
| 7 | M | 314 | VAL | N-CA | 5.56 | 1.53 | 1.46 |
| 7 | M | 417 | SER | C-N | 5.56 | 1.39 | 1.33 |
| 8 | P | 690 | LEU | CB-CG | 5.56 | 1.64 | 1.53 |
| 8 | P | 879 | ILE | CA-C | -5.56 | 1.45 | 1.52 |
| 9 | R | 551 | ARG | CA-C | 5.56 | 1.60 | 1.52 |
| 1 | Y | 245 | ILE | C-N | 5.56 | 1.41 | 1.33 |
| 12 | u | 143 | VAL | N-CA | -5.56 | 1.39 | 1.46 |
| 21 | q | 75 | HIS | ND1-CE1 | 5.56 | 1.38 | 1.32 |
| 19 | f | 391 | HIS | CA-CB | 5.56 | 1.61 | 1.53 |
| 14 | a | 856 | ILE | CA-CB | 5.56 | 1.61 | 1.54 |
| 9 | S | 550 | PRO | CA-C | -5.56 | 1.44 | 1.52 |
| 2 | 1 | 1070 | ASP | C-N | 5.56 | 1.41 | 1.34 |
| 6 | I | 471 | SER | C-N | 5.56 | 1.41 | 1.33 |
| 7 | M | 66 | VAL | CA-C | -5.56 | 1.46 | 1.52 |
| 8 | N | 519 | SER | C-N | 5.56 | 1.39 | 1.33 |
| 2 | Z | 505 | GLY | CA-C | -5.56 | 1.44 | 1.51 |
| 15 | i | 142 | ALA | CA-C | -5.56 | 1.45 | 1.52 |
| 18 | e | 82 | LYS | CA-CB | 5.56 | 1.60 | 1.53 |
| 18 | e | 135 | ARG | CZ-NH2 | 5.56 | 1.40 | 1.33 |
| 19 | f | 117 | TYR | CA-CB | 5.56 | 1.61 | 1.53 |
| 2 | 1 | 721 | SER | C-N | 5.56 | 1.41 | 1.33 |
| 7 | M | 295 | ARG | NE-CZ | 5.56 | 1.39 | 1.33 |
| 7 | O | 298 | ASP | C-N | 5.56 | 1.41 | 1.33 |
| 20 | n | 538 | ILE | C-N | 5.56 | 1.40 | 1.33 |
| 21 | q | 11 | VAL | CA-CB | -5.56 | 1.47 | 1.54 |
| 15 | b | 435 | GLU | N-CA | -5.56 | 1.38 | 1.46 |
| 2 | Z | 820 | ASP | C-N | 5.56 | 1.41 | 1.34 |
| 13 | w | 1117 | TYR | N-CA | -5.56 | 1.39 | 1.46 |
| 4 | D | 770 | ASN | C-N | 5.55 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | H | 389 | LYS | C-N | 5.55 | 1.41 | 1.33 |
| 7 | M | 442 | ILE | C-N | 5.55 | 1.41 | 1.33 |
| 7 | O | 1154 | ARG | CD-NE | 5.55 | 1.54 | 1.46 |
| 9 | Q | 607 | ARG | CZ-NH1 | 5.55 | 1.40 | 1.32 |
| 9 | S | 373 | ALA | C-N | 5.55 | 1.41 | 1.33 |
| 2 | Z | 646 | TYR | N-CA | -5.55 | 1.39 | 1.46 |
| 15 | b | 531 | LEU | CA-CB | 5.55 | 1.58 | 1.53 |
| 16 | c | 587 | VAL | N-CA | -5.55 | 1.38 | 1.46 |
| 5 | E | 329 | HIS | CE1-NE2 | -5.55 | 1.26 | 1.32 |
| 7 | O | 932 | VAL | CA-CB | -5.55 | 1.47 | 1.55 |
| 9 | R | 624 | THR | C-N | 5.55 | 1.41 | 1.33 |
| 2 | Z | 728 | VAL | CA-CB | -5.55 | 1.47 | 1.54 |
| 12 | v | 156 | ILE | N-CA | -5.55 | 1.39 | 1.46 |
| 5 | H | 466 | LEU | CB-CG | 5.55 | 1.64 | 1.53 |
| 7 | O | 243 | SER | N-CA | -5.55 | 1.39 | 1.46 |
| 8 | P | 1029 | ASN | N-CA | -5.55 | 1.39 | 1.46 |
| 4 | z | 663 | ASN | N-CA | -5.55 | 1.39 | 1.46 |
| 14 | h | 776 | ILE | CA-C | -5.55 | 1.45 | 1.52 |
| 19 | m | 177 | ASP | N-CA | -5.55 | 1.39 | 1.46 |
| 2 | 1 | 1325 | LEU | CA-C | 5.55 | 1.60 | 1.52 |
| 7 | M | 145 | LEU | C-N | 5.55 | 1.41 | 1.33 |
| 7 | O | 1109 | ILE | C-N | 5.55 | 1.41 | 1.34 |
| 12 | u | 707 | GLU | N-CA | -5.55 | 1.39 | 1.46 |
| 15 | b | 109 | SER | N-CA | -5.55 | 1.39 | 1.46 |
| 17 | d | 13 | HIS | ND1-CE1 | 5.55 | 1.38 | 1.32 |
| 20 | g | 508 | ASN | CA-C | -5.55 | 1.45 | 1.52 |
| 14 | a | 924 | ARG | N-CA | -5.55 | 1.39 | 1.46 |
| 1 | 0 | 1189 | LYS | C-N | 5.55 | 1.41 | 1.33 |
| 8 | N | 654 | ILE | C-N | 5.55 | 1.41 | 1.33 |
| 2 | Z | 435 | LYS | CA-C | 5.55 | 1.59 | 1.52 |
| 12 | v | 69 | PHE | C-N | 5.55 | 1.41 | 1.33 |
| 21 | t | 74 | GLY | CA-C | 5.55 | 1.59 | 1.51 |
| 1 | 0 | 233 | LEU | CA-C | 5.55 | 1.59 | 1.52 |
| 8 | N | 349 | PHE | C-N | 5.55 | 1.41 | 1.33 |
| 8 | N | 389 | PHE | CA-CB | 5.55 | 1.62 | 1.53 |
| 7 | O | 1579 | ASN | C-N | 5.55 | 1.40 | 1.33 |
| 9 | Q | 787 | HIS | CA-CB | 5.55 | 1.62 | 1.53 |
| 9 | R | 432 | ILE | CA-CB | -5.55 | 1.47 | 1.54 |
| 2 | Z | 203 | LYS | C-N | 5.55 | 1.40 | 1.33 |
| 16 | j | 417 | PRO | C-N | 5.55 | 1.41 | 1.34 |
| 21 | p | 84 | LEU | CA-CB | 5.55 | 1.60 | 1.53 |
| 18 | e | 45 | TRP | CA-C | -5.55 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | f | 119 | ILE | C-N | 5.55 | 1.41 | 1.33 |
| 19 | f | 364 | GLU | CA-CB | 5.55 | 1.64 | 1.53 |
| 4 | A | 657 | GLN | N-CA | -5.54 | 1.39 | 1.46 |
| 7 | M | 951 | ARG | NE-CZ | 5.54 | 1.39 | 1.33 |
| 7 | O | 347 | LEU | C-N | 5.54 | 1.41 | 1.33 |
| 9 | Q | 430 | LEU | C-N | 5.54 | 1.40 | 1.33 |
| 7 | M | 47 | SER | C-O | -5.54 | 1.17 | 1.24 |
| 8 | N | 1548 | ILE | C-N | -5.54 | 1.26 | 1.33 |
| 8 | P | 617 | TYR | C-N | 5.54 | 1.41 | 1.33 |
| 9 | T | 701 | GLY | N-CA | 5.54 | 1.52 | 1.45 |
| 18 | l | 72 | ILE | CA-C | -5.54 | 1.45 | 1.52 |
| 18 | l | 342 | MET | C-N | 5.54 | 1.40 | 1.33 |
| 19 | m | 122 | VAL | CA-C | 5.54 | 1.60 | 1.52 |
| 9 | R | 546 | ARG | CA-CB | 5.54 | 1.62 | 1.53 |
| 9 | S | 323 | SER | CA-C | -5.54 | 1.45 | 1.52 |
| 15 | i | 369 | GLU | CA-C | -5.54 | 1.45 | 1.52 |
| 16 | j | 399 | LEU | CA-CB | 5.54 | 1.61 | 1.53 |
| 19 | m | 168 | VAL | CA-CB | 5.54 | 1.61 | 1.54 |
| 19 | m | 586 | GLN | N-CA | -5.54 | 1.38 | 1.46 |
| 20 | g | 758 | ILE | CA-CB | -5.54 | 1.48 | 1.54 |
| 1 | 0 | 848 | ILE | C-N | 5.54 | 1.41 | 1.33 |
| 8 | P | 1606 | LEU | CB-CG | 5.54 | 1.64 | 1.53 |
| 9 | R | 792 | SER | N-CA | -5.54 | 1.39 | 1.46 |
| 10 | W | 267 | ILE | CB-CG1 | 5.54 | 1.64 | 1.53 |
| 16 | c | 451 | TRP | N-CA | -5.54 | 1.39 | 1.46 |
| 2 | 1 | 808 | ALA | C-O | -5.54 | 1.16 | 1.24 |
| 2 | 1 | 1166 | ILE | CA-CB | -5.54 | 1.47 | 1.54 |
| 5 | E | 373 | ARG | NE-CZ | 5.54 | 1.39 | 1.33 |
| 7 | O | 845 | ASP | CA-CB | 5.54 | 1.62 | 1.53 |
| 9 | R | 158 | ASN | C-N | 5.54 | 1.41 | 1.33 |
| 9 | R | 214 | ASN | CA-CB | 5.54 | 1.63 | 1.53 |
| 9 | R | 290 | TYR | CA-CB | 5.54 | 1.62 | 1.53 |
| 15 | i | 82 | ILE | CA-CB | -5.54 | 1.47 | 1.54 |
| 20 | g | 1035 | LYS | C-O | -5.54 | 1.17 | 1.24 |
| 2 | 1 | 1331 | ASN | CA-C | -5.54 | 1.45 | 1.52 |
| 8 | P | 418 | ASN | CA-CB | 5.54 | 1.62 | 1.53 |
| 9 | S | 620 | LEU | CA-C | 5.54 | 1.60 | 1.52 |
| 16 | c | 329 | ASP | C-N | 5.54 | 1.39 | 1.34 |
| 1 | 0 | 265 | VAL | C-N | 5.54 | 1.41 | 1.33 |
| 2 | 1 | 400 | SER | C-N | 5.54 | 1.41 | 1.33 |
| 2 | 1 | 912 | ALA | N-CA | -5.54 | 1.38 | 1.46 |
| 7 | M | 439 | LEU | N-CA | -5.54 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 11 | V | 395 | LEU | CA-CB | 5.54 | 1.62 | 1.53 |
| 15 | i | 724 | MET | CA-CB | 5.54 | 1.60 | 1.53 |
| 17 | d | 216 | VAL | CA-C | -5.54 | 1.46 | 1.52 |
| 8 | N | 141 | LEU | CA-C | -5.53 | 1.45 | 1.52 |
| 20 | n | 74 | THR | CB-OG1 | -5.53 | 1.34 | 1.43 |
| 14 | a | 87 | ALA | C-N | 5.53 | 1.42 | 1.33 |
| 7 | M | 1560 | GLY | C-N | 5.53 | 1.41 | 1.33 |
| 7 | O | 916 | ILE | C-N | 5.53 | 1.41 | 1.33 |
| 1 | 0 | 1417 | ILE | CA-C | -5.53 | 1.45 | 1.52 |
| 2 | 1 | 501 | ILE | C-N | 5.53 | 1.40 | 1.33 |
| 7 | O | 120 | ILE | CB-CG1 | 5.53 | 1.64 | 1.53 |
| 7 | O | 428 | GLN | N-CA | -5.53 | 1.39 | 1.46 |
| 9 | Q | 774 | LEU | CA-CB | 5.53 | 1.62 | 1.53 |
| 9 | R | 409 | LEU | CA-C | -5.53 | 1.45 | 1.52 |
| 12 | u | 655 | LEU | CA-C | -5.53 | 1.45 | 1.52 |
| 14 | a | 161 | ARG | CD-NE | 5.53 | 1.53 | 1.46 |
| 6 | I | 461 | HIS | CA-C | 5.53 | 1.60 | 1.52 |
| 6 | C | 275 | GLN | C-N | 5.53 | 1.41 | 1.33 |
| 8 | P | 1612 | LEU | C-N | 5.53 | 1.41 | 1.33 |
| 9 | S | 232 | PHE | CA-CB | 5.53 | 1.65 | 1.53 |
| 20 | n | 475 | LEU | C-N | 5.53 | 1.41 | 1.33 |
| 21 | p | 69 | VAL | CA-CB | -5.53 | 1.47 | 1.54 |
| 18 | e | 101 | LEU | N-CA | -5.53 | 1.40 | 1.46 |
| 18 | e | 201 | LYS | CA-C | -5.53 | 1.45 | 1.52 |
| 14 | a | 246 | TRP | CD2-CE2 | 5.53 | 1.50 | 1.41 |
| 8 | N | 713 | LYS | C-N | 5.53 | 1.41 | 1.33 |
| 8 | N | 1264 | SER | C-N | 5.53 | 1.41 | 1.33 |
| 7 | O | 992 | ASP | CA-C | -5.53 | 1.45 | 1.52 |
| 4 | y | 640 | LEU | N-CA | -5.53 | 1.39 | 1.46 |
| 14 | h | 419 | ILE | CA-CB | -5.53 | 1.46 | 1.54 |
| 19 | m | 534 | SER | N-CA | 5.53 | 1.52 | 1.46 |
| 20 | n | 107 | ILE | C-N | 5.53 | 1.41 | 1.33 |
| 16 | c | 319 | SER | C-N | 5.53 | 1.41 | 1.33 |
| 8 | P | 779 | LEU | C-N | 5.52 | 1.40 | 1.33 |
| 9 | S | 65 | ASP | C-N | 5.52 | 1.40 | 1.33 |
| 12 | v | 40 | ASP | CA-CB | 5.52 | 1.59 | 1.52 |
| 20 | g | 750 | TYR | CA-CB | 5.52 | 1.62 | 1.53 |
| 2 | 1 | 262 | ASN | C-O | -5.52 | 1.17 | 1.23 |
| 8 | N | 137 | VAL | C-N | 5.52 | 1.40 | 1.33 |
| 8 | N | 1025 | ASN | CA-C | -5.52 | 1.46 | 1.52 |
| 8 | P | 834 | ILE | N-CA | -5.52 | 1.39 | 1.46 |
| 9 | S | 732 | TRP | CA-C | -5.52 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | T | 315 | LYS | CA-C | -5.52 | 1.44 | 1.52 |
| 11 | V | 280 | ILE | N-CA | -5.52 | 1.39 | 1.46 |
| 1 | Y | 1151 | LYS | CA-C | -5.52 | 1.45 | 1.52 |
| 19 | m | 642 | ASN | CA-C | -5.52 | 1.46 | 1.52 |
| 15 | b | 320 | SER | C-N | 5.52 | 1.40 | 1.33 |
| 7 | M | 1278 | GLU | N-CA | -5.52 | 1.39 | 1.46 |
| 8 | N | 1030 | SER | CA-CB | 5.52 | 1.62 | 1.53 |
| 8 | P | 863 | GLY | CA-C | -5.52 | 1.44 | 1.51 |
| 14 | a | 495 | TYR | CA-CB | 5.52 | 1.63 | 1.53 |
| 5 | H | 330 | VAL | N-CA | -5.52 | 1.39 | 1.46 |
| 7 | O | 1137 | ASN | CA-CB | 5.52 | 1.64 | 1.53 |
| 9 | S | 790 | ASN | C-N | 5.52 | 1.41 | 1.33 |
| 1 | Y | 1464 | ASP | N-CA | -5.52 | 1.39 | 1.46 |
| 4 | y | 769 | ILE | CA-C | -5.52 | 1.45 | 1.52 |
| 14 | h | 24 | VAL | CA-C | -5.52 | 1.45 | 1.52 |
| 19 | m | 199 | GLU | C-N | 5.52 | 1.41 | 1.33 |
| 6 | C | 277 | ILE | N-CA | -5.52 | 1.40 | 1.46 |
| 5 | E | 449 | ASP | CA-C | -5.52 | 1.47 | 1.53 |
| 7 | M | 469 | LEU | CA-C | -5.52 | 1.45 | 1.52 |
| 8 | P | 723 | LEU | CA-C | -5.52 | 1.45 | 1.52 |
| 9 | S | 534 | PHE | C-N | 5.52 | 1.42 | 1.33 |
| 9 | T | 563 | ASN | N-CA | -5.52 | 1.39 | 1.45 |
| 15 | b | 497 | ARG | NE-CZ | 5.52 | 1.39 | 1.33 |
| 17 | d | 174 | VAL | CA-CB | -5.52 | 1.47 | 1.54 |
| 12 | v | 142 | ILE | CA-CB | 5.52 | 1.60 | 1.54 |
| 1 | 0 | 668 | PRO | CA-C | -5.51 | 1.45 | 1.53 |
| 8 | P | 23 | ASN | CA-C | -5.51 | 1.45 | 1.52 |
| 8 | P | 499 | LEU | CA-C | -5.51 | 1.46 | 1.52 |
| 12 | v | 358 | ARG | CD-NE | 5.51 | 1.53 | 1.46 |
| 14 | h | 493 | TRP | N-CA | -5.51 | 1.39 | 1.46 |
| 19 | m | 339 | SER | CA-CB | 5.51 | 1.62 | 1.53 |
| 21 | o | 29 | LYS | CA-C | 5.51 | 1.59 | 1.52 |
| 1 | 0 | 774 | ALA | N-CA | -5.51 | 1.39 | 1.46 |
| 19 | m | 269 | GLY | CA-C | 5.51 | 1.59 | 1.51 |
| 21 | o | 76 | PHE | C-O | -5.51 | 1.17 | 1.23 |
| 2 | 1 | 1221 | ARG | CA-C | -5.51 | 1.45 | 1.52 |
| 7 | M | 1398 | SER | C-N | 5.51 | 1.40 | 1.33 |
| 8 | N | 1264 | SER | CA-CB | 5.51 | 1.62 | 1.53 |
| 10 | W | 326 | ARG | CA-C | -5.51 | 1.45 | 1.52 |
| 15 | b | 743 | PHE | C-N | 5.51 | 1.41 | 1.33 |
| 1 | 0 | 691 | LYS | N-CA | -5.51 | 1.39 | 1.47 |
| 7 | M | 1294 | LYS | C-N | 5.51 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | O | 61 | GLY | CA-C | -5.51 | 1.44 | 1.51 |
| 8 | P | 851 | SER | C-N | 5.51 | 1.40 | 1.33 |
| 14 | h | 26 | LEU | CA-CB | 5.51 | 1.62 | 1.53 |
| 17 | k | 276 | ASN | CB-CG | 5.51 | 1.65 | 1.52 |
| 15 | b | 113 | GLU | C-O | -5.51 | 1.17 | 1.24 |
| 19 | f | 236 | GLY | CA-C | -5.51 | 1.44 | 1.52 |
| 14 | a | 802 | TYR | CA-CB | 5.51 | 1.59 | 1.52 |
| 2 | 1 | 99 | GLN | N-CA | -5.51 | 1.39 | 1.46 |
| 4 | A | 640 | LEU | CA-CB | 5.51 | 1.62 | 1.53 |
| 5 | H | 520 | ILE | N-CA | -5.51 | 1.40 | 1.46 |
| 9 | Q | 797 | SER | CA-CB | 5.51 | 1.62 | 1.53 |
| 15 | i | 356 | SER | C-N | 5.51 | 1.41 | 1.34 |
| 5 | K | 401 | ALA | N-CA | -5.51 | 1.39 | 1.46 |
| 7 | O | 534 | SER | CA-C | -5.51 | 1.45 | 1.52 |
| 18 | l | 150 | LEU | C-N | 5.51 | 1.40 | 1.33 |
| 20 | g | 178 | ILE | C-N | 5.51 | 1.41 | 1.33 |
| 14 | a | 79 | LEU | CA-CB | 5.51 | 1.60 | 1.52 |
| 14 | a | 119 | VAL | CA-C | -5.51 | 1.46 | 1.52 |
| 10 | U | 330 | GLU | C-N | 5.50 | 1.42 | 1.33 |
| 1 | Y | 588 | THR | C-N | 5.50 | 1.41 | 1.33 |
| 15 | i | 542 | LEU | C-O | -5.50 | 1.17 | 1.24 |
| 20 | g | 251 | PRO | C-N | 5.50 | 1.41 | 1.33 |
| 20 | g | 278 | LYS | CA-CB | 5.50 | 1.61 | 1.53 |
| 8 | N | 1413 | ASN | CA-CB | 5.50 | 1.61 | 1.53 |
| 9 | S | 477 | TYR | N-CA | -5.50 | 1.38 | 1.46 |
| 9 | S | 560 | ILE | C-N | 5.50 | 1.41 | 1.33 |
| 12 | v | 396 | CYS | C-N | 5.50 | 1.40 | 1.34 |
| 16 | j | 779 | LYS | CA-C | 5.50 | 1.60 | 1.52 |
| 15 | b | 218 | GLU | N-CA | -5.50 | 1.38 | 1.45 |
| 19 | f | 405 | GLU | N-CA | -5.50 | 1.39 | 1.46 |
| 2 | 1 | 1384 | LYS | CA-C | 5.50 | 1.60 | 1.53 |
| 9 | S | 542 | THR | CA-C | -5.50 | 1.45 | 1.52 |
| 9 | T | 763 | LEU | CA-CB | 5.50 | 1.62 | 1.53 |
| 10 | W | 324 | LYS | N-CA | -5.50 | 1.39 | 1.46 |
| 1 | Y | 603 | GLY | N-CA | 5.50 | 1.50 | 1.43 |
| 21 | o | 10 | ILE | C-N | 5.50 | 1.41 | 1.33 |
| 15 | b | 658 | LEU | CA-CB | 5.50 | 1.62 | 1.53 |
| 1 | 0 | 1263 | GLN | C-N | 5.50 | 1.41 | 1.33 |
| 7 | M | 762 | ALA | C-O | -5.50 | 1.17 | 1.24 |
| 8 | N | 301 | ALA | C-N | 5.50 | 1.40 | 1.33 |
| 8 | N | 1239 | ASP | CA-CB | 5.50 | 1.62 | 1.53 |
| 7 | O | 315 | GLU | CA-C | 5.50 | 1.60 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1579 | ASN | CA-C | -5.50 | 1.45 | 1.52 |
| 1 | Y | 860 | ILE | C-N | 5.50 | 1.41 | 1.33 |
| 15 | i | 566 | GLU | CA-C | -5.50 | 1.45 | 1.52 |
| 16 | j | 204 | SER | CA-CB | 5.50 | 1.63 | 1.53 |
| 15 | b | 699 | TRP | C-N | 5.50 | 1.41 | 1.33 |
| 19 | f | 240 | HIS | C-N | 5.50 | 1.42 | 1.33 |
| 20 | g | 548 | PRO | CA-C | 5.50 | 1.59 | 1.52 |
| 4 | G | 755 | LEU | CA-C | -5.50 | 1.45 | 1.52 |
| 5 | H | 419 | LEU | CB-CG | 5.50 | 1.64 | 1.53 |
| 8 | P | 780 | HIS | ND1-CE1 | 5.50 | 1.38 | 1.32 |
| 1 | Y | 1150 | LEU | C-N | 5.50 | 1.41 | 1.33 |
| 2 | Z | 1112 | ALA | C-N | 5.50 | 1.41 | 1.33 |
| 12 | u | 150 | THR | C-N | 5.50 | 1.40 | 1.33 |
| 19 | m | 706 | GLN | N-CA | 5.50 | 1.52 | 1.45 |
| 5 | H | 456 | THR | CA-C | 5.50 | 1.59 | 1.52 |
| 8 | N | 1193 | ASN | C-N | 5.50 | 1.41 | 1.33 |
| 7 | O | 1655 | SER | C-N | 5.50 | 1.41 | 1.33 |
| 8 | P | 1506 | LEU | C-N | 5.50 | 1.41 | 1.33 |
| 12 | u | 80 | LEU | N-CA | -5.50 | 1.39 | 1.46 |
| 14 | h | 84 | LEU | CA-C | 5.50 | 1.60 | 1.52 |
| 21 | q | 13 | ALA | CA-C | -5.50 | 1.45 | 1.52 |
| 16 | c | 663 | GLN | C-N | 5.50 | 1.42 | 1.33 |
| 19 | f | 421 | LYS | N-CA | 5.50 | 1.53 | 1.46 |
| 14 | a | 669 | ARG | CD-NE | 5.50 | 1.53 | 1.46 |
| 4 | G | 688 | HIS | N-CA | -5.50 | 1.39 | 1.46 |
| 9 | R | 440 | LEU | N-CA | -5.50 | 1.39 | 1.46 |
| 9 | R | 669 | ASP | C-N | 5.50 | 1.40 | 1.33 |
| 14 | h | 572 | ASP | CA-CB | 5.50 | 1.62 | 1.53 |
| 14 | h | 648 | GLY | CA-C | 5.50 | 1.58 | 1.52 |
| 15 | i | 369 | GLU | CA-CB | 5.50 | 1.62 | 1.53 |
| 16 | j | 130 | ASP | CA-CB | 5.50 | 1.63 | 1.53 |
| 16 | j | 390 | CYS | CA-C | -5.50 | 1.45 | 1.52 |
| 16 | j | 463 | ARG | NE-CZ | 5.50 | 1.39 | 1.33 |
| 16 | c | 459 | PHE | CA-CB | 5.50 | 1.62 | 1.53 |
| 7 | M | 248 | PRO | C-O | -5.49 | 1.17 | 1.23 |
| 8 | N | 208 | ILE | CA-CB | -5.49 | 1.46 | 1.54 |
| 8 | N | 675 | TYR | C-N | 5.49 | 1.41 | 1.33 |
| 8 | P | 1168 | LYS | CA-CB | 5.49 | 1.62 | 1.53 |
| 9 | R | 487 | LEU | C-N | 5.49 | 1.40 | 1.33 |
| 9 | R | 826 | ARG | CD-NE | 5.49 | 1.53 | 1.46 |
| 9 | T | 497 | THR | C-N | 5.49 | 1.41 | 1.33 |
| 2 | Z | 1107 | HIS | CA-CB | 5.49 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 16 | j | 419 | GLY | C-N | 5.49 | 1.40 | 1.34 |
| 18 | l | 25 | ALA | C-N | 5.49 | 1.41 | 1.33 |
| 20 | n | 556 | HIS | ND1-CE1 | 5.49 | 1.38 | 1.32 |
| 15 | b | 529 | TRP | CD2-CE3 | -5.49 | 1.31 | 1.40 |
| 14 | a | 414 | ARG | CD-NE | 5.49 | 1.53 | 1.46 |
| 6 | C | 323 | SER | CA-C | -5.49 | 1.45 | 1.52 |
| 6 | L | 469 | SER | CA-C | 5.49 | 1.59 | 1.52 |
| 9 | S | 260 | LEU | CA-C | 5.49 | 1.60 | 1.52 |
| 1 | 0 | 382 | ILE | CA-C | -5.49 | 1.45 | 1.52 |
| 9 | R | 315 | LYS | C-N | 5.49 | 1.42 | 1.33 |
| 9 | S | 690 | ARG | CD-NE | 5.49 | 1.53 | 1.46 |
| 9 | T | 340 | LEU | N-CA | -5.49 | 1.39 | 1.46 |
| 1 | Y | 266 | GLN | CA-CB | 5.49 | 1.62 | 1.53 |
| 15 | i | 673 | PRO | CA-C | 5.49 | 1.58 | 1.52 |
| 19 | m | 552 | ARG | C-N | 5.49 | 1.41 | 1.33 |
| 20 | n | 467 | VAL | CA-CB | -5.49 | 1.47 | 1.54 |
| 19 | f | 308 | VAL | N-CA | -5.49 | 1.39 | 1.46 |
| 14 | a | 319 | ILE | CA-CB | -5.49 | 1.47 | 1.54 |
| 1 | 0 | 1408 | VAL | C-N | 5.49 | 1.41 | 1.33 |
| 6 | F | 386 | ASP | C-N | 5.49 | 1.41 | 1.34 |
| 9 | S | 257 | TRP | NE1-CE2 | -5.49 | 1.31 | 1.37 |
| 11 | V | 384 | CYS | C-N | 5.49 | 1.38 | 1.33 |
| 1 | Y | 235 | SER | N-CA | 5.49 | 1.52 | 1.45 |
| 1 | Y | 1445 | ASN | CA-CB | 5.49 | 1.62 | 1.53 |
| 2 | Z | 251 | LEU | N-CA | -5.49 | 1.39 | 1.46 |
| 20 | n | 478 | PHE | CA-C | 5.49 | 1.59 | 1.52 |
| 21 | p | 69 | VAL | C-N | 5.49 | 1.41 | 1.33 |
| 16 | c | 598 | ILE | C-N | 5.49 | 1.40 | 1.33 |
| 6 | L | 350 | PHE | CA-CB | 5.49 | 1.63 | 1.53 |
| 7 | O | 648 | PRO | CA-C | 5.49 | 1.57 | 1.52 |
| 9 | S | 566 | PRO | C-N | 5.49 | 1.40 | 1.33 |
| 9 | S | 683 | THR | N-CA | -5.49 | 1.40 | 1.46 |
| 14 | h | 826 | TYR | CA-CB | 5.49 | 1.62 | 1.53 |
| 7 | O | 104 | VAL | CA-C | 5.49 | 1.59 | 1.52 |
| 1 | Y | 1303 | SER | CA-CB | 5.49 | 1.62 | 1.53 |
| 15 | b | 552 | ILE | N-CA | -5.49 | 1.39 | 1.46 |
| 18 | e | 38 | LEU | C-O | -5.49 | 1.17 | 1.24 |
| 19 | f | 403 | SER | C-N | 5.49 | 1.40 | 1.33 |
| 8 | N | 680 | ASP | C-N | 5.48 | 1.41 | 1.33 |
| 8 | N | 880 | ASN | N-CA | -5.48 | 1.39 | 1.46 |
| 19 | f | 18 | THR | C-N | 5.48 | 1.41 | 1.33 |
| 6 | I | 348 | GLN | N-CA | 5.48 | 1.52 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | K | 445 | GLN | CA-CB | 5.48 | 1.62 | 1.53 |
| 7 | M | 86 | ILE | N-CA | 5.48 | 1.53 | 1.46 |
| 7 | O | 319 | ILE | C-N | 5.48 | 1.41 | 1.33 |
| 7 | O | 658 | SER | CA-C | 5.48 | 1.60 | 1.52 |
| 8 | P | 327 | PHE | CA-CB | 5.48 | 1.62 | 1.53 |
| 8 | P | 921 | SER | CA-C | 5.48 | 1.59 | 1.52 |
| 9 | Q | 353 | LEU | CB-CG | 5.48 | 1.64 | 1.53 |
| 20 | n | 78 | SER | C-N | 5.48 | 1.41 | 1.33 |
| 20 | n | 344 | SER | CA-CB | 5.48 | 1.61 | 1.53 |
| 17 | d | 19 | TYR | C-O | -5.48 | 1.17 | 1.24 |
| 1 | 0 | 1313 | VAL | C-N | 5.48 | 1.40 | 1.34 |
| 7 | M | 1258 | HIS | CE1-NE2 | -5.48 | 1.27 | 1.32 |
| 7 | O | 218 | HIS | ND1-CE1 | 5.48 | 1.38 | 1.32 |
| 2 | Z | 804 | SER | C-N | 5.48 | 1.40 | 1.33 |
| 14 | h | 725 | ARG | CA-C | 5.48 | 1.59 | 1.52 |
| 15 | i | 647 | ARG | CD-NE | 5.48 | 1.53 | 1.46 |
| 15 | b | 403 | HIS | ND1-CE1 | 5.48 | 1.38 | 1.32 |
| 8 | P | 1645 | LYS | CA-C | 5.48 | 1.59 | 1.52 |
| 2 | Z | 867 | LEU | CA-C | -5.48 | 1.45 | 1.52 |
| 12 | v | 532 | SER | C-N | 5.48 | 1.41 | 1.33 |
| 19 | m | 318 | PRO | N-CD | -5.48 | 1.40 | 1.47 |
| 8 | N | 1060 | LEU | CA-C | -5.48 | 1.45 | 1.52 |
| 8 | N | 1176 | PRO | CA-CB | 5.48 | 1.62 | 1.53 |
| 9 | Q | 304 | LYS | CA-C | -5.48 | 1.45 | 1.52 |
| 12 | u | 251 | LYS | CA-CB | 5.48 | 1.61 | 1.53 |
| 13 | x | 1269 | LEU | CA-C | -5.48 | 1.45 | 1.52 |
| 16 | c | 517 | LEU | CA-CB | -5.48 | 1.46 | 1.54 |
| 2 | 1 | 1227 | GLN | CA-CB | 5.48 | 1.62 | 1.53 |
| 4 | A | 722 | LEU | C-N | 5.48 | 1.41 | 1.33 |
| 8 | N | 1320 | GLU | N-CA | -5.48 | 1.39 | 1.46 |
| 9 | Q | 578 | GLU | CA-C | -5.48 | 1.44 | 1.52 |
| 11 | X | 373 | ASN | CA-CB | 5.48 | 1.63 | 1.53 |
| 2 | 1 | 275 | THR | N-CA | -5.47 | 1.39 | 1.45 |
| 9 | S | 130 | ASN | C-N | 5.47 | 1.40 | 1.33 |
| 2 | Z | 708 | ARG | C-N | 5.47 | 1.41 | 1.33 |
| 12 | v | 362 | SER | C-N | 5.47 | 1.41 | 1.33 |
| 20 | g | 605 | ARG | C-N | 5.47 | 1.41 | 1.33 |
| 5 | B | 379 | ILE | N-CA | -5.47 | 1.39 | 1.46 |
| 9 | Q | 724 | ARG | CZ-NH1 | 5.47 | 1.40 | 1.32 |
| 9 | T | 106 | SER | N-CA | -5.47 | 1.39 | 1.46 |
| 1 | Y | 1158 | HIS | CB-CG | 5.47 | 1.57 | 1.50 |
| 15 | i | 664 | VAL | N-CA | -5.47 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 16 | j | 248 | TYR | N-CA | 5.47 | 1.52 | 1.45 |
| 19 | f | 270 | ALA | C-N | 5.47 | 1.39 | 1.33 |
| 19 | f | 643 | PHE | CA-CB | 5.47 | 1.62 | 1.53 |
| 20 | g | 164 | LEU | CA-C | -5.47 | 1.45 | 1.52 |
| 20 | g | 552 | THR | C-N | 5.47 | 1.42 | 1.33 |
| 4 | G | 753 | GLU | CA-CB | 5.47 | 1.62 | 1.53 |
| 2 | Z | 664 | PHE | CA-C | -5.47 | 1.45 | 1.52 |
| 19 | m | 684 | ILE | CA-CB | 5.47 | 1.60 | 1.54 |
| 1 | 0 | 227 | ALA | C-N | 5.47 | 1.41 | 1.33 |
| 1 | 0 | 1078 | LYS | C-N | 5.47 | 1.40 | 1.33 |
| 7 | O | 442 | ILE | C-N | 5.47 | 1.40 | 1.33 |
| 8 | P | 362 | LEU | CA-CB | 5.47 | 1.61 | 1.53 |
| 8 | P | 1129 | LYS | CA-CB | 5.47 | 1.57 | 1.53 |
| 9 | S | 659 | SER | N-CA | 5.47 | 1.53 | 1.46 |
| 16 | c | 606 | GLU | CA-C | -5.47 | 1.45 | 1.52 |
| 20 | g | 961 | SER | N-CA | -5.47 | 1.39 | 1.46 |
| 14 | a | 694 | ASN | N-CA | -5.47 | 1.39 | 1.46 |
| 2 | Z | 173 | TRP | CA-CB | 5.47 | 1.60 | 1.53 |
| 19 | m | 175 | GLU | N-CA | 5.47 | 1.53 | 1.46 |
| 1 | 0 | 1303 | SER | CA-C | -5.47 | 1.46 | 1.52 |
| 7 | M | 1285 | HIS | ND1-CE1 | 5.47 | 1.38 | 1.32 |
| 8 | N | 444 | ASN | C-N | 5.47 | 1.41 | 1.33 |
| 8 | N | 721 | GLU | CA-C | -5.47 | 1.45 | 1.52 |
| 7 | O | 878 | TYR | C-N | 5.47 | 1.42 | 1.33 |
| 2 | Z | 615 | ARG | CZ-NH2 | 5.47 | 1.40 | 1.33 |
| 12 | v | 564 | LEU | N-CA | -5.47 | 1.39 | 1.46 |
| 18 | l | 204 | VAL | N-CA | 5.47 | 1.53 | 1.46 |
| 20 | n | 811 | LEU | CA-C | -5.47 | 1.46 | 1.52 |
| 20 | g | 1073 | ASN | CA-C | -5.47 | 1.44 | 1.52 |
| 14 | a | 327 | ALA | C-N | 5.47 | 1.41 | 1.33 |
| 7 | O | 65 | LYS | CA-CB | 5.46 | 1.60 | 1.53 |
| 2 | Z | 1078 | GLN | C-O | -5.46 | 1.17 | 1.23 |
| 12 | u | 172 | SER | N-CA | -5.46 | 1.39 | 1.46 |
| 12 | u | 345 | ASN | CA-C | -5.46 | 1.46 | 1.53 |
| 20 | n | 410 | THR | C-N | 5.46 | 1.41 | 1.33 |
| 1 | 0 | 524 | THR | C-N | 5.46 | 1.40 | 1.33 |
| 5 | K | 449 | ASP | CA-CB | 5.46 | 1.61 | 1.53 |
| 8 | P | 1531 | SER | CA-C | 5.46 | 1.59 | 1.52 |
| 9 | Q | 792 | SER | CA-C | -5.46 | 1.46 | 1.52 |
| 1 | Y | 629 | ALA | C-N | 5.46 | 1.41 | 1.33 |
| 20 | g | 649 | PHE | C-N | 5.46 | 1.41 | 1.34 |
| 14 | a | 108 | LEU | CA-C | -5.46 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | F | 286 | LYS | N-CA | 5.46 | 1.53 | 1.46 |
| 9 | R | 662 | SER | C-N | 5.46 | 1.40 | 1.33 |
| 1 | Y | 279 | SER | C-N | 5.46 | 1.39 | 1.33 |
| 1 | Y | 454 | ARG | NE-CZ | 5.46 | 1.39 | 1.33 |
| 1 | Y | 1219 | ARG | CZ-NH2 | 5.46 | 1.40 | 1.33 |
| 15 | i | 140 | HIS | CA-C | -5.46 | 1.45 | 1.52 |
| 19 | f | 381 | ASP | CA-CB | 5.46 | 1.61 | 1.53 |
| 8 | N | 425 | LEU | N-CA | -5.46 | 1.39 | 1.46 |
| 16 | j | 252 | ASN | CA-C | -5.46 | 1.46 | 1.52 |
| 21 | r | 76 | PHE | C-N | 5.46 | 1.39 | 1.33 |
| 21 | s | 51 | VAL | CA-C | 5.46 | 1.59 | 1.52 |
| 20 | g | 552 | THR | C-O | 5.46 | 1.31 | 1.24 |
| 1 | 0 | 1386 | PRO | C-N | 5.46 | 1.39 | 1.34 |
| 2 | 1 | 885 | VAL | CA-CB | -5.46 | 1.47 | 1.54 |
| 6 | F | 345 | LEU | N-CA | -5.46 | 1.39 | 1.46 |
| 5 | K | 537 | TYR | CA-CB | 5.46 | 1.61 | 1.53 |
| 7 | M | 1645 | LEU | N-CA | 5.46 | 1.52 | 1.46 |
| 7 | O | 1302 | VAL | C-N | 5.46 | 1.40 | 1.33 |
| 8 | P | 659 | GLU | CA-C | -5.46 | 1.45 | 1.52 |
| 9 | T | 720 | ILE | C-N | 5.46 | 1.41 | 1.33 |
| 10 | U | 312 | GLY | C-N | -5.46 | 1.26 | 1.33 |
| 2 | Z | 1266 | SER | C-N | 5.46 | 1.41 | 1.33 |
| 13 | w | 1226 | THR | CA-C | -5.46 | 1.45 | 1.52 |
| 14 | h | 135 | LEU | CA-C | -5.46 | 1.43 | 1.52 |
| 20 | n | 646 | PHE | N-CA | -5.46 | 1.39 | 1.46 |
| 21 | s | 22 | GLU | CA-C | -5.46 | 1.45 | 1.52 |
| 14 | a | 74 | SER | CA-CB | 5.46 | 1.62 | 1.53 |
| 7 | M | 1124 | GLY | CA-C | -5.46 | 1.44 | 1.51 |
| 9 | R | 627 | ALA | N-CA | 5.46 | 1.52 | 1.46 |
| 1 | Y | 703 | LEU | CA-C | -5.46 | 1.46 | 1.53 |
| 1 | Y | 1458 | SER | CA-C | -5.46 | 1.45 | 1.52 |
| 17 | d | 272 | SER | CA-C | -5.46 | 1.46 | 1.52 |
| 18 | e | 8 | HIS | CA-CB | 5.46 | 1.62 | 1.53 |
| 7 | M | 1122 | TRP | C-N | 5.46 | 1.41 | 1.33 |
| 7 | O | 16 | GLU | CA-CB | 5.46 | 1.61 | 1.53 |
| 8 | P | 1396 | THR | N-CA | -5.46 | 1.39 | 1.46 |
| 1 | 0 | 695 | LEU | CA-CB | 5.45 | 1.63 | 1.53 |
| 21 | s | 74 | GLY | N-CA | -5.45 | 1.36 | 1.45 |
| 16 | c | 498 | ASN | CA-C | 5.45 | 1.59 | 1.52 |
| 17 | d | 132 | GLU | CA-C | -5.45 | 1.45 | 1.52 |
| 14 | a | 609 | GLY | CA-C | -5.45 | 1.45 | 1.52 |
| 9 | Q | 42 | ILE | CA-C | -5.45 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | i | 188 | MET | C-N | 5.45 | 1.41 | 1.33 |
| 19 | f | 412 | LEU | N-CA | -5.45 | 1.39 | 1.46 |
| 20 | g | 1036 | PHE | CA-C | -5.45 | 1.45 | 1.52 |
| 12 | v | 353 | ARG | CD-NE | 5.45 | 1.53 | 1.46 |
| 17 | k | 23 | ARG | CA-CB | 5.45 | 1.62 | 1.53 |
| 17 | k | 37 | GLU | C-N | 5.45 | 1.39 | 1.33 |
| 16 | c | 243 | PRO | N-CD | -5.45 | 1.40 | 1.47 |
| 18 | e | 223 | SER | C-N | 5.45 | 1.40 | 1.33 |
| 2 | 1 | 583 | PRO | N-CA | -5.45 | 1.40 | 1.47 |
| 8 | N | 1225 | GLY | CA-C | -5.45 | 1.45 | 1.52 |
| 9 | S | 318 | LYS | CA-C | -5.45 | 1.45 | 1.52 |
| 9 | S | 787 | HIS | ND1-CE1 | 5.45 | 1.38 | 1.32 |
| 9 | T | 279 | GLU | CA-C | -5.45 | 1.45 | 1.52 |
| 1 | Y | 1487 | TYR | N-CA | -5.45 | 1.39 | 1.46 |
| 14 | h | 200 | ASN | CA-CB | 5.45 | 1.62 | 1.53 |
| 19 | m | 358 | VAL | C-O | -5.45 | 1.17 | 1.24 |
| 19 | m | 625 | LYS | CA-CB | 5.45 | 1.61 | 1.53 |
| 19 | m | 642 | ASN | N-CA | -5.45 | 1.39 | 1.45 |
| 15 | b | 548 | SER | CA-CB | 5.45 | 1.60 | 1.53 |
| 18 | e | 6 | SER | C-N | 5.45 | 1.40 | 1.33 |
| 1 | 0 | 1453 | HIS | ND1-CE1 | 5.45 | 1.38 | 1.32 |
| 7 | M | 457 | GLU | CA-CB | 5.45 | 1.62 | 1.53 |
| 7 | M | 1408 | LEU | C-N | 5.45 | 1.40 | 1.33 |
| 1 | Y | 154 | PHE | N-CA | -5.45 | 1.39 | 1.46 |
| 6 | L | 280 | LEU | CA-C | -5.45 | 1.45 | 1.52 |
| 7 | O | 495 | TYR | CA-C | -5.45 | 1.45 | 1.52 |
| 7 | O | 1105 | PHE | CA-C | 5.45 | 1.59 | 1.52 |
| 9 | R | 304 | LYS | C-N | 5.45 | 1.41 | 1.33 |
| 9 | R | 463 | GLN | C-N | 5.45 | 1.41 | 1.33 |
| 9 | T | 68 | LYS | N-CA | -5.45 | 1.39 | 1.46 |
| 18 | l | 328 | VAL | N-CA | -5.45 | 1.39 | 1.46 |
| 17 | d | 127 | VAL | C-N | 5.45 | 1.39 | 1.33 |
| 19 | f | 19 | LEU | CA-C | 5.45 | 1.59 | 1.52 |
| 19 | f | 182 | LYS | CA-CB | 5.45 | 1.61 | 1.53 |
| 19 | f | 245 | ARG | CD-NE | 5.45 | 1.53 | 1.46 |
| 19 | f | 548 | GLN | CA-C | -5.45 | 1.45 | 1.52 |
| 7 | M | 120 | ILE | CA-CB | 5.44 | 1.60 | 1.54 |
| 7 | O | 978 | ILE | CB-CG1 | 5.44 | 1.64 | 1.53 |
| 9 | T | 72 | LEU | C-O | -5.44 | 1.17 | 1.24 |
| 17 | k | 41 | GLU | CA-C | -5.44 | 1.45 | 1.52 |
| 4 | D | 671 | LYS | CA-CB | 5.44 | 1.61 | 1.53 |
| 4 | D | 702 | ARG | CA-C | -5.44 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | J | 818 | ILE | CA-C | -5.44 | 1.45 | 1.52 |
| 7 | M | 214 | LEU | CA-CB | 5.44 | 1.61 | 1.53 |
| 8 | N | 771 | LEU | CA-C | -5.44 | 1.45 | 1.52 |
| 7 | O | 181 | PHE | C-N | 5.44 | 1.41 | 1.33 |
| 9 | T | 288 | ASN | N-CA | -5.44 | 1.39 | 1.46 |
| 1 | Y | 1421 | VAL | CA-C | -5.44 | 1.45 | 1.52 |
| 2 | Z | 924 | SER | CA-C | -5.44 | 1.46 | 1.52 |
| 12 | v | 182 | ILE | N-CA | -5.44 | 1.39 | 1.46 |
| 14 | h | 255 | GLN | CD-NE2 | 5.44 | 1.44 | 1.33 |
| 17 | k | 28 | SER | C-N | 5.44 | 1.41 | 1.33 |
| 18 | l | 135 | ARG | C-N | 5.44 | 1.41 | 1.33 |
| 1 | 0 | 1096 | GLN | C-N | 5.44 | 1.40 | 1.33 |
| 2 | 1 | 863 | ILE | C-N | 5.44 | 1.40 | 1.33 |
| 8 | P | 466 | THR | CA-C | 5.44 | 1.60 | 1.53 |
| 8 | P | 1597 | ARG | CZ-NH2 | 5.44 | 1.40 | 1.33 |
| 9 | R | 727 | TYR | C-N | 5.44 | 1.41 | 1.33 |
| 9 | R | 775 | LEU | CA-C | -5.44 | 1.45 | 1.52 |
| 13 | x | 1443 | MET | CA-CB | 5.44 | 1.61 | 1.53 |
| 19 | f | 173 | ASP | CA-C | 5.44 | 1.60 | 1.52 |
| 9 | T | 473 | ARG | NE-CZ | 5.44 | 1.39 | 1.33 |
| 16 | j | 566 | ASP | CA-C | 5.44 | 1.59 | 1.52 |
| 19 | f | 244 | ARG | CA-C | 5.44 | 1.59 | 1.52 |
| 4 | D | 696 | SER | C-N | 5.44 | 1.42 | 1.33 |
| 8 | N | 420 | THR | CB-OG1 | -5.44 | 1.35 | 1.43 |
| 7 | O | 44 | ASN | N-CA | 5.44 | 1.52 | 1.46 |
| 7 | O | 240 | LEU | CA-C | -5.44 | 1.45 | 1.52 |
| 8 | P | 766 | GLU | C-N | 5.44 | 1.40 | 1.33 |
| 8 | P | 904 | LEU | CA-CB | 5.44 | 1.61 | 1.53 |
| 8 | P | 1462 | ASN | N-CA | 5.44 | 1.52 | 1.46 |
| 9 | R | 575 | ALA | C-N | 5.44 | 1.40 | 1.33 |
| 1 | Y | 530 | ILE | N-CA | -5.44 | 1.39 | 1.46 |
| 12 | v | 572 | SER | C-N | 5.44 | 1.41 | 1.33 |
| 18 | l | 144 | ASP | C-N | 5.44 | 1.40 | 1.33 |
| 18 | l | 301 | ASP | CA-CB | 5.44 | 1.60 | 1.53 |
| 20 | g | 470 | LYS | CA-CB | 5.44 | 1.62 | 1.54 |
| 2 | 1 | 877 | SER | CA-CB | 5.44 | 1.62 | 1.53 |
| 7 | O | 712 | LEU | CA-CB | 5.44 | 1.61 | 1.53 |
| 1 | Y | 927 | LEU | C-N | 5.44 | 1.40 | 1.33 |
| 16 | j | 231 | TYR | CA-CB | 5.44 | 1.61 | 1.53 |
| 16 | j | 547 | ARG | C-N | 5.44 | 1.41 | 1.33 |
| 15 | b | 580 | CYS | N-CA | -5.44 | 1.39 | 1.46 |
| 16 | c | 288 | SER | CA-C | -5.44 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 765 | ASP | C-N | 5.43 | 1.41 | 1.33 |
| 9 | R | 124 | SER | CA-CB | 5.43 | 1.62 | 1.53 |
| 9 | T | 644 | TYR | CA-C | -5.43 | 1.46 | 1.52 |
| 2 | Z | 1351 | TYR | C-N | 5.43 | 1.41 | 1.33 |
| 17 | k | 43 | HIS | CB-CG | 5.43 | 1.57 | 1.50 |
| 16 | c | 289 | ASN | N-CA | -5.43 | 1.39 | 1.46 |
| 14 | a | 256 | ASP | CA-C | -5.43 | 1.46 | 1.52 |
| 2 | 1 | 452 | LYS | CA-CB | 5.43 | 1.59 | 1.52 |
| 5 | K | 402 | GLN | C-N | 5.43 | 1.41 | 1.33 |
| 8 | P | 389 | PHE | C-N | 5.43 | 1.39 | 1.33 |
| 2 | Z | 143 | VAL | N-CA | 5.43 | 1.52 | 1.46 |
| 2 | Z | 1051 | ASN | CG-ND2 | 5.43 | 1.44 | 1.33 |
| 4 | y | 774 | ASN | CA-C | -5.43 | 1.46 | 1.52 |
| 14 | h | 755 | VAL | C-N | 5.43 | 1.41 | 1.33 |
| 14 | h | 912 | ASP | C-N | 5.43 | 1.40 | 1.33 |
| 15 | i | 365 | ILE | CA-C | 5.43 | 1.56 | 1.52 |
| 20 | n | 298 | SER | C-N | 5.43 | 1.41 | 1.34 |
| 18 | e | 233 | THR | CA-C | 5.43 | 1.58 | 1.52 |
| 20 | g | 333 | ILE | CA-C | -5.43 | 1.46 | 1.53 |
| 8 | N | 556 | LEU | N-CA | -5.43 | 1.39 | 1.46 |
| 19 | f | 185 | TYR | CA-CB | 5.43 | 1.61 | 1.53 |
| 20 | g | 969 | VAL | CA-C | 5.43 | 1.59 | 1.52 |
| 2 | 1 | 445 | SER | C-O | -5.43 | 1.17 | 1.23 |
| 4 | J | 762 | LEU | CA-CB | 5.43 | 1.61 | 1.53 |
| 7 | O | 930 | VAL | C-N | 5.43 | 1.41 | 1.33 |
| 1 | Y | 284 | PHE | N-CA | -5.43 | 1.39 | 1.46 |
| 12 | u | 394 | SER | CA-C | -5.43 | 1.45 | 1.52 |
| 16 | j | 158 | MET | C-N | 5.43 | 1.40 | 1.33 |
| 20 | n | 496 | SER | N-CA | -5.43 | 1.39 | 1.46 |
| 21 | s | 74 | GLY | C-N | 5.43 | 1.41 | 1.33 |
| 20 | g | 1006 | TYR | CA-C | -5.43 | 1.46 | 1.52 |
| 6 | I | 324 | GLN | CA-C | -5.43 | 1.45 | 1.52 |
| 4 | J | 810 | ASN | CA-CB | 5.43 | 1.61 | 1.53 |
| 7 | O | 254 | LEU | C-N | 5.43 | 1.40 | 1.33 |
| 1 | 0 | 294 | TRP | C-N | 5.43 | 1.40 | 1.33 |
| 4 | A | 794 | ILE | C-N | 5.43 | 1.41 | 1.33 |
| 12 | u | 359 | GLU | CA-C | -5.43 | 1.45 | 1.52 |
| 14 | h | 667 | LEU | CA-C | -5.43 | 1.47 | 1.53 |
| 20 | n | 903 | LEU | CA-C | 5.43 | 1.60 | 1.52 |
| 20 | n | 1080 | SER | C-O | -5.43 | 1.17 | 1.23 |
| 4 | D | 676 | ILE | CB-CG1 | 5.42 | 1.64 | 1.53 |
| 7 | O | 1181 | VAL | CA-CB | -5.42 | 1.48 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | R | 147 | ASP | CA-C | -5.42 | 1.45 | 1.52 |
| 10 | W | 275 | GLU | CA-CB | 5.42 | 1.62 | 1.53 |
| 12 | v | 66 | ASP | CA-C | -5.42 | 1.46 | 1.52 |
| 14 | h | 325 | ALA | C-N | 5.42 | 1.41 | 1.33 |
| 19 | m | 46 | ALA | CA-C | -5.42 | 1.45 | 1.52 |
| 19 | m | 669 | LYS | N-CA | -5.42 | 1.39 | 1.46 |
| 20 | n | 436 | SER | N-CA | -5.42 | 1.39 | 1.46 |
| 5 | B | 288 | ILE | CA-CB | -5.42 | 1.47 | 1.54 |
| 7 | M | 1527 | ARG | C-N | 5.42 | 1.40 | 1.33 |
| 7 | O | 763 | HIS | ND1-CE1 | 5.42 | 1.38 | 1.32 |
| 14 | a | 903 | ASN | CA-C | -5.42 | 1.45 | 1.52 |
| 6 | C | 276 | GLU | C-O | -5.42 | 1.17 | 1.24 |
| 5 | K | 530 | ASP | C-N | 5.42 | 1.41 | 1.33 |
| 9 | T | 271 | VAL | CA-CB | 5.42 | 1.61 | 1.54 |
| 1 | Y | 579 | SER | N-CA | -5.42 | 1.39 | 1.46 |
| 1 | Y | 709 | GLY | N-CA | -5.42 | 1.37 | 1.45 |
| 12 | u | 589 | ASP | CA-C | 5.42 | 1.59 | 1.52 |
| 14 | a | 220 | TYR | N-CA | 5.42 | 1.52 | 1.45 |
| 14 | a | 757 | GLU | N-CA | -5.42 | 1.39 | 1.46 |
| 9 | S | 40 | GLY | C-N | 5.42 | 1.40 | 1.33 |
| 12 | u | 247 | ARG | CZ-NH2 | 5.42 | 1.40 | 1.33 |
| 19 | m | 528 | HIS | ND1-CE1 | 5.42 | 1.38 | 1.32 |
| 6 | C | 373 | PHE | CA-C | -5.42 | 1.45 | 1.52 |
| 8 | N | 142 | ILE | C-N | 5.42 | 1.41 | 1.33 |
| 8 | N | 1342 | LEU | CA-CB | 5.42 | 1.62 | 1.53 |
| 7 | O | 722 | ARG | C-N | 5.42 | 1.40 | 1.33 |
| 14 | h | 882 | PHE | CA-CB | 5.42 | 1.62 | 1.53 |
| 17 | d | 218 | LEU | C-N | 5.42 | 1.41 | 1.33 |
| 19 | f | 303 | LEU | CA-C | -5.42 | 1.45 | 1.52 |
| 19 | f | 391 | HIS | N-CA | 5.42 | 1.52 | 1.46 |
| 20 | g | 392 | ASP | N-CA | -5.42 | 1.39 | 1.46 |
| 20 | g | 796 | ASN | N-CA | -5.42 | 1.40 | 1.46 |
| 5 | H | 437 | TRP | CA-CB | 5.42 | 1.62 | 1.53 |
| 8 | N | 713 | LYS | CA-C | 5.42 | 1.59 | 1.52 |
| 8 | N | 729 | HIS | ND1-CE1 | 5.42 | 1.38 | 1.32 |
| 9 | Q | 484 | LEU | CA-CB | 5.42 | 1.61 | 1.53 |
| 12 | u | 156 | ILE | C-N | 5.42 | 1.43 | 1.34 |
| 15 | i | 538 | ILE | CA-C | -5.42 | 1.46 | 1.52 |
| 20 | n | 948 | GLN | CA-C | -5.42 | 1.45 | 1.52 |
| 1 | 0 | 251 | THR | N-CA | -5.42 | 1.38 | 1.46 |
| 1 | 0 | 664 | ASP | N-CA | -5.42 | 1.39 | 1.46 |
| 2 | 1 | 653 | LYS | CA-CB | 5.42 | 1.63 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 61 | GLY | CA-C | -5.42 | 1.46 | 1.52 |
| 8 | N | 648 | ARG | NE-CZ | 5.42 | 1.39 | 1.33 |
| 9 | R | 141 | ASN | CA-C | -5.42 | 1.46 | 1.52 |
| 1 | Y | 511 | LYS | C-N | 5.42 | 1.40 | 1.33 |
| 15 | b | 293 | LYS | C-N | 5.42 | 1.40 | 1.33 |
| 8 | N | 1025 | ASN | CA-CB | 5.41 | 1.62 | 1.53 |
| 7 | O | 50 | GLN | C-N | 5.41 | 1.41 | 1.33 |
| 9 | S | 359 | ASN | N-CA | -5.41 | 1.39 | 1.46 |
| 1 | Y | 771 | TYR | C-N | 5.41 | 1.40 | 1.33 |
| 19 | m | 722 | ALA | N-CA | -5.41 | 1.39 | 1.46 |
| 2 | 1 | 852 | LEU | N-CA | 5.41 | 1.53 | 1.46 |
| 4 | D | 699 | TYR | N-CA | -5.41 | 1.38 | 1.46 |
| 9 | R | 765 | ASP | C-N | 5.41 | 1.41 | 1.33 |
| 2 | Z | 441 | ARG | N-CA | -5.41 | 1.40 | 1.46 |
| 12 | u | 337 | TRP | NE1-CE2 | -5.41 | 1.31 | 1.37 |
| 14 | h | 877 | ILE | CA-CB | -5.41 | 1.48 | 1.54 |
| 2 | 1 | 566 | GLU | CA-CB | 5.41 | 1.62 | 1.53 |
| 1 | Y | 1471 | ILE | CA-CB | -5.41 | 1.48 | 1.54 |
| 2 | Z | 985 | SER | C-N | 5.41 | 1.41 | 1.34 |
| 2 | Z | 1161 | HIS | ND1-CE1 | 5.41 | 1.38 | 1.32 |
| 13 | x | 1294 | LYS | N-CA | -5.41 | 1.39 | 1.46 |
| 13 | x | 1397 | LYS | N-CA | -5.41 | 1.40 | 1.46 |
| 19 | m | 338 | GLU | CA-CB | 5.41 | 1.62 | 1.53 |
| 16 | c | 559 | LEU | C-N | 5.41 | 1.40 | 1.33 |
| 14 | a | 321 | THR | C-N | 5.41 | 1.41 | 1.33 |
| 14 | a | 461 | SER | C-N | 5.41 | 1.40 | 1.33 |
| 14 | a | 613 | ILE | C-N | -5.41 | 1.26 | 1.33 |
| 6 | F | 332 | LYS | N-CA | -5.41 | 1.39 | 1.46 |
| 9 | Q | 731 | GLN | C-O | -5.41 | 1.17 | 1.24 |
| 10 | U | 252 | ALA | C-N | 5.41 | 1.40 | 1.33 |
| 14 | h | 681 | LYS | N-CA | -5.41 | 1.39 | 1.46 |
| 14 | h | 984 | TYR | CG-CD1 | 5.41 | 1.50 | 1.39 |
| 20 | n | 745 | ILE | CA-C | -5.41 | 1.44 | 1.52 |
| 20 | n | 1145 | ASN | CA-CB | 5.41 | 1.60 | 1.52 |
| 5 | H | 453 | LEU | N-CA | -5.41 | 1.39 | 1.46 |
| 5 | H | 518 | ARG | CZ-NH2 | 5.41 | 1.40 | 1.33 |
| 9 | S | 136 | PHE | C-N | 5.41 | 1.40 | 1.33 |
| 13 | w | 1357 | ASN | C-N | 5.41 | 1.41 | 1.33 |
| 19 | m | 244 | ARG | CA-CB | 5.41 | 1.61 | 1.53 |
| 15 | b | 530 | ARG | C-N | 5.41 | 1.37 | 1.33 |
| 20 | g | 406 | ASN | N-CA | 5.41 | 1.53 | 1.45 |
| 2 | 1 | 266 | TYR | CA-C | -5.41 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 1008 | ILE | CA-C | -5.41 | 1.46 | 1.52 |
| 5 | B | 451 | ALA | C-O | -5.41 | 1.17 | 1.24 |
| 12 | u | 112 | PHE | CA-C | -5.41 | 1.45 | 1.52 |
| 12 | v | 73 | SER | CA-CB | 5.41 | 1.61 | 1.53 |
| 19 | m | 117 | TYR | CA-C | -5.41 | 1.45 | 1.52 |
| 20 | n | 1030 | ASN | CA-CB | 5.41 | 1.62 | 1.53 |
| 9 | T | 161 | ILE | N-CA | -5.40 | 1.40 | 1.46 |
| 2 | Z | 642 | SER | CA-C | -5.40 | 1.45 | 1.52 |
| 2 | Z | 963 | THR | C-O | -5.40 | 1.17 | 1.24 |
| 20 | n | 777 | ILE | CA-CB | 5.40 | 1.61 | 1.54 |
| 16 | c | 773 | PRO | N-CD | -5.40 | 1.40 | 1.47 |
| 1 | 0 | 127 | TYR | C-N | 5.40 | 1.41 | 1.33 |
| 7 | M | 1031 | VAL | CA-C | -5.40 | 1.45 | 1.52 |
| 8 | P | 699 | GLU | N-CA | -5.40 | 1.39 | 1.45 |
| 10 | U | 311 | ASP | CA-C | -5.40 | 1.45 | 1.52 |
| 1 | Y | 972 | ASN | N-CA | 5.40 | 1.53 | 1.46 |
| 12 | u | 70 | HIS | ND1-CE1 | 5.40 | 1.38 | 1.32 |
| 19 | f | 150 | SER | CA-CB | 5.40 | 1.61 | 1.53 |
| 2 | 1 | 1294 | GLU | CA-C | -5.40 | 1.45 | 1.52 |
| 6 | L | 333 | ILE | N-CA | -5.40 | 1.40 | 1.46 |
| 6 | L | 406 | PHE | N-CA | 5.40 | 1.53 | 1.46 |
| 7 | O | 558 | ILE | N-CA | -5.40 | 1.40 | 1.46 |
| 9 | Q | 795 | GLN | C-N | 5.40 | 1.40 | 1.33 |
| 9 | S | 614 | ARG | NE-CZ | 5.40 | 1.39 | 1.33 |
| 2 | Z | 1222 | ILE | CA-C | -5.40 | 1.45 | 1.52 |
| 12 | v | 337 | TRP | CA-C | -5.40 | 1.45 | 1.52 |
| 17 | k | 120 | SER | C-N | 5.40 | 1.40 | 1.33 |
| 20 | n | 1148 | ILE | CA-CB | 5.40 | 1.60 | 1.54 |
| 16 | c | 429 | GLU | CA-C | -5.40 | 1.45 | 1.52 |
| 18 | e | 14 | ASP | N-CA | -5.40 | 1.39 | 1.45 |
| 20 | g | 884 | HIS | CD2-NE2 | 5.40 | 1.43 | 1.37 |
| 14 | a | 183 | LEU | N-CA | 5.40 | 1.52 | 1.45 |
| 2 | 1 | 364 | ARG | CD-NE | 5.40 | 1.53 | 1.46 |
| 8 | P | 1095 | GLU | CA-C | 5.40 | 1.60 | 1.52 |
| 5 | B | 347 | THR | CA-C | 5.40 | 1.59 | 1.52 |
| 6 | C | 301 | HIS | CB-CG | -5.40 | 1.42 | 1.50 |
| 8 | N | 449 | ASP | CA-C | -5.40 | 1.45 | 1.52 |
| 8 | N | 1472 | SER | C-N | 5.40 | 1.41 | 1.33 |
| 7 | O | 1351 | GLU | CA-C | -5.40 | 1.46 | 1.52 |
| 8 | P | 348 | LYS | C-O | -5.40 | 1.17 | 1.24 |
| 2 | Z | 138 | PHE | CA-C | -5.40 | 1.46 | 1.52 |
| 2 | Z | 638 | SER | C-N | 5.40 | 1.42 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 12 | v | 698 | ASN | N-CA | -5.40 | 1.40 | 1.46 |
| 14 | h | 317 | ASN | N-CA | -5.40 | 1.38 | 1.46 |
| 14 | h | 611 | THR | N-CA | -5.40 | 1.38 | 1.45 |
| 19 | m | 540 | ASN | CA-CB | 5.40 | 1.62 | 1.53 |
| 20 | g | 939 | LEU | CA-C | -5.40 | 1.46 | 1.53 |
| 5 | B | 331 | LEU | N-CA | -5.40 | 1.39 | 1.46 |
| 8 | N | 202 | THR | N-CA | -5.40 | 1.38 | 1.45 |
| 7 | O | 1344 | GLU | C-N | 5.40 | 1.41 | 1.33 |
| 4 | y | 696 | SER | CA-C | 5.40 | 1.59 | 1.52 |
| 4 | D | 755 | LEU | C-N | 5.39 | 1.41 | 1.33 |
| 8 | N | 278 | SER | CA-CB | 5.39 | 1.62 | 1.53 |
| 8 | N | 405 | SER | C-N | 5.39 | 1.40 | 1.33 |
| 1 | Y | 109 | ASP | N-CA | -5.39 | 1.39 | 1.46 |
| 2 | Z | 930 | THR | CA-C | -5.39 | 1.45 | 1.52 |
| 12 | u | 137 | TYR | CZ-OH | 5.39 | 1.49 | 1.38 |
| 19 | m | 535 | ARG | NE-CZ | 5.39 | 1.39 | 1.33 |
| 15 | b | 662 | TYR | CA-C | -5.39 | 1.46 | 1.52 |
| 20 | g | 272 | ASN | CA-C | -5.39 | 1.46 | 1.53 |
| 20 | g | 379 | SER | C-O | -5.39 | 1.17 | 1.24 |
| 14 | a | 937 | LEU | N-CA | -5.39 | 1.38 | 1.45 |
| 8 | N | 1517 | GLU | CA-CB | 5.39 | 1.61 | 1.53 |
| 8 | P | 1431 | ILE | C-N | 5.39 | 1.41 | 1.33 |
| 20 | n | 945 | ARG | CD-NE | 5.39 | 1.53 | 1.46 |
| 18 | e | 169 | PHE | N-CA | -5.39 | 1.39 | 1.46 |
| 14 | a | 354 | LEU | C-O | 5.39 | 1.30 | 1.24 |
| 7 | M | 354 | ARG | NE-CZ | 5.39 | 1.39 | 1.33 |
| 20 | n | 1026 | GLY | CA-C | -5.39 | 1.42 | 1.51 |
| 18 | e | 154 | MET | CA-CB | 5.39 | 1.60 | 1.53 |
| 2 | 1 | 1286 | HIS | ND1-CE1 | 5.39 | 1.38 | 1.32 |
| 5 | K | 336 | ASP | CA-C | -5.39 | 1.45 | 1.52 |
| 7 | M | 342 | TYR | C-N | 5.39 | 1.41 | 1.33 |
| 7 | O | 185 | PHE | C-O | -5.39 | 1.17 | 1.24 |
| 11 | V | 295 | MET | N-CA | -5.39 | 1.40 | 1.46 |
| 13 | x | 1141 | PRO | C-N | 5.39 | 1.41 | 1.33 |
| 17 | k | 288 | LYS | C-N | 5.39 | 1.41 | 1.33 |
| 19 | f | 463 | GLU | CA-C | -5.39 | 1.45 | 1.52 |
| 1 | 0 | 1352 | ASN | C-O | 5.39 | 1.30 | 1.24 |
| 1 | 0 | 1442 | SER | CA-C | -5.39 | 1.45 | 1.52 |
| 10 | U | 326 | ARG | CD-NE | 5.39 | 1.53 | 1.46 |
| 17 | k | 195 | VAL | C-N | 5.39 | 1.41 | 1.33 |
| 20 | n | 350 | SER | CA-CB | 5.39 | 1.59 | 1.52 |
| 15 | b | 100 | THR | CA-C | -5.39 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | O | 701 | THR | C-N | 5.39 | 1.39 | 1.33 |
| 8 | P | 134 | ARG | N-CA | -5.39 | 1.39 | 1.46 |
| 9 | R | 481 | THR | C-N | 5.39 | 1.40 | 1.33 |
| 9 | S | 346 | ILE | C-N | 5.39 | 1.40 | 1.33 |
| 12 | u | 48 | VAL | CA-C | -5.39 | 1.47 | 1.53 |
| 12 | v | 167 | ASN | CA-CB | 5.39 | 1.62 | 1.53 |
| 13 | w | 1225 | PHE | N-CA | -5.39 | 1.39 | 1.46 |
| 19 | m | 118 | GLN | C-N | 5.39 | 1.40 | 1.33 |
| 19 | m | 462 | ILE | C-N | 5.39 | 1.41 | 1.33 |
| 4 | A | 788 | ASP | C-N | 5.38 | 1.41 | 1.33 |
| 6 | L | 348 | GLN | CA-C | -5.38 | 1.46 | 1.52 |
| 7 | O | 38 | ASN | CA-CB | 5.38 | 1.62 | 1.53 |
| 9 | R | 511 | ALA | C-N | 5.38 | 1.41 | 1.33 |
| 9 | S | 695 | ILE | CA-CB | 5.38 | 1.61 | 1.54 |
| 9 | T | 345 | LEU | CA-C | -5.38 | 1.46 | 1.53 |
| 2 | Z | 1386 | ARG | NE-CZ | 5.38 | 1.39 | 1.33 |
| 12 | v | 64 | VAL | C-O | 5.38 | 1.29 | 1.24 |
| 14 | h | 683 | SER | C-O | -5.38 | 1.18 | 1.23 |
| 20 | n | 999 | LEU | N-CA | -5.38 | 1.39 | 1.46 |
| 21 | o | 71 | HIS | ND1-CE1 | 5.38 | 1.38 | 1.32 |
| 1 | 0 | 975 | ILE | CB-CG1 | 5.38 | 1.64 | 1.53 |
| 4 | A | 653 | SER | CA-C | 5.38 | 1.59 | 1.52 |
| 6 | I | 311 | ASP | C-N | 5.38 | 1.40 | 1.33 |
| 7 | O | 893 | HIS | N-CA | -5.38 | 1.38 | 1.46 |
| 7 | O | 1669 | LEU | N-CA | -5.38 | 1.39 | 1.46 |
| 5 | B | 517 | GLN | CA-CB | 5.38 | 1.62 | 1.53 |
| 6 | C | 310 | ARG | CD-NE | 5.38 | 1.53 | 1.46 |
| 12 | v | 304 | THR | N-CA | -5.38 | 1.39 | 1.46 |
| 20 | n | 135 | ALA | CA-C | -5.38 | 1.45 | 1.52 |
| 1 | 0 | 101 | LEU | C-N | 5.38 | 1.41 | 1.33 |
| 1 | 0 | 957 | ASP | CA-CB | 5.38 | 1.59 | 1.52 |
| 6 | F | 321 | ALA | CA-C | -5.38 | 1.45 | 1.52 |
| 7 | O | 1328 | ILE | N-CA | 5.38 | 1.53 | 1.46 |
| 14 | a | 562 | PHE | CA-CB | 5.38 | 1.62 | 1.53 |
| 14 | a | 657 | LEU | C-O | -5.38 | 1.17 | 1.24 |
| 1 | 0 | 455 | PHE | CA-C | 5.38 | 1.59 | 1.52 |
| 2 | 1 | 420 | LEU | C-N | 5.38 | 1.41 | 1.33 |
| 2 | 1 | 1064 | VAL | C-N | 5.38 | 1.40 | 1.33 |
| 8 | N | 918 | PHE | CA-C | -5.38 | 1.45 | 1.52 |
| 8 | N | 1510 | PHE | CA-C | -5.38 | 1.45 | 1.52 |
| 11 | X | 395 | LEU | C-N | 5.38 | 1.41 | 1.33 |
| 12 | u | 558 | PHE | CA-CB | 5.38 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 12 | v | 638 | ILE | CA-C | 5.38 | 1.59 | 1.52 |
| 20 | g | 461 | ASP | CA-C | -5.38 | 1.46 | 1.52 |
| 14 | a | 508 | LYS | C-N | 5.38 | 1.40 | 1.33 |
| 1 | 0 | 177 | PRO | CA-C | -5.38 | 1.44 | 1.52 |
| 1 | 0 | 598 | PHE | N-CA | -5.38 | 1.39 | 1.46 |
| 6 | L | 281 | ASP | CA-CB | 5.38 | 1.61 | 1.53 |
| 8 | N | 1419 | LYS | CA-C | -5.38 | 1.46 | 1.52 |
| 8 | N | 1519 | CYS | N-CA | -5.38 | 1.39 | 1.46 |
| 7 | O | 56 | ILE | CA-C | -5.38 | 1.45 | 1.52 |
| 9 | S | 832 | LEU | N-CA | -5.38 | 1.39 | 1.46 |
| 15 | i | 108 | VAL | CA-CB | -5.38 | 1.48 | 1.54 |
| 19 | f | 469 | ARG | CA-C | -5.38 | 1.45 | 1.52 |
| 19 | f | 708 | SER | CA-CB | 5.38 | 1.62 | 1.53 |
| 20 | g | 838 | GLU | C-N | 5.38 | 1.41 | 1.33 |
| 7 | M | 1126 | PRO | N-CD | -5.38 | 1.40 | 1.47 |
| 7 | O | 1654 | ASN | N-CA | 5.38 | 1.52 | 1.46 |
| 9 | R | 336 | LEU | CA-C | -5.38 | 1.45 | 1.52 |
| 9 | S | 97 | GLU | C-N | 5.38 | 1.40 | 1.34 |
| 1 | Y | 1287 | SER | CA-C | -5.38 | 1.45 | 1.52 |
| 1 | Y | 1476 | GLU | CA-C | -5.38 | 1.46 | 1.52 |
| 14 | h | 674 | LEU | CA-CB | 5.38 | 1.60 | 1.53 |
| 7 | M | 1493 | LYS | CA-C | -5.37 | 1.45 | 1.52 |
| 8 | N | 163 | ASP | CA-C | -5.37 | 1.45 | 1.52 |
| 8 | N | 602 | VAL | C-O | -5.37 | 1.18 | 1.24 |
| 8 | P | 1644 | ILE | C-O | -5.37 | 1.16 | 1.24 |
| 9 | T | 661 | LEU | N-CA | -5.37 | 1.39 | 1.46 |
| 14 | h | 1032 | ASP | C-N | 5.37 | 1.40 | 1.33 |
| 16 | j | 143 | ARG | CD-NE | 5.37 | 1.53 | 1.46 |
| 20 | n | 522 | LEU | N-CA | -5.37 | 1.39 | 1.46 |
| 20 | g | 806 | GLU | C-O | 5.37 | 1.30 | 1.24 |
| 1 | 0 | 899 | MET | C-O | -5.37 | 1.17 | 1.24 |
| 2 | 1 | 187 | ASN | N-CA | -5.37 | 1.39 | 1.45 |
| 6 | L | 341 | ASP | C-N | 5.37 | 1.41 | 1.33 |
| 6 | L | 395 | GLU | N-CA | -5.37 | 1.39 | 1.46 |
| 7 | M | 462 | LEU | CA-C | -5.37 | 1.45 | 1.52 |
| 9 | Q | 22 | LEU | CA-CB | 5.37 | 1.61 | 1.53 |
| 9 | T | 58 | SER | C-O | -5.37 | 1.16 | 1.24 |
| 14 | h | 250 | SER | C-N | 5.37 | 1.41 | 1.33 |
| 17 | k | 41 | GLU | C-N | 5.37 | 1.41 | 1.33 |
| 20 | n | 390 | ILE | CA-C | -5.37 | 1.46 | 1.52 |
| 16 | c | 762 | LYS | N-CA | -5.37 | 1.39 | 1.46 |
| 20 | g | 1054 | GLY | CA-C | -5.37 | 1.44 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | F | 370 | ASP | C-N | 5.37 | 1.40 | 1.33 |
| 5 | K | 393 | ASP | C-N | 5.37 | 1.41 | 1.33 |
| 7 | M | 178 | ASN | CA-C | -5.37 | 1.45 | 1.52 |
| 8 | N | 1545 | SER | N-CA | 5.37 | 1.52 | 1.46 |
| 12 | u | 220 | GLU | N-CA | 5.37 | 1.52 | 1.46 |
| 12 | v | 70 | HIS | CG-ND1 | 5.37 | 1.44 | 1.38 |
| 13 | x | 1217 | THR | C-N | 5.37 | 1.41 | 1.33 |
| 15 | i | 517 | ASP | CA-CB | 5.37 | 1.61 | 1.53 |
| 2 | 1 | 645 | LEU | CA-C | -5.37 | 1.46 | 1.52 |
| 9 | R | 456 | ARG | NE-CZ | 5.37 | 1.39 | 1.33 |
| 9 | R | 684 | ASN | C-N | 5.37 | 1.40 | 1.34 |
| 9 | S | 50 | ARG | C-N | -5.37 | 1.26 | 1.33 |
| 4 | y | 764 | SER | CA-CB | 5.37 | 1.61 | 1.53 |
| 20 | n | 160 | GLU | CA-C | -5.37 | 1.46 | 1.52 |
| 16 | c | 203 | LYS | CA-C | -5.37 | 1.46 | 1.52 |
| 7 | M | 757 | PHE | CA-CB | 5.37 | 1.61 | 1.53 |
| 8 | P | 201 | ASN | N-CA | -5.37 | 1.38 | 1.46 |
| 8 | P | 986 | SER | N-CA | -5.37 | 1.39 | 1.46 |
| 9 | R | 54 | PHE | CA-C | 5.37 | 1.59 | 1.52 |
| 2 | Z | 131 | GLY | C-N | 5.37 | 1.40 | 1.33 |
| 13 | w | 1308 | GLU | C-O | 5.37 | 1.30 | 1.24 |
| 15 | b | 150 | ALA | C-N | 5.37 | 1.39 | 1.34 |
| 17 | d | 78 | LYS | C-N | 5.37 | 1.40 | 1.33 |
| 5 | B | 381 | GLU | C-N | 5.37 | 1.41 | 1.33 |
| 8 | N | 217 | GLN | C-O | -5.37 | 1.16 | 1.24 |
| 7 | O | 1410 | ASN | N-CA | -5.37 | 1.40 | 1.46 |
| 9 | T | 577 | ARG | NE-CZ | 5.37 | 1.39 | 1.33 |
| 2 | Z | 1167 | ALA | C-N | 5.37 | 1.41 | 1.33 |
| 2 | Z | 1234 | ILE | CA-C | -5.37 | 1.46 | 1.52 |
| 12 | u | 57 | LEU | CA-C | -5.37 | 1.45 | 1.53 |
| 12 | u | 215 | VAL | CA-C | -5.37 | 1.46 | 1.52 |
| 4 | y | 761 | ASN | CA-C | -5.37 | 1.45 | 1.52 |
| 17 | k | 201 | GLU | CA-CB | 5.37 | 1.62 | 1.53 |
| 15 | b | 396 | ASP | CA-CB | 5.37 | 1.62 | 1.53 |
| 19 | f | 68 | TRP | N-CA | 5.37 | 1.53 | 1.46 |
| 19 | f | 400 | ASN | CA-CB | 5.37 | 1.61 | 1.53 |
| 1 | 0 | 377 | ILE | CA-CB | 5.36 | 1.60 | 1.53 |
| 2 | 1 | 356 | THR | N-CA | -5.36 | 1.39 | 1.46 |
| 2 | 1 | 1106 | GLU | CD-OE2 | 5.36 | 1.35 | 1.25 |
| 5 | K | 309 | ARG | CA-CB | -5.36 | 1.46 | 1.53 |
| 8 | P | 765 | PHE | C-N | 5.36 | 1.41 | 1.33 |
| 8 | P | 990 | LYS | N-CA | -5.36 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 12 | u | 606 | SER | CA-C | 5.36 | 1.60 | 1.52 |
| 20 | n | 811 | LEU | CA-CB | 5.36 | 1.60 | 1.53 |
| 17 | d | 136 | THR | CA-C | -5.36 | 1.46 | 1.52 |
| 14 | a | 381 | SER | N-CA | -5.36 | 1.39 | 1.46 |
| 4 | A | 769 | ILE | C-N | 5.36 | 1.41 | 1.33 |
| 7 | O | 776 | VAL | CA-C | -5.36 | 1.45 | 1.52 |
| 4 | z | 757 | SER | C-N | 5.36 | 1.40 | 1.33 |
| 14 | h | 273 | VAL | N-CA | -5.36 | 1.39 | 1.46 |
| 20 | n | 178 | ILE | C-N | 5.36 | 1.41 | 1.33 |
| 17 | d | 25 | ALA | CA-C | -5.36 | 1.46 | 1.52 |
| 6 | C | 380 | TYR | CB-CG | 5.36 | 1.63 | 1.51 |
| 6 | F | 280 | LEU | C-N | 5.36 | 1.41 | 1.33 |
| 7 | M | 512 | GLU | N-CA | -5.36 | 1.39 | 1.46 |
| 7 | O | 1249 | ILE | N-CA | -5.36 | 1.40 | 1.46 |
| 9 | T | 787 | HIS | CG-CD2 | 5.36 | 1.41 | 1.35 |
| 11 | V | 287 | HIS | CG-CD2 | 5.36 | 1.41 | 1.35 |
| 2 | Z | 1189 | LYS | N-CA | -5.36 | 1.39 | 1.46 |
| 13 | x | 1442 | ALA | C-O | -5.36 | 1.18 | 1.24 |
| 14 | h | 555 | LYS | CA-C | -5.36 | 1.45 | 1.52 |
| 15 | i | 713 | ILE | CA-C | 5.36 | 1.59 | 1.52 |
| 20 | n | 974 | ARG | N-CA | -5.36 | 1.39 | 1.46 |
| 4 | D | 654 | HIS | N-CA | -5.36 | 1.39 | 1.46 |
| 7 | M | 474 | LEU | N-CA | -5.36 | 1.40 | 1.46 |
| 7 | O | 483 | LEU | CA-CB | 5.36 | 1.61 | 1.53 |
| 2 | Z | 815 | PHE | C-N | 5.36 | 1.41 | 1.33 |
| 12 | u | 446 | THR | CA-C | -5.36 | 1.46 | 1.52 |
| 16 | j | 168 | SER | N-CA | -5.36 | 1.39 | 1.46 |
| 20 | n | 928 | LYS | N-CA | -5.36 | 1.40 | 1.46 |
| 16 | c | 650 | HIS | CA-C | -5.36 | 1.45 | 1.52 |
| 6 | L | 305 | ILE | CB-CG1 | 5.36 | 1.64 | 1.53 |
| 7 | M | 1472 | GLU | N-CA | -5.36 | 1.42 | 1.47 |
| 8 | N | 162 | HIS | CA-C | -5.36 | 1.45 | 1.52 |
| 8 | N | 1311 | LEU | N-CA | -5.36 | 1.39 | 1.46 |
| 9 | Q | 481 | THR | C-N | 5.36 | 1.41 | 1.33 |
| 9 | S | 818 | GLY | CA-C | -5.36 | 1.46 | 1.52 |
| 9 | T | 745 | LEU | N-CA | 5.36 | 1.49 | 1.46 |
| 17 | d | 272 | SER | N-CA | -5.36 | 1.39 | 1.46 |
| 7 | M | 152 | HIS | CA-C | -5.36 | 1.45 | 1.52 |
| 8 | P | 933 | LYS | N-CA | -5.36 | 1.40 | 1.46 |
| 7 | M | 192 | ILE | N-CA | -5.35 | 1.40 | 1.46 |
| 8 | P | 1030 | SER | N-CA | -5.35 | 1.39 | 1.46 |
| 1 | Y | 1088 | PHE | C-N | 5.35 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 715 | LEU | CA-C | -5.35 | 1.46 | 1.52 |
| 12 | u | 372 | LYS | CA-C | -5.35 | 1.46 | 1.52 |
| 16 | j | 266 | CYS | C-O | 5.35 | 1.31 | 1.24 |
| 20 | g | 154 | ASN | C-N | 5.35 | 1.40 | 1.34 |
| 20 | g | 682 | LEU | N-CA | -5.35 | 1.40 | 1.46 |
| 8 | N | 1027 | TRP | CA-C | 5.35 | 1.59 | 1.52 |
| 8 | N | 1493 | ASN | CG-ND2 | 5.35 | 1.44 | 1.33 |
| 9 | S | 280 | GLN | C-N | 5.35 | 1.41 | 1.33 |
| 10 | U | 281 | ARG | CA-C | -5.35 | 1.45 | 1.52 |
| 1 | Y | 965 | GLU | C-N | 5.35 | 1.40 | 1.33 |
| 20 | n | 368 | PHE | CA-C | -5.35 | 1.45 | 1.52 |
| 14 | a | 738 | ARG | CZ-NH1 | 5.35 | 1.40 | 1.32 |
| 5 | H | 527 | LEU | C-N | 5.35 | 1.41 | 1.33 |
| 9 | Q | 479 | LEU | CA-CB | 5.35 | 1.62 | 1.53 |
| 1 | Y | 1276 | LEU | C-N | 5.35 | 1.41 | 1.33 |
| 2 | Z | 998 | TYR | CA-C | -5.35 | 1.45 | 1.52 |
| 12 | u | 289 | PRO | C-N | 5.35 | 1.41 | 1.33 |
| 12 | u | 399 | GLU | CA-C | -5.35 | 1.45 | 1.52 |
| 13 | w | 1273 | GLN | C-N | 5.35 | 1.40 | 1.33 |
| 7 | M | 729 | MET | C-N | 5.35 | 1.41 | 1.33 |
| 8 | N | 722 | SER | CA-C | -5.35 | 1.46 | 1.52 |
| 9 | R | 81 | GLU | C-O | -5.35 | 1.17 | 1.23 |
| 1 | 0 | 387 | LEU | CA-CB | 5.35 | 1.61 | 1.53 |
| 1 | 0 | 1228 | THR | C-N | 5.35 | 1.41 | 1.33 |
| 2 | 1 | 118 | SER | CA-C | 5.35 | 1.59 | 1.52 |
| 4 | A | 772 | VAL | CA-CB | 5.35 | 1.61 | 1.54 |
| 7 | M | 83 | LEU | N-CA | -5.35 | 1.39 | 1.46 |
| 8 | N | 111 | HIS | ND1-CE1 | 5.35 | 1.37 | 1.32 |
| 8 | P | 712 | LEU | CA-C | -5.35 | 1.46 | 1.52 |
| 11 | X | 371 | GLN | CA-C | -5.35 | 1.46 | 1.52 |
| 1 | Y | 185 | THR | CA-C | -5.35 | 1.46 | 1.52 |
| 13 | x | 1338 | GLN | C-N | 5.35 | 1.41 | 1.33 |
| 19 | m | 122 | VAL | N-CA | 5.35 | 1.53 | 1.46 |
| 20 | n | 874 | PHE | CA-C | -5.35 | 1.45 | 1.52 |
| 21 | t | 50 | ASP | CA-C | 5.35 | 1.59 | 1.52 |
| 16 | c | 189 | TYR | CA-C | -5.35 | 1.46 | 1.52 |
| 16 | c | 358 | TYR | CA-CB | 5.35 | 1.63 | 1.53 |
| 4 | J | 768 | GLU | C-N | 5.35 | 1.40 | 1.33 |
| 9 | T | 513 | LEU | C-N | 5.35 | 1.41 | 1.33 |
| 15 | b | 278 | CYS | N-CA | 5.35 | 1.52 | 1.45 |
| 1 | 0 | 233 | LEU | CB-CG | 5.34 | 1.64 | 1.53 |
| 2 | 1 | 503 | SER | C-N | 5.34 | 1.38 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 1072 | PRO | N-CD | -5.34 | 1.40 | 1.47 |
| 7 | M | 1439 | GLU | N-CA | -5.34 | 1.40 | 1.46 |
| 7 | O | 168 | LEU | N-CA | 5.34 | 1.53 | 1.46 |
| 8 | P | 118 | VAL | N-CA | -5.34 | 1.40 | 1.46 |
| 1 | Y | 1008 | GLU | CA-C | -5.34 | 1.45 | 1.52 |
| 14 | h | 348 | TYR | CA-C | -5.34 | 1.45 | 1.52 |
| 14 | h | 363 | LEU | CA-C | -5.34 | 1.46 | 1.53 |
| 15 | b | 556 | ILE | CA-C | 5.34 | 1.60 | 1.52 |
| 20 | g | 814 | LEU | N-CA | -5.34 | 1.39 | 1.46 |
| 2 | Z | 562 | ASP | CA-CB | 5.34 | 1.60 | 1.53 |
| 19 | f | 669 | LYS | C-N | 5.34 | 1.41 | 1.33 |
| 1 | 0 | 966 | ILE | C-N | 5.34 | 1.41 | 1.33 |
| 7 | O | 748 | GLY | C-N | 5.34 | 1.41 | 1.33 |
| 9 | S | 456 | ARG | CZ-NH1 | 5.34 | 1.40 | 1.32 |
| 2 | Z | 1172 | ASP | C-N | 5.34 | 1.40 | 1.33 |
| 14 | h | 384 | LYS | C-N | 5.34 | 1.40 | 1.33 |
| 15 | i | 325 | SER | CA-C | 5.34 | 1.59 | 1.52 |
| 18 | l | 76 | SER | CA-C | -5.34 | 1.45 | 1.53 |
| 20 | n | 974 | ARG | CZ-NH2 | 5.34 | 1.40 | 1.33 |
| 15 | b | 647 | ARG | CA-CB | 5.34 | 1.62 | 1.53 |
| 18 | e | 230 | LEU | C-N | 5.34 | 1.40 | 1.33 |
| 1 | 0 | 1284 | ARG | NE-CZ | 5.34 | 1.39 | 1.33 |
| 7 | M | 738 | THR | CB-OG1 | -5.34 | 1.35 | 1.43 |
| 7 | M | 964 | LYS | CA-C | 5.34 | 1.60 | 1.52 |
| 8 | P | 151 | ASN | C-N | 5.34 | 1.41 | 1.33 |
| 14 | h | 436 | HIS | CB-CG | 5.34 | 1.57 | 1.50 |
| 15 | i | 639 | ARG | NE-CZ | 5.34 | 1.39 | 1.33 |
| 16 | j | 305 | ARG | CZ-NH2 | 5.34 | 1.40 | 1.33 |
| 1 | 0 | 1342 | GLU | CA-CB | 5.34 | 1.62 | 1.53 |
| 2 | 1 | 113 | ASN | CG-ND2 | 5.34 | 1.44 | 1.33 |
| 6 | I | 371 | LYS | CA-CB | 5.34 | 1.62 | 1.53 |
| 15 | i | 375 | LEU | C-O | -5.34 | 1.17 | 1.24 |
| 18 | e | 53 | ALA | C-N | 5.34 | 1.41 | 1.33 |
| 2 | 1 | 857 | ALA | C-N | 5.34 | 1.41 | 1.33 |
| 8 | N | 525 | LYS | CA-C | -5.34 | 1.46 | 1.52 |
| 7 | O | 633 | LYS | C-N | 5.34 | 1.38 | 1.33 |
| 8 | P | 670 | HIS | ND1-CE1 | 5.34 | 1.37 | 1.32 |
| 9 | Q | 533 | ARG | N-CA | 5.34 | 1.56 | 1.46 |
| 10 | W | 345 | TYR | CZ-OH | 5.34 | 1.49 | 1.38 |
| 2 | Z | 185 | ILE | CA-C | -5.34 | 1.46 | 1.52 |
| 12 | u | 405 | LEU | CA-C | -5.34 | 1.45 | 1.52 |
| 13 | w | 1144 | HIS | C-N | 5.34 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 18 | l | 317 | THR | C-N | 5.34 | 1.39 | 1.33 |
| 19 | m | 73 | ARG | CA-CB | 5.34 | 1.62 | 1.53 |
| 19 | m | 238 | LYS | C-N | 5.34 | 1.40 | 1.33 |
| 20 | n | 253 | LYS | C-N | 5.34 | 1.41 | 1.33 |
| 15 | b | 185 | LEU | CA-CB | 5.34 | 1.61 | 1.53 |
| 7 | M | 285 | PHE | CA-C | -5.33 | 1.45 | 1.52 |
| 7 | M | 839 | SER | C-N | 5.33 | 1.40 | 1.33 |
| 12 | v | 378 | ASP | C-N | 5.33 | 1.43 | 1.34 |
| 15 | i | 82 | ILE | C-N | 5.33 | 1.40 | 1.33 |
| 20 | n | 399 | ILE | CB-CG1 | 5.33 | 1.64 | 1.53 |
| 19 | f | 384 | TYR | CA-CB | 5.33 | 1.61 | 1.53 |
| 1 | 0 | 1348 | ARG | CD-NE | 5.33 | 1.53 | 1.46 |
| 2 | 1 | 768 | ILE | CA-CB | -5.33 | 1.48 | 1.54 |
| 5 | B | 356 | GLU | C-N | 5.33 | 1.40 | 1.33 |
| 4 | D | 790 | ASN | CA-CB | 5.33 | 1.62 | 1.53 |
| 5 | H | 462 | ARG | CD-NE | 5.33 | 1.53 | 1.46 |
| 8 | N | 183 | SER | C-N | 5.33 | 1.40 | 1.33 |
| 8 | N | 663 | MET | CA-CB | 5.33 | 1.62 | 1.53 |
| 7 | O | 612 | LEU | CA-CB | 5.33 | 1.62 | 1.53 |
| 12 | u | 582 | GLU | C-N | 5.33 | 1.41 | 1.33 |
| 12 | v | 225 | LEU | C-N | 5.33 | 1.40 | 1.33 |
| 14 | h | 727 | TYR | CA-C | -5.33 | 1.46 | 1.52 |
| 18 | l | 51 | TRP | C-N | 5.33 | 1.41 | 1.33 |
| 19 | m | 456 | GLN | C-N | 5.33 | 1.40 | 1.33 |
| 15 | b | 244 | TYR | C-N | 5.33 | 1.41 | 1.33 |
| 16 | c | 604 | ASP | CA-CB | 5.33 | 1.61 | 1.53 |
| 14 | a | 921 | THR | C-N | 5.33 | 1.40 | 1.33 |
| 6 | F | 439 | ILE | C-N | 5.33 | 1.40 | 1.33 |
| 7 | O | 306 | VAL | CA-C | -5.33 | 1.46 | 1.52 |
| 9 | Q | 740 | GLU | C-N | 5.33 | 1.40 | 1.33 |
| 9 | S | 154 | GLU | C-N | 5.33 | 1.40 | 1.33 |
| 2 | Z | 963 | THR | CA-C | 5.33 | 1.59 | 1.52 |
| 13 | x | 1305 | GLN | N-CA | -5.33 | 1.40 | 1.46 |
| 17 | k | 231 | CYS | C-N | 5.33 | 1.40 | 1.33 |
| 20 | n | 790 | HIS | CA-C | -5.33 | 1.45 | 1.52 |
| 20 | g | 351 | ILE | CA-CB | 5.33 | 1.60 | 1.54 |
| 20 | g | 411 | ASN | C-O | -5.33 | 1.17 | 1.24 |
| 1 | 0 | 767 | SER | C-N | -5.33 | 1.27 | 1.34 |
| 2 | 1 | 1066 | ASN | CA-CB | 5.33 | 1.61 | 1.53 |
| 6 | L | 329 | ASP | N-CA | -5.33 | 1.40 | 1.46 |
| 8 | P | 919 | LEU | N-CA | -5.33 | 1.39 | 1.46 |
| 9 | S | 289 | LEU | CA-CB | 5.33 | 1.61 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | R | 505 | HIS | ND1-CE1 | 5.33 | 1.37 | 1.32 |
| 14 | h | 938 | ARG | CZ-NH2 | 5.33 | 1.40 | 1.33 |
| 2 | Z | 345 | LEU | CA-CB | 5.33 | 1.62 | 1.53 |
| 12 | u | 44 | ARG | C-N | 5.33 | 1.40 | 1.33 |
| 19 | m | 188 | ILE | CA-C | 5.33 | 1.60 | 1.52 |
| 20 | n | 1012 | GLU | N-CA | -5.33 | 1.39 | 1.46 |
| 15 | b | 640 | GLU | C-N | 5.33 | 1.41 | 1.33 |
| 16 | c | 423 | GLN | N-CA | 5.33 | 1.52 | 1.46 |
| 4 | J | 695 | GLN | CA-C | -5.33 | 1.46 | 1.52 |
| 8 | P | 1205 | LYS | CA-CB | 5.33 | 1.62 | 1.53 |
| 8 | P | 1313 | ARG | CZ-NH2 | 5.33 | 1.40 | 1.33 |
| 13 | w | 1453 | PHE | N-CA | -5.33 | 1.40 | 1.46 |
| 16 | c | 547 | ARG | CA-C | -5.33 | 1.45 | 1.52 |
| 19 | f | 212 | LEU | CA-CB | 5.33 | 1.62 | 1.53 |
| 20 | g | 752 | GLN | N-CA | -5.33 | 1.39 | 1.46 |
| 14 | a | 462 | SER | N-CA | 5.33 | 1.52 | 1.45 |
| 2 | 1 | 423 | ALA | C-N | 5.32 | 1.40 | 1.33 |
| 6 | F | 335 | SER | N-CA | 5.32 | 1.52 | 1.46 |
| 7 | O | 73 | GLU | C-N | 5.32 | 1.41 | 1.33 |
| 7 | O | 157 | GLU | C-N | 5.32 | 1.40 | 1.33 |
| 7 | O | 637 | ASP | N-CA | -5.32 | 1.40 | 1.46 |
| 7 | O | 1374 | LYS | CA-CB | 5.32 | 1.62 | 1.53 |
| 8 | P | 1547 | LEU | CA-C | -5.32 | 1.45 | 1.52 |
| 1 | Y | 781 | LEU | CA-CB | -5.32 | 1.46 | 1.53 |
| 12 | v | 134 | PRO | CA-C | -5.32 | 1.44 | 1.52 |
| 18 | e | 15 | VAL | C-O | -5.32 | 1.18 | 1.24 |
| 20 | g | 547 | PRO | CA-CB | 5.32 | 1.61 | 1.54 |
| 1 | 0 | 1025 | ASN | CA-C | -5.32 | 1.46 | 1.52 |
| 7 | M | 893 | HIS | C-O | -5.32 | 1.17 | 1.24 |
| 7 | O | 674 | PHE | C-O | -5.32 | 1.18 | 1.24 |
| 9 | R | 670 | LEU | CB-CG | 5.32 | 1.64 | 1.53 |
| 15 | b | 738 | LYS | C-N | 5.32 | 1.41 | 1.33 |
| 18 | e | 107 | SER | C-N | 5.32 | 1.41 | 1.33 |
| 14 | a | 533 | LEU | CA-CB | 5.32 | 1.61 | 1.53 |
| 1 | 0 | 1425 | LYS | CA-C | -5.32 | 1.46 | 1.52 |
| 7 | M | 1029 | SER | N-CA | -5.32 | 1.39 | 1.46 |
| 8 | N | 187 | PHE | C-N | 5.32 | 1.40 | 1.33 |
| 8 | P | 163 | ASP | C-N | 5.32 | 1.41 | 1.33 |
| 16 | j | 563 | SER | CA-C | -5.32 | 1.45 | 1.53 |
| 17 | d | 29 | SER | C-O | -5.32 | 1.17 | 1.24 |
| 20 | g | 313 | TYR | CZ-OH | 5.32 | 1.49 | 1.38 |
| 20 | g | 342 | GLU | C-N | 5.32 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | G | 702 | ARG | NE-CZ | 5.32 | 1.39 | 1.33 |
| 9 | R | 628 | ALA | CA-CB | 5.32 | 1.61 | 1.53 |
| 15 | i | 651 | LEU | N-CA | 5.32 | 1.52 | 1.46 |
| 20 | g | 135 | ALA | C-N | 5.32 | 1.39 | 1.34 |
| 2 | 1 | 214 | PHE | CA-C | -5.32 | 1.45 | 1.52 |
| 2 | 1 | 581 | SER | CA-C | 5.32 | 1.59 | 1.53 |
| 2 | 1 | 769 | HIS | CA-CB | 5.32 | 1.61 | 1.53 |
| 6 | C | 400 | GLY | CA-C | -5.32 | 1.46 | 1.52 |
| 7 | M | 1328 | ILE | CA-CB | -5.32 | 1.48 | 1.54 |
| 8 | P | 756 | TRP | CA-C | -5.32 | 1.46 | 1.52 |
| 15 | i | 403 | HIS | C-N | 5.32 | 1.41 | 1.33 |
| 19 | m | 273 | ASN | C-N | 5.32 | 1.41 | 1.33 |
| 19 | m | 627 | THR | CA-C | -5.32 | 1.45 | 1.52 |
| 16 | c | 267 | ARG | N-CA | -5.32 | 1.40 | 1.46 |
| 14 | a | 1006 | VAL | CA-C | -5.32 | 1.46 | 1.53 |
| 7 | M | 1446 | VAL | CA-C | -5.32 | 1.47 | 1.53 |
| 8 | N | 614 | ILE | N-CA | -5.32 | 1.39 | 1.46 |
| 8 | P | 461 | CYS | CA-C | -5.32 | 1.46 | 1.52 |
| 8 | P | 1070 | LYS | CA-CB | 5.32 | 1.62 | 1.53 |
| 8 | P | 1215 | VAL | CA-C | 5.32 | 1.59 | 1.52 |
| 9 | Q | 644 | TYR | CG-CD1 | 5.32 | 1.50 | 1.39 |
| 9 | T | 639 | ASP | C-N | 5.32 | 1.41 | 1.33 |
| 1 | Y | 362 | ASP | CA-CB | 5.32 | 1.60 | 1.53 |
| 12 | u | 210 | PRO | C-N | 5.32 | 1.40 | 1.33 |
| 12 | v | 600 | GLU | C-N | 5.32 | 1.41 | 1.33 |
| 15 | i | 478 | ASP | CA-CB | 5.32 | 1.61 | 1.53 |
| 19 | f | 616 | LEU | C-N | 5.32 | 1.40 | 1.33 |
| 15 | b | 423 | ILE | CA-C | -5.31 | 1.47 | 1.53 |
| 17 | d | 254 | PRO | N-CD | 5.31 | 1.55 | 1.47 |
| 20 | g | 643 | PRO | C-N | 5.31 | 1.40 | 1.33 |
| 14 | a | 880 | ARG | CD-NE | 5.31 | 1.53 | 1.46 |
| 4 | A | 792 | GLN | C-O | -5.31 | 1.17 | 1.24 |
| 4 | G | 705 | ASP | N-CA | -5.31 | 1.38 | 1.46 |
| 7 | M | 47 | SER | N-CA | -5.31 | 1.40 | 1.46 |
| 8 | N | 366 | SER | C-N | 5.31 | 1.40 | 1.33 |
| 7 | O | 1647 | ARG | N-CA | 5.31 | 1.52 | 1.46 |
| 8 | P | 563 | SER | CA-C | -5.31 | 1.45 | 1.52 |
| 13 | x | 1273 | GLN | C-N | 5.31 | 1.41 | 1.33 |
| 20 | n | 579 | ILE | CA-C | -5.31 | 1.46 | 1.52 |
| 6 | F | 389 | ARG | NE-CZ | 5.31 | 1.38 | 1.33 |
| 6 | I | 344 | LEU | C-N | 5.31 | 1.41 | 1.34 |
| 7 | O | 1513 | TYR | CA-CB | 5.31 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 10 | W | 342 | CYS | CA-C | -5.31 | 1.46 | 1.52 |
| 13 | x | 1439 | VAL | N-CA | -5.31 | 1.40 | 1.46 |
| 14 | h | 924 | ARG | CA-C | -5.31 | 1.46 | 1.52 |
| 15 | b | 610 | ASP | CA-C | -5.31 | 1.45 | 1.52 |
| 1 | 0 | 1218 | TYR | CZ-OH | 5.31 | 1.49 | 1.38 |
| 2 | 1 | 907 | GLY | CA-C | -5.31 | 1.46 | 1.52 |
| 4 | A | 702 | ARG | C-N | 5.31 | 1.41 | 1.33 |
| 5 | K | 422 | LEU | CA-C | -5.31 | 1.45 | 1.52 |
| 5 | K | 508 | LYS | CA-C | -5.31 | 1.45 | 1.52 |
| 8 | P | 1171 | ARG | N-CA | -5.31 | 1.39 | 1.46 |
| 9 | R | 477 | TYR | CA-CB | 5.31 | 1.62 | 1.53 |
| 10 | U | 324 | LYS | CA-C | -5.31 | 1.45 | 1.52 |
| 4 | z | 659 | THR | CA-CB | 5.31 | 1.61 | 1.53 |
| 14 | h | 232 | ARG | CD-NE | 5.31 | 1.53 | 1.46 |
| 16 | j | 577 | GLY | N-CA | 5.31 | 1.51 | 1.44 |
| 17 | k | 216 | VAL | CA-CB | -5.31 | 1.47 | 1.54 |
| 20 | g | 204 | GLY | CA-C | -5.31 | 1.47 | 1.52 |
| 20 | g | 631 | THR | CA-C | -5.31 | 1.45 | 1.52 |
| 2 | 1 | 906 | ALA | C-N | 5.31 | 1.39 | 1.33 |
| 7 | M | 795 | VAL | C-N | 5.31 | 1.40 | 1.33 |
| 8 | N | 705 | TYR | CA-CB | 5.31 | 1.61 | 1.53 |
| 9 | T | 267 | ASP | N-CA | -5.31 | 1.40 | 1.46 |
| 1 | Y | 1078 | LYS | CA-C | 5.31 | 1.60 | 1.52 |
| 20 | n | 494 | VAL | CA-C | -5.31 | 1.46 | 1.52 |
| 14 | a | 591 | MET | C-N | 5.31 | 1.40 | 1.33 |
| 2 | 1 | 1062 | TRP | CA-CB | 5.31 | 1.61 | 1.53 |
| 9 | S | 789 | LEU | CA-CB | 5.31 | 1.62 | 1.53 |
| 9 | T | 777 | ILE | CA-CB | -5.31 | 1.48 | 1.54 |
| 16 | j | 305 | ARG | N-CA | 5.31 | 1.52 | 1.46 |
| 2 | 1 | 438 | ILE | CA-C | -5.30 | 1.46 | 1.52 |
| 5 | B | 395 | ALA | N-CA | -5.30 | 1.39 | 1.46 |
| 7 | O | 995 | VAL | CA-C | -5.30 | 1.46 | 1.52 |
| 9 | R | 630 | ARG | C-N | 5.30 | 1.40 | 1.33 |
| 12 | u | 214 | SER | C-N | 5.30 | 1.40 | 1.33 |
| 15 | b | 392 | GLN | N-CA | -5.30 | 1.38 | 1.46 |
| 15 | b | 605 | VAL | C-O | 5.30 | 1.30 | 1.24 |
| 2 | 1 | 142 | GLN | C-N | 5.30 | 1.40 | 1.33 |
| 7 | M | 1157 | TRP | N-CA | -5.30 | 1.40 | 1.46 |
| 7 | M | 1545 | ARG | C-N | 5.30 | 1.40 | 1.34 |
| 14 | a | 440 | GLU | C-O | -5.30 | 1.18 | 1.23 |
| 8 | N | 1092 | SER | CA-CB | 5.30 | 1.62 | 1.53 |
| 8 | N | 1199 | TYR | N-CA | -5.30 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 639 | VAL | CA-C | 5.30 | 1.58 | 1.52 |
| 1 | Y | 1152 | TYR | CA-C | 5.30 | 1.59 | 1.52 |
| 14 | h | 619 | LEU | CA-C | -5.30 | 1.46 | 1.52 |
| 16 | j | 274 | SER | C-N | 5.30 | 1.41 | 1.33 |
| 19 | m | 455 | PRO | N-CA | 5.30 | 1.54 | 1.47 |
| 15 | b | 224 | ILE | CB-CG1 | 5.30 | 1.64 | 1.53 |
| 1 | 0 | 704 | THR | CA-CB | -5.30 | 1.44 | 1.53 |
| 6 | L | 314 | TYR | CA-C | -5.30 | 1.45 | 1.52 |
| 7 | O | 837 | TYR | C-N | 5.30 | 1.40 | 1.33 |
| 8 | P | 766 | GLU | N-CA | -5.30 | 1.40 | 1.46 |
| 9 | Q | 704 | ARG | CD-NE | 5.30 | 1.53 | 1.46 |
| 9 | T | 646 | LEU | C-N | 5.30 | 1.41 | 1.33 |
| 15 | i | 504 | ILE | CB-CG1 | 5.30 | 1.64 | 1.53 |
| 19 | m | 457 | VAL | CA-CB | -5.30 | 1.47 | 1.54 |
| 18 | e | 186 | SER | N-CA | -5.30 | 1.39 | 1.46 |
| 14 | a | 658 | HIS | CG-ND1 | -5.30 | 1.32 | 1.38 |
| 14 | a | 658 | HIS | ND1-CE1 | 5.30 | 1.37 | 1.32 |
| 14 | a | 677 | GLU | CA-C | -5.30 | 1.45 | 1.52 |
| 19 | m | 304 | GLU | C-N | 5.30 | 1.41 | 1.33 |
| 15 | b | 210 | ASN | CA-CB | 5.30 | 1.62 | 1.53 |
| 20 | g | 972 | CYS | CA-C | -5.30 | 1.46 | 1.52 |
| 8 | N | 756 | TRP | CA-C | 5.30 | 1.59 | 1.52 |
| 8 | P | 1449 | GLU | C-N | 5.30 | 1.40 | 1.33 |
| 9 | T | 471 | PRO | CA-CB | 5.30 | 1.61 | 1.53 |
| 2 | Z | 647 | LEU | C-N | 5.30 | 1.41 | 1.33 |
| 20 | n | 401 | ILE | CA-C | -5.30 | 1.47 | 1.52 |
| 20 | n | 722 | PHE | C-N | 5.30 | 1.42 | 1.33 |
| 19 | f | 69 | GLU | N-CA | -5.30 | 1.40 | 1.46 |
| 2 | 1 | 1177 | VAL | CA-CB | 5.29 | 1.62 | 1.54 |
| 7 | O | 1383 | GLN | CA-C | -5.29 | 1.45 | 1.52 |
| 4 | z | 755 | LEU | C-N | 5.29 | 1.40 | 1.33 |
| 14 | h | 83 | PRO | CA-CB | 5.29 | 1.60 | 1.53 |
| 14 | h | 420 | PHE | CA-CB | 5.29 | 1.61 | 1.53 |
| 4 | J | 710 | PHE | N-CA | -5.29 | 1.40 | 1.46 |
| 8 | N | 1416 | GLY | C-N | 5.29 | 1.40 | 1.33 |
| 9 | T | 251 | ALA | N-CA | -5.29 | 1.40 | 1.46 |
| 11 | X | 384 | CYS | CA-CB | 5.29 | 1.63 | 1.53 |
| 15 | i | 696 | GLU | C-N | 5.29 | 1.41 | 1.33 |
| 19 | m | 50 | ALA | CA-C | -5.29 | 1.45 | 1.52 |
| 19 | m | 294 | LEU | N-CA | -5.29 | 1.39 | 1.46 |
| 20 | n | 558 | SER | C-N | 5.29 | 1.40 | 1.33 |
| 16 | c | 359 | LYS | C-N | 5.29 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | f | 428 | ASN | CA-C | -5.29 | 1.45 | 1.52 |
| 14 | a | 436 | HIS | ND1-CE1 | 5.29 | 1.37 | 1.32 |
| 1 | 0 | 1397 | PHE | N-CA | -5.29 | 1.39 | 1.46 |
| 6 | I | 375 | LYS | CA-C | -5.29 | 1.46 | 1.52 |
| 7 | M | 1013 | TYR | CA-C | -5.29 | 1.45 | 1.52 |
| 8 | N | 451 | GLU | CA-CB | 5.29 | 1.60 | 1.53 |
| 8 | N | 1309 | ARG | CA-CB | 5.29 | 1.60 | 1.53 |
| 9 | S | 134 | LYS | C-N | 5.29 | 1.40 | 1.33 |
| 1 | Y | 1314 | PRO | CA-C | 5.29 | 1.59 | 1.52 |
| 13 | w | 1392 | ARG | C-N | 5.29 | 1.40 | 1.33 |
| 21 | o | 12 | LYS | CB-CG | 5.29 | 1.68 | 1.52 |
| 21 | q | 57 | TRP | CA-CB | 5.29 | 1.61 | 1.53 |
| 4 | D | 715 | GLU | CA-CB | 5.29 | 1.61 | 1.53 |
| 6 | L | 373 | PHE | CA-C | -5.29 | 1.46 | 1.52 |
| 7 | M | 624 | ASP | C-N | 5.29 | 1.40 | 1.33 |
| 8 | N | 452 | PHE | N-CA | -5.29 | 1.39 | 1.46 |
| 1 | Y | 1238 | ARG | C-N | 5.29 | 1.40 | 1.33 |
| 2 | Z | 1160 | ILE | CA-CB | -5.29 | 1.47 | 1.54 |
| 12 | u | 58 | ASN | N-CA | -5.29 | 1.39 | 1.46 |
| 16 | j | 233 | LEU | CB-CG | 5.29 | 1.64 | 1.53 |
| 16 | j | 382 | LEU | CA-CB | 5.29 | 1.61 | 1.53 |
| 19 | m | 701 | ILE | N-CA | -5.29 | 1.40 | 1.46 |
| 20 | n | 280 | THR | C-N | 5.29 | 1.40 | 1.33 |
| 19 | f | 322 | LEU | CA-C | -5.29 | 1.46 | 1.52 |
| 20 | g | 420 | PHE | CA-CB | 5.29 | 1.62 | 1.54 |
| 2 | 1 | 409 | ILE | CA-C | -5.29 | 1.48 | 1.53 |
| 9 | R | 606 | GLU | N-CA | -5.29 | 1.39 | 1.46 |
| 9 | R | 825 | PRO | CA-C | -5.29 | 1.46 | 1.52 |
| 12 | v | 231 | LEU | CB-CG | 5.29 | 1.64 | 1.53 |
| 7 | O | 1582 | LEU | C-N | 5.29 | 1.40 | 1.33 |
| 8 | P | 147 | SER | N-CA | 5.29 | 1.53 | 1.46 |
| 10 | W | 344 | SER | C-N | 5.29 | 1.40 | 1.33 |
| 19 | m | 215 | ILE | CB-CG1 | 5.29 | 1.64 | 1.53 |
| 15 | b | 461 | MET | CA-C | -5.29 | 1.46 | 1.52 |
| 1 | 0 | 178 | GLU | C-N | 5.28 | 1.41 | 1.33 |
| 2 | 1 | 819 | ILE | C-O | -5.28 | 1.19 | 1.24 |
| 2 | 1 | 1368 | LYS | N-CA | -5.28 | 1.38 | 1.46 |
| 4 | G | 641 | VAL | N-CA | -5.28 | 1.39 | 1.46 |
| 7 | O | 1139 | ILE | N-CA | -5.28 | 1.39 | 1.46 |
| 8 | P | 1031 | LYS | C-N | 5.28 | 1.40 | 1.33 |
| 9 | R | 114 | ARG | CA-C | -5.28 | 1.46 | 1.52 |
| 9 | T | 762 | ASN | C-N | 5.28 | 1.37 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 1102 | LEU | CA-C | -5.28 | 1.45 | 1.52 |
| 17 | k | 226 | SER | CA-C | -5.28 | 1.46 | 1.52 |
| 18 | l | 210 | GLY | CA-C | -5.28 | 1.43 | 1.51 |
| 15 | b | 460 | GLY | C-N | 5.28 | 1.41 | 1.33 |
| 16 | c | 428 | ASN | C-N | 5.28 | 1.41 | 1.33 |
| 17 | d | 277 | LYS | N-CA | 5.28 | 1.52 | 1.46 |
| 20 | g | 1083 | LEU | N-CA | -5.28 | 1.39 | 1.46 |
| 9 | R | 763 | LEU | CA-C | -5.28 | 1.45 | 1.52 |
| 19 | m | 69 | GLU | N-CA | -5.28 | 1.40 | 1.46 |
| 14 | a | 370 | ASP | N-CA | -5.28 | 1.40 | 1.46 |
| 14 | a | 446 | LEU | CA-CB | 5.28 | 1.61 | 1.53 |
| 6 | C | 402 | ASP | N-CA | 5.28 | 1.52 | 1.46 |
| 9 | Q | 66 | TYR | N-CA | 5.28 | 1.52 | 1.45 |
| 9 | Q | 689 | ALA | CA-C | -5.28 | 1.46 | 1.52 |
| 9 | S | 649 | GLU | CA-C | -5.28 | 1.46 | 1.52 |
| 14 | h | 316 | GLN | C-N | 5.28 | 1.41 | 1.33 |
| 16 | j | 349 | SER | CA-C | -5.28 | 1.45 | 1.52 |
| 7 | M | 490 | ALA | C-O | -5.28 | 1.17 | 1.23 |
| 7 | O | 172 | ASN | CA-C | -5.28 | 1.46 | 1.52 |
| 13 | w | 1434 | PHE | CA-C | 5.28 | 1.59 | 1.52 |
| 18 | e | 298 | SER | C-O | 5.28 | 1.30 | 1.23 |
| 2 | 1 | 157 | THR | CA-C | -5.28 | 1.46 | 1.52 |
| 6 | F | 452 | ASP | CA-CB | 5.28 | 1.61 | 1.53 |
| 5 | K | 365 | GLN | CA-C | 5.28 | 1.59 | 1.52 |
| 7 | M | 823 | PRO | CA-C | -5.28 | 1.45 | 1.52 |
| 7 | M | 1109 | ILE | C-N | 5.28 | 1.41 | 1.34 |
| 7 | O | 707 | LEU | C-N | 5.28 | 1.40 | 1.33 |
| 8 | P | 729 | HIS | CD2-NE2 | 5.28 | 1.43 | 1.37 |
| 9 | R | 370 | TYR | CA-C | -5.28 | 1.45 | 1.52 |
| 21 | q | 64 | ASN | C-N | 5.28 | 1.39 | 1.33 |
| 21 | s | 39 | ARG | NE-CZ | 5.28 | 1.38 | 1.33 |
| 19 | f | 330 | ARG | CZ-NH2 | 5.28 | 1.40 | 1.33 |
| 1 | 0 | 1429 | ILE | CA-C | 5.28 | 1.59 | 1.52 |
| 2 | 1 | 185 | ILE | CA-C | -5.28 | 1.46 | 1.52 |
| 2 | 1 | 751 | GLN | CA-C | -5.28 | 1.46 | 1.52 |
| 2 | 1 | 976 | LYS | N-CA | 5.28 | 1.53 | 1.46 |
| 6 | C | 351 | SER | CA-C | -5.28 | 1.45 | 1.52 |
| 7 | M | 716 | LEU | N-CA | 5.28 | 1.52 | 1.46 |
| 8 | N | 748 | HIS | ND1-CE1 | 5.28 | 1.37 | 1.32 |
| 7 | O | 1500 | ASN | CA-CB | 5.28 | 1.62 | 1.53 |
| 16 | j | 571 | ALA | C-N | 5.28 | 1.40 | 1.33 |
| 18 | l | 146 | ARG | NE-CZ | 5.28 | 1.38 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 17 | d | 259 | ARG | NE-CZ | 5.28 | 1.38 | 1.33 |
| 18 | e | 331 | TRP | CA-C | -5.28 | 1.46 | 1.52 |
| 14 | a | 684 | SER | CA-C | -5.28 | 1.45 | 1.52 |
| 4 | D | 647 | GLN | C-N | 5.27 | 1.40 | 1.33 |
| 9 | R | 473 | ARG | C-N | 5.27 | 1.42 | 1.33 |
| 9 | T | 59 | LYS | CA-C | -5.27 | 1.45 | 1.52 |
| 15 | i | 206 | GLU | CA-CB | 5.27 | 1.61 | 1.53 |
| 20 | n | 379 | SER | C-N | 5.27 | 1.40 | 1.33 |
| 15 | b | 292 | LEU | CA-C | -5.27 | 1.45 | 1.52 |
| 15 | b | 406 | LEU | C-N | 5.27 | 1.41 | 1.33 |
| 14 | a | 400 | LYS | C-N | 5.27 | 1.40 | 1.33 |
| 8 | N | 211 | GLN | N-CA | -5.27 | 1.39 | 1.46 |
| 8 | N | 668 | TYR | CA-C | 5.27 | 1.59 | 1.52 |
| 8 | N | 1595 | LYS | N-CA | -5.27 | 1.39 | 1.46 |
| 8 | P | 1248 | THR | C-N | 5.27 | 1.41 | 1.33 |
| 9 | T | 726 | LEU | C-N | 5.27 | 1.41 | 1.33 |
| 1 | Y | 697 | SER | C-N | 5.27 | 1.41 | 1.34 |
| 15 | i | 250 | ASN | CA-CB | 5.27 | 1.61 | 1.53 |
| 15 | i | 547 | LEU | N-CA | -5.27 | 1.39 | 1.46 |
| 20 | n | 859 | ASP | C-N | 5.27 | 1.40 | 1.33 |
| 20 | n | 1110 | ARG | NE-CZ | 5.27 | 1.38 | 1.33 |
| 21 | s | 79 | PHE | CA-C | -5.27 | 1.46 | 1.52 |
| 15 | b | 672 | TYR | CA-C | -5.27 | 1.46 | 1.52 |
| 16 | c | 356 | LYS | CA-CB | 5.27 | 1.62 | 1.53 |
| 20 | g | 353 | ASP | CA-C | -5.27 | 1.46 | 1.52 |
| 8 | N | 104 | SER | N-CA | -5.27 | 1.39 | 1.46 |
| 2 | Z | 722 | GLN | N-CA | -5.27 | 1.39 | 1.46 |
| 17 | d | 281 | TRP | N-CA | 5.27 | 1.53 | 1.46 |
| 2 | 1 | 947 | LEU | CA-CB | 5.27 | 1.61 | 1.53 |
| 6 | F | 449 | LEU | N-CA | -5.27 | 1.39 | 1.46 |
| 9 | S | 89 | ASP | N-CA | -5.27 | 1.40 | 1.46 |
| 11 | V | 382 | ILE | CA-C | -5.27 | 1.46 | 1.52 |
| 2 | Z | 761 | VAL | C-N | 5.27 | 1.41 | 1.33 |
| 2 | Z | 1249 | PRO | CA-CB | 5.27 | 1.62 | 1.53 |
| 20 | n | 749 | LEU | N-CA | -5.27 | 1.39 | 1.46 |
| 15 | b | 116 | ARG | NE-CZ | 5.27 | 1.38 | 1.33 |
| 19 | f | 604 | VAL | C-N | 5.27 | 1.41 | 1.33 |
| 20 | g | 438 | SER | C-N | 5.27 | 1.41 | 1.33 |
| 1 | 0 | 151 | GLN | CA-CB | 5.27 | 1.62 | 1.53 |
| 7 | O | 620 | THR | CA-C | -5.27 | 1.45 | 1.52 |
| 9 | T | 63 | SER | N-CA | -5.27 | 1.39 | 1.45 |
| 15 | i | 211 | TRP | CA-CB | 5.27 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | g | 1056 | LYS | CA-C | -5.27 | 1.45 | 1.52 |
| 7 | M | 354 | ARG | CD-NE | 5.27 | 1.53 | 1.46 |
| 7 | O | 1531 | THR | C-N | 5.27 | 1.40 | 1.33 |
| 2 | Z | 354 | LEU | CA-CB | 5.27 | 1.59 | 1.52 |
| 1 | 0 | 891 | ILE | CA-C | 5.26 | 1.59 | 1.52 |
| 2 | 1 | 1070 | ASP | N-CA | -5.26 | 1.39 | 1.46 |
| 4 | J | 644 | TRP | CA-CB | -5.26 | 1.44 | 1.53 |
| 7 | O | 43 | LYS | C-N | 5.26 | 1.40 | 1.33 |
| 7 | O | 677 | SER | CA-CB | 5.26 | 1.61 | 1.53 |
| 8 | P | 864 | SER | C-N | 5.26 | 1.40 | 1.33 |
| 9 | Q | 754 | ARG | CD-NE | 5.26 | 1.53 | 1.46 |
| 12 | u | 339 | VAL | C-N | 5.26 | 1.41 | 1.33 |
| 20 | n | 625 | GLN | C-N | 5.26 | 1.40 | 1.33 |
| 16 | c | 442 | THR | N-CA | -5.26 | 1.39 | 1.46 |
| 14 | a | 595 | ILE | CA-CB | -5.26 | 1.47 | 1.53 |
| 1 | 0 | 1360 | SER | CA-C | 5.26 | 1.59 | 1.52 |
| 8 | N | 1353 | SER | N-CA | -5.26 | 1.39 | 1.46 |
| 7 | O | 1303 | LEU | N-CA | -5.26 | 1.40 | 1.46 |
| 2 | Z | 652 | ASN | CG-ND2 | 5.26 | 1.44 | 1.33 |
| 14 | h | 75 | ARG | NE-CZ | 5.26 | 1.38 | 1.33 |
| 1 | 0 | 117 | ASN | CA-C | -5.26 | 1.46 | 1.52 |
| 2 | 1 | 1289 | MET | CA-C | -5.26 | 1.45 | 1.52 |
| 6 | C | 331 | LYS | CA-C | -5.26 | 1.46 | 1.52 |
| 4 | G | 680 | TYR | N-CA | -5.26 | 1.40 | 1.46 |
| 6 | I | 272 | GLN | N-CA | -5.26 | 1.39 | 1.46 |
| 8 | N | 179 | LEU | C-N | 5.26 | 1.41 | 1.33 |
| 7 | O | 772 | ASN | N-CA | -5.26 | 1.38 | 1.46 |
| 8 | P | 517 | LEU | CA-C | -5.26 | 1.45 | 1.52 |
| 9 | Q | 684 | ASN | CA-C | 5.26 | 1.57 | 1.52 |
| 9 | S | 567 | THR | CA-C | -5.26 | 1.45 | 1.52 |
| 9 | T | 142 | HIS | C-N | 5.26 | 1.40 | 1.33 |
| 2 | Z | 812 | ILE | CA-C | 5.26 | 1.60 | 1.52 |
| 12 | v | 654 | ASP | N-CA | -5.26 | 1.39 | 1.46 |
| 14 | h | 705 | LEU | N-CA | -5.26 | 1.39 | 1.46 |
| 18 | l | 196 | ARG | CA-CB | 5.26 | 1.62 | 1.53 |
| 20 | n | 672 | LEU | N-CA | -5.26 | 1.40 | 1.47 |
| 14 | a | 817 | VAL | N-CA | 5.26 | 1.53 | 1.46 |
| 5 | B | 361 | ARG | NE-CZ | 5.26 | 1.38 | 1.33 |
| 8 | N | 1333 | SER | CA-C | -5.26 | 1.46 | 1.52 |
| 7 | O | 1525 | LEU | C-N | 5.26 | 1.40 | 1.33 |
| 1 | Y | 1435 | GLU | C-N | 5.26 | 1.40 | 1.33 |
| 12 | u | 64 | VAL | C-N | 5.26 | 1.41 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 18 | l | 344 | VAL | CA-C | -5.26 | 1.48 | 1.53 |
| 20 | n | 857 | LEU | CA-C | 5.26 | 1.59 | 1.52 |
| 20 | g | 66 | ARG | CZ-NH1 | 5.26 | 1.40 | 1.32 |
| 7 | M | 873 | ASN | C-N | 5.26 | 1.41 | 1.34 |
| 9 | Q | 638 | TYR | N-CA | -5.26 | 1.39 | 1.46 |
| 20 | n | 512 | ILE | CA-C | -5.26 | 1.46 | 1.52 |
| 19 | f | 37 | ASN | CA-C | -5.26 | 1.46 | 1.52 |
| 14 | a | 291 | LEU | CA-CB | 5.26 | 1.62 | 1.52 |
| 1 | 0 | 1168 | GLN | N-CA | -5.26 | 1.39 | 1.46 |
| 6 | C | 458 | ALA | C-N | 5.26 | 1.40 | 1.33 |
| 4 | J | 670 | VAL | C-N | 5.26 | 1.40 | 1.33 |
| 7 | M | 227 | ASP | CA-CB | 5.26 | 1.61 | 1.53 |
| 8 | P | 705 | TYR | N-CA | -5.26 | 1.39 | 1.46 |
| 2 | Z | 424 | VAL | C-N | 5.26 | 1.40 | 1.33 |
| 20 | n | 570 | PHE | C-N | 5.26 | 1.40 | 1.33 |
| 21 | o | 30 | ASP | C-N | 5.26 | 1.40 | 1.33 |
| 15 | b | 156 | GLU | CA-C | -5.26 | 1.46 | 1.52 |
| 19 | f | 104 | LEU | N-CA | -5.26 | 1.39 | 1.46 |
| 2 | 1 | 1260 | SER | CA-C | -5.25 | 1.46 | 1.52 |
| 7 | M | 1469 | ARG | C-N | 5.25 | 1.41 | 1.33 |
| 8 | N | 333 | ARG | CZ-NH1 | 5.25 | 1.40 | 1.32 |
| 8 | N | 732 | LYS | N-CA | -5.25 | 1.40 | 1.46 |
| 7 | O | 938 | ALA | CA-CB | 5.25 | 1.61 | 1.53 |
| 1 | Y | 641 | VAL | N-CA | -5.25 | 1.39 | 1.46 |
| 20 | n | 528 | GLU | CA-CB | 5.25 | 1.60 | 1.53 |
| 14 | a | 901 | ARG | NE-CZ | 5.25 | 1.38 | 1.33 |
| 1 | 0 | 956 | ASN | CA-C | -5.25 | 1.45 | 1.52 |
| 4 | D | 713 | ASN | CA-C | -5.25 | 1.45 | 1.52 |
| 5 | E | 315 | LYS | N-CA | 5.25 | 1.52 | 1.46 |
| 12 | u | 374 | TYR | CA-CB | 5.25 | 1.60 | 1.53 |
| 14 | h | 106 | TYR | CZ-OH | 5.25 | 1.49 | 1.38 |
| 16 | j | 155 | THR | CA-C | 5.25 | 1.59 | 1.52 |
| 20 | g | 569 | THR | C-N | 5.25 | 1.40 | 1.33 |
| 14 | a | 6 | ARG | N-CA | 5.25 | 1.52 | 1.46 |
| 14 | a | 617 | GLU | CA-C | -5.25 | 1.45 | 1.52 |
| 7 | M | 1484 | ARG | NE-CZ | 5.25 | 1.38 | 1.33 |
| 8 | P | 424 | LYS | C-N | 5.25 | 1.41 | 1.33 |
| 9 | R | 478 | TYR | C-N | 5.25 | 1.40 | 1.33 |
| 9 | S | 760 | PHE | CG-CD1 | 5.25 | 1.49 | 1.38 |
| 9 | T | 76 | SER | C-N | 5.25 | 1.40 | 1.33 |
| 17 | k | 285 | LEU | CA-CB | 5.25 | 1.62 | 1.53 |
| 20 | n | 159 | ASP | CA-CB | 5.25 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | b | 562 | ALA | CA-CB | 5.25 | 1.62 | 1.53 |
| 19 | f | 549 | PHE | CA-CB | 5.25 | 1.62 | 1.53 |
| 14 | a | 655 | LEU | C-N | 5.25 | 1.41 | 1.33 |
| 1 | Y | 419 | LYS | CA-CB | 5.25 | 1.60 | 1.53 |
| 1 | Y | 1161 | MET | N-CA | -5.25 | 1.40 | 1.46 |
| 21 | s | 83 | PRO | C-N | 5.25 | 1.40 | 1.33 |
| 14 | a | 832 | PHE | CA-CB | 5.25 | 1.61 | 1.53 |
| 1 | 0 | 587 | LYS | CA-C | -5.25 | 1.45 | 1.52 |
| 2 | 1 | 395 | ASN | N-CA | 5.25 | 1.52 | 1.45 |
| 9 | Q | 82 | ASP | C-N | 5.25 | 1.40 | 1.33 |
| 9 | Q | 798 | THR | CA-CB | 5.25 | 1.62 | 1.53 |
| 9 | T | 282 | PHE | CA-C | 5.25 | 1.59 | 1.52 |
| 12 | v | 185 | LEU | C-N | 5.25 | 1.40 | 1.33 |
| 19 | m | 197 | LEU | CA-CB | 5.25 | 1.61 | 1.53 |
| 20 | n | 1063 | LYS | N-CA | -5.25 | 1.40 | 1.46 |
| 18 | e | 241 | ARG | CA-C | -5.25 | 1.47 | 1.53 |
| 14 | a | 292 | PRO | N-CD | -5.25 | 1.40 | 1.47 |
| 8 | P | 775 | PHE | N-CA | -5.25 | 1.40 | 1.46 |
| 2 | Z | 191 | TYR | CA-C | -5.25 | 1.46 | 1.53 |
| 12 | u | 275 | GLU | N-CA | -5.25 | 1.39 | 1.46 |
| 4 | y | 639 | ASP | C-N | 5.25 | 1.40 | 1.33 |
| 15 | i | 528 | GLU | N-CA | -5.25 | 1.40 | 1.46 |
| 17 | k | 23 | ARG | CD-NE | 5.25 | 1.53 | 1.46 |
| 20 | g | 782 | ASP | C-N | 5.25 | 1.41 | 1.33 |
| 14 | a | 209 | THR | N-CA | 5.25 | 1.52 | 1.45 |
| 1 | 0 | 772 | GLY | CA-C | -5.25 | 1.46 | 1.52 |
| 1 | 0 | 1227 | ILE | CA-CB | -5.25 | 1.47 | 1.55 |
| 8 | N | 1091 | ASP | CA-C | -5.25 | 1.47 | 1.53 |
| 7 | O | 1280 | ILE | N-CA | 5.25 | 1.52 | 1.46 |
| 1 | Y | 1404 | LYS | CA-CB | 5.25 | 1.62 | 1.53 |
| 13 | x | 1455 | ASN | N-CA | -5.25 | 1.39 | 1.46 |
| 16 | j | 625 | LEU | N-CA | -5.25 | 1.39 | 1.46 |
| 21 | p | 38 | GLU | CA-CB | 5.25 | 1.61 | 1.53 |
| 20 | g | 794 | LYS | N-CA | 5.25 | 1.52 | 1.46 |
| 8 | N | 1080 | GLU | N-CA | -5.24 | 1.40 | 1.46 |
| 7 | O | 297 | ALA | C-N | 5.24 | 1.41 | 1.33 |
| 14 | h | 784 | GLU | CA-CB | 5.24 | 1.61 | 1.53 |
| 18 | l | 83 | LEU | N-CA | -5.24 | 1.39 | 1.46 |
| 19 | m | 663 | LEU | C-O | 5.24 | 1.30 | 1.24 |
| 21 | q | 40 | ASP | C-N | 5.24 | 1.40 | 1.33 |
| 18 | e | 167 | SER | CA-C | 5.24 | 1.58 | 1.52 |
| 14 | a | 857 | GLN | CA-CB | 5.24 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 1484 | ARG | C-N | 5.24 | 1.40 | 1.33 |
| 9 | R | 260 | LEU | CA-CB | -5.24 | 1.45 | 1.53 |
| 9 | S | 206 | ASN | C-N | 5.24 | 1.40 | 1.33 |
| 19 | f | 608 | SER | CA-C | -5.24 | 1.45 | 1.52 |
| 1 | 0 | 1487 | TYR | CA-C | 5.24 | 1.59 | 1.52 |
| 4 | D | 820 | SER | CA-CB | 5.24 | 1.62 | 1.53 |
| 7 | M | 126 | GLU | C-N | 5.24 | 1.41 | 1.33 |
| 8 | N | 1175 | GLU | CA-C | 5.24 | 1.59 | 1.52 |
| 7 | O | 903 | ASN | C-O | 5.24 | 1.31 | 1.24 |
| 9 | T | 208 | LEU | C-N | 5.24 | 1.41 | 1.34 |
| 1 | Y | 1483 | PRO | CA-CB | -5.24 | 1.46 | 1.53 |
| 15 | i | 244 | TYR | C-N | 5.24 | 1.41 | 1.33 |
| 15 | i | 633 | PHE | CA-C | 5.24 | 1.60 | 1.52 |
| 20 | n | 892 | LEU | CA-CB | 5.24 | 1.62 | 1.53 |
| 15 | b | 123 | VAL | C-N | 5.24 | 1.41 | 1.33 |
| 17 | d | 269 | LEU | CA-C | -5.24 | 1.46 | 1.52 |
| 6 | C | 327 | LYS | C-N | 5.24 | 1.41 | 1.34 |
| 7 | M | 132 | GLN | CA-C | -5.24 | 1.46 | 1.52 |
| 7 | O | 242 | ALA | CA-C | 5.24 | 1.59 | 1.52 |
| 7 | O | 455 | ASP | N-CA | -5.24 | 1.39 | 1.46 |
| 8 | P | 184 | ASP | N-CA | -5.24 | 1.40 | 1.46 |
| 17 | k | 153 | TRP | CG-CD2 | 5.24 | 1.53 | 1.43 |
| 19 | m | 360 | HIS | CA-CB | 5.24 | 1.61 | 1.53 |
| 14 | a | 606 | LYS | C-N | 5.24 | 1.41 | 1.33 |
| 8 | P | 830 | THR | CA-C | -5.24 | 1.47 | 1.53 |
| 9 | R | 816 | TYR | C-N | 5.24 | 1.40 | 1.33 |
| 9 | S | 698 | ASP | C-N | 5.24 | 1.40 | 1.33 |
| 1 | 0 | 1032 | THR | N-CA | -5.24 | 1.39 | 1.45 |
| 6 | C | 334 | SER | C-N | 5.24 | 1.40 | 1.33 |
| 7 | O | 838 | LYS | CA-C | -5.24 | 1.46 | 1.52 |
| 9 | T | 788 | ILE | C-N | 5.24 | 1.41 | 1.33 |
| 2 | Z | 1012 | VAL | N-CA | 5.24 | 1.52 | 1.46 |
| 2 | Z | 1257 | GLY | CA-C | -5.24 | 1.45 | 1.51 |
| 12 | u | 28 | SER | CA-C | 5.24 | 1.58 | 1.52 |
| 20 | n | 417 | LEU | CA-C | -5.24 | 1.45 | 1.52 |
| 18 | e | 54 | HIS | ND1-CE1 | 5.24 | 1.37 | 1.32 |
| 20 | g | 359 | THR | N-CA | -5.24 | 1.40 | 1.46 |
| 14 | a | 572 | ASP | CA-CB | 5.24 | 1.61 | 1.53 |
| 2 | 1 | 345 | LEU | C-N | 5.23 | 1.40 | 1.33 |
| 5 | B | 463 | LEU | CA-C | -5.23 | 1.45 | 1.52 |
| 8 | N | 330 | TYR | CA-CB | 5.23 | 1.61 | 1.53 |
| 7 | O | 925 | HIS | CD2-NE2 | 5.23 | 1.43 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | P | 959 | LEU | N-CA | -5.23 | 1.39 | 1.46 |
| 11 | V | 347 | TYR | CA-C | -5.23 | 1.46 | 1.52 |
| 2 | 1 | 604 | LEU | CA-CB | 5.23 | 1.61 | 1.53 |
| 9 | R | 127 | GLN | CA-CB | 5.23 | 1.61 | 1.53 |
| 9 | R | 408 | ARG | CA-C | -5.23 | 1.46 | 1.52 |
| 4 | y | 676 | ILE | N-CA | -5.23 | 1.40 | 1.46 |
| 15 | i | 507 | LEU | N-CA | -5.23 | 1.39 | 1.46 |
| 16 | j | 314 | LYS | CA-CB | 5.23 | 1.61 | 1.53 |
| 2 | 1 | 228 | PHE | N-CA | 5.23 | 1.52 | 1.46 |
| 2 | 1 | 1116 | TYR | CA-CB | 5.23 | 1.61 | 1.53 |
| 7 | O | 323 | LEU | CA-C | 5.23 | 1.59 | 1.52 |
| 9 | Q | 457 | TYR | C-N | 5.23 | 1.40 | 1.33 |
| 9 | R | 632 | ASP | C-O | -5.23 | 1.18 | 1.24 |
| 9 | T | 80 | PHE | C-N | 5.23 | 1.40 | 1.33 |
| 9 | T | 322 | ILE | CA-C | -5.23 | 1.47 | 1.53 |
| 1 | Y | 367 | ILE | CA-C | -5.23 | 1.46 | 1.52 |
| 2 | Z | 708 | ARG | CD-NE | 5.23 | 1.53 | 1.46 |
| 15 | i | 552 | ILE | CA-C | -5.23 | 1.46 | 1.52 |
| 20 | n | 760 | ILE | N-CA | -5.23 | 1.39 | 1.46 |
| 18 | e | 292 | LEU | C-N | 5.23 | 1.40 | 1.33 |
| 14 | a | 648 | GLY | C-N | 5.23 | 1.40 | 1.33 |
| 2 | 1 | 1093 | GLU | C-N | 5.23 | 1.40 | 1.33 |
| 7 | O | 263 | LEU | CA-C | -5.23 | 1.46 | 1.52 |
| 8 | P | 1539 | ASN | CA-C | -5.23 | 1.46 | 1.52 |
| 1 | Y | 201 | TYR | CA-CB | 5.23 | 1.63 | 1.53 |
| 2 | Z | 176 | SER | CA-C | 5.23 | 1.59 | 1.52 |
| 2 | Z | 1226 | SER | C-N | 5.23 | 1.41 | 1.33 |
| 19 | m | 286 | LEU | CA-CB | 5.23 | 1.61 | 1.53 |
| 14 | a | 65 | SER | CA-C | 5.23 | 1.59 | 1.52 |
| 1 | 0 | 978 | GLY | C-N | 5.23 | 1.41 | 1.33 |
| 7 | O | 330 | SER | C-N | 5.23 | 1.40 | 1.33 |
| 8 | P | 994 | ILE | N-CA | -5.23 | 1.39 | 1.46 |
| 8 | P | 1014 | CYS | CA-C | -5.23 | 1.45 | 1.52 |
| 9 | Q | 293 | ASN | CA-CB | 5.23 | 1.62 | 1.53 |
| 1 | Y | 902 | SER | N-CA | -5.23 | 1.39 | 1.46 |
| 16 | j | 186 | ASP | N-CA | -5.23 | 1.40 | 1.46 |
| 19 | m | 112 | ASP | CA-CB | 5.23 | 1.61 | 1.53 |
| 19 | m | 285 | ASP | CA-CB | 5.23 | 1.61 | 1.53 |
| 16 | c | 146 | ALA | C-O | -5.23 | 1.17 | 1.23 |
| 9 | R | 482 | LEU | N-CA | -5.23 | 1.40 | 1.46 |
| 9 | R | 584 | LYS | C-N | 5.23 | 1.40 | 1.33 |
| 1 | Y | 1174 | LEU | CA-C | -5.23 | 1.48 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | n | 723 | PHE | CA-C | -5.23 | 1.45 | 1.52 |
| 7 | M | 487 | PHE | C-N | 5.22 | 1.41 | 1.33 |
| 8 | N | 1605 | PHE | CA-CB | 5.22 | 1.61 | 1.53 |
| 7 | O | 499 | PHE | CG-CD2 | 5.22 | 1.49 | 1.38 |
| 9 | Q | 337 | ILE | C-N | 5.22 | 1.41 | 1.34 |
| 9 | R | 284 | GLN | CA-CB | -5.22 | 1.46 | 1.54 |
| 9 | T | 459 | LEU | CA-CB | 5.22 | 1.61 | 1.53 |
| 9 | T | 494 | TYR | CA-CB | 5.22 | 1.61 | 1.53 |
| 12 | v | 278 | LEU | C-O | -5.22 | 1.17 | 1.24 |
| 13 | w | 1298 | TYR | CA-C | -5.22 | 1.45 | 1.52 |
| 16 | j | 663 | GLN | N-CA | -5.22 | 1.39 | 1.46 |
| 19 | f | 404 | VAL | C-O | -5.22 | 1.18 | 1.24 |
| 2 | 1 | 1051 | ASN | CA-CB | 5.22 | 1.61 | 1.53 |
| 7 | O | 1525 | LEU | N-CA | -5.22 | 1.40 | 1.46 |
| 9 | T | 828 | THR | CA-CB | -5.22 | 1.45 | 1.53 |
| 12 | v | 250 | ILE | CA-CB | -5.22 | 1.48 | 1.54 |
| 12 | v | 315 | VAL | CA-CB | 5.22 | 1.59 | 1.53 |
| 17 | k | 119 | ALA | C-N | 5.22 | 1.40 | 1.33 |
| 19 | m | 548 | GLN | N-CA | -5.22 | 1.39 | 1.46 |
| 21 | s | 71 | HIS | C-N | 5.22 | 1.40 | 1.33 |
| 15 | b | 529 | TRP | NE1-CE2 | -5.22 | 1.31 | 1.37 |
| 7 | M | 1338 | LYS | N-CA | -5.22 | 1.38 | 1.45 |
| 9 | T | 64 | LYS | C-N | 5.22 | 1.38 | 1.32 |
| 14 | h | 568 | LYS | C-N | 5.22 | 1.40 | 1.34 |
| 19 | m | 330 | ARG | CD-NE | 5.22 | 1.53 | 1.46 |
| 20 | g | 831 | LEU | CB-CG | 5.22 | 1.63 | 1.53 |
| 2 | 1 | 408 | LYS | CA-C | -5.22 | 1.45 | 1.52 |
| 7 | M | 350 | ARG | NE-CZ | 5.22 | 1.38 | 1.33 |
| 7 | M | 1613 | VAL | N-CA | 5.22 | 1.54 | 1.46 |
| 8 | N | 1216 | LYS | C-N | 5.22 | 1.40 | 1.33 |
| 7 | O | 1182 | ASN | C-N | 5.22 | 1.40 | 1.33 |
| 7 | O | 1447 | TYR | CA-CB | 5.22 | 1.62 | 1.53 |
| 8 | P | 207 | ASP | CA-CB | 5.22 | 1.62 | 1.53 |
| 8 | P | 823 | ILE | C-O | -5.22 | 1.18 | 1.24 |
| 10 | W | 264 | ASN | CA-C | -5.22 | 1.45 | 1.52 |
| 10 | W | 311 | ASP | CA-C | -5.22 | 1.46 | 1.52 |
| 19 | m | 212 | LEU | C-N | 5.22 | 1.41 | 1.34 |
| 20 | n | 462 | SER | C-N | 5.22 | 1.41 | 1.33 |
| 15 | b | 661 | HIS | CE1-NE2 | 5.22 | 1.37 | 1.32 |
| 17 | d | 147 | GLY | CA-C | -5.22 | 1.44 | 1.51 |
| 17 | d | 156 | ALA | CA-C | -5.22 | 1.45 | 1.52 |
| 19 | f | 271 | ILE | CB-CG1 | 5.22 | 1.63 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | H | 443 | LEU | CA-CB | 5.22 | 1.62 | 1.53 |
| 8 | N | 822 | ASN | N-CA | -5.22 | 1.42 | 1.47 |
| 18 | l | 14 | ASP | C-N | 5.22 | 1.40 | 1.33 |
| 21 | q | 78 | TYR | CA-C | -5.22 | 1.46 | 1.52 |
| 14 | a | 728 | ILE | CA-CB | 5.22 | 1.60 | 1.54 |
| 6 | L | 395 | GLU | C-N | 5.22 | 1.41 | 1.33 |
| 7 | O | 133 | GLU | CA-CB | 5.22 | 1.62 | 1.53 |
| 9 | R | 122 | LEU | N-CA | -5.22 | 1.40 | 1.46 |
| 9 | S | 712 | GLU | C-N | 5.22 | 1.39 | 1.34 |
| 11 | V | 351 | THR | CA-C | 5.22 | 1.58 | 1.52 |
| 15 | i | 713 | ILE | N-CA | 5.22 | 1.52 | 1.46 |
| 20 | n | 555 | GLN | N-CA | -5.22 | 1.39 | 1.46 |
| 21 | t | 68 | TYR | N-CA | -5.22 | 1.39 | 1.46 |
| 16 | c | 136 | LYS | CA-C | 5.22 | 1.59 | 1.52 |
| 16 | c | 645 | TYR | C-N | 5.22 | 1.41 | 1.33 |
| 19 | f | 286 | LEU | CA-CB | 5.22 | 1.61 | 1.53 |
| 1 | 0 | 1190 | ALA | N-CA | 5.21 | 1.52 | 1.46 |
| 6 | L | 385 | GLU | N-CA | -5.21 | 1.39 | 1.46 |
| 8 | P | 340 | SER | CA-C | -5.21 | 1.45 | 1.52 |
| 9 | Q | 121 | ILE | C-O | 5.21 | 1.30 | 1.24 |
| 9 | T | 283 | LEU | N-CA | 5.21 | 1.52 | 1.46 |
| 1 | Y | 389 | GLY | C-N | 5.21 | 1.40 | 1.33 |
| 20 | n | 266 | SER | CA-CB | 5.21 | 1.60 | 1.53 |
| 2 | Z | 186 | ASN | C-N | 5.21 | 1.40 | 1.33 |
| 15 | i | 587 | ASP | CA-C | -5.21 | 1.45 | 1.52 |
| 21 | q | 51 | VAL | CA-CB | -5.21 | 1.48 | 1.54 |
| 2 | 1 | 507 | TYR | N-CA | 5.21 | 1.52 | 1.46 |
| 5 | K | 340 | GLU | N-CA | -5.21 | 1.39 | 1.46 |
| 7 | M | 1329 | LEU | CA-C | 5.21 | 1.59 | 1.52 |
| 9 | Q | 359 | ASN | CA-C | -5.21 | 1.46 | 1.52 |
| 9 | Q | 753 | ALA | N-CA | 5.21 | 1.56 | 1.46 |
| 15 | b | 79 | MET | N-CA | -5.21 | 1.39 | 1.46 |
| 16 | c | 155 | THR | CA-C | 5.21 | 1.59 | 1.52 |
| 20 | g | 829 | VAL | CA-CB | -5.21 | 1.49 | 1.54 |
| 7 | O | 715 | ASN | CA-C | -5.21 | 1.46 | 1.52 |
| 17 | d | 144 | HIS | CA-C | -5.21 | 1.46 | 1.52 |
| 14 | a | 757 | GLU | C-N | 5.21 | 1.40 | 1.33 |
| 8 | N | 89 | PHE | CA-C | -5.21 | 1.45 | 1.52 |
| 8 | P | 1641 | SER | CA-CB | 5.21 | 1.61 | 1.53 |
| 9 | T | 342 | ARG | CZ-NH2 | 5.21 | 1.40 | 1.33 |
| 11 | V | 290 | HIS | ND1-CE1 | 5.21 | 1.37 | 1.32 |
| 1 | Y | 919 | VAL | CA-C | -5.21 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 1306 | SER | C-N | 5.21 | 1.39 | 1.33 |
| 14 | h | 728 | ILE | C-N | 5.21 | 1.40 | 1.33 |
| 16 | j | 220 | ALA | C-N | 5.21 | 1.40 | 1.33 |
| 18 | l | 38 | LEU | CA-CB | 5.21 | 1.60 | 1.53 |
| 15 | b | 499 | ALA | CA-C | -5.21 | 1.45 | 1.52 |
| 19 | f | 595 | ARG | C-N | 5.21 | 1.41 | 1.33 |
| 2 | 1 | 498 | ALA | C-N | -5.21 | 1.26 | 1.33 |
| 4 | D | 772 | VAL | C-N | 5.21 | 1.41 | 1.33 |
| 7 | M | 1404 | ASP | CA-C | 5.21 | 1.59 | 1.52 |
| 8 | N | 83 | VAL | N-CA | -5.21 | 1.39 | 1.46 |
| 8 | N | 1219 | THR | N-CA | -5.21 | 1.39 | 1.46 |
| 7 | O | 1476 | LEU | N-CA | -5.21 | 1.40 | 1.46 |
| 9 | T | 236 | ASN | C-N | 5.21 | 1.41 | 1.34 |
| 9 | T | 535 | ALA | N-CA | -5.21 | 1.39 | 1.46 |
| 12 | u | 76 | SER | N-CA | -5.21 | 1.39 | 1.46 |
| 14 | h | 861 | LEU | N-CA | -5.21 | 1.39 | 1.46 |
| 16 | j | 338 | LEU | C-O | -5.21 | 1.18 | 1.24 |
| 20 | g | 464 | SER | N-CA | -5.21 | 1.39 | 1.45 |
| 4 | G | 654 | HIS | ND1-CE1 | 5.21 | 1.37 | 1.32 |
| 8 | N | 687 | LYS | CA-C | -5.21 | 1.46 | 1.52 |
| 7 | O | 1623 | VAL | N-CA | -5.21 | 1.39 | 1.46 |
| 9 | S | 605 | GLU | N-CA | -5.21 | 1.39 | 1.46 |
| 10 | W | 261 | THR | CA-CB | 5.21 | 1.61 | 1.53 |
| 4 | G | 746 | LYS | C-N | 5.20 | 1.40 | 1.33 |
| 8 | N | 1025 | ASN | C-N | 5.20 | 1.41 | 1.33 |
| 8 | N | 1048 | LYS | CA-C | -5.20 | 1.47 | 1.53 |
| 8 | P | 1171 | ARG | NE-CZ | 5.20 | 1.38 | 1.33 |
| 9 | S | 342 | ARG | CZ-NH1 | 5.20 | 1.40 | 1.32 |
| 1 | Y | 1218 | TYR | CA-CB | 5.20 | 1.61 | 1.53 |
| 19 | m | 49 | LEU | N-CA | -5.20 | 1.40 | 1.46 |
| 18 | e | 215 | ILE | N-CA | -5.20 | 1.39 | 1.46 |
| 20 | g | 608 | ASP | N-CA | -5.20 | 1.39 | 1.46 |
| 14 | a | 474 | ASN | C-N | 5.20 | 1.40 | 1.33 |
| 1 | 0 | 1051 | VAL | CA-CB | -5.20 | 1.47 | 1.54 |
| 6 | L | 452 | ASP | C-N | 5.20 | 1.40 | 1.33 |
| 7 | M | 898 | TYR | C-N | 5.20 | 1.41 | 1.33 |
| 8 | N | 554 | ILE | CA-C | -5.20 | 1.46 | 1.52 |
| 13 | x | 1294 | LYS | C-N | 5.20 | 1.40 | 1.33 |
| 1 | 0 | 937 | SER | C-O | -5.20 | 1.17 | 1.23 |
| 1 | 0 | 959 | THR | CA-CB | -5.20 | 1.45 | 1.54 |
| 6 | F | 337 | LYS | N-CA | -5.20 | 1.40 | 1.46 |
| 8 | N | 398 | ARG | N-CA | -5.20 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | N | 677 | ASN | N-CA | -5.20 | 1.40 | 1.46 |
| 7 | O | 17 | SER | CA-C | -5.20 | 1.45 | 1.52 |
| 9 | Q | 630 | ARG | NE-CZ | 5.20 | 1.38 | 1.33 |
| 9 | S | 237 | GLU | C-N | 5.20 | 1.41 | 1.33 |
| 13 | w | 1309 | ASP | N-CA | -5.20 | 1.40 | 1.46 |
| 16 | j | 777 | PRO | C-O | -5.20 | 1.18 | 1.23 |
| 18 | l | 61 | ILE | C-N | 5.20 | 1.40 | 1.33 |
| 20 | n | 97 | GLY | N-CA | -5.20 | 1.39 | 1.45 |
| 19 | f | 444 | ALA | CA-CB | 5.20 | 1.61 | 1.53 |
| 14 | a | 391 | SER | N-CA | -5.20 | 1.39 | 1.46 |
| 1 | 0 | 1069 | ASN | CA-C | 5.20 | 1.59 | 1.52 |
| 2 | 1 | 679 | SER | C-N | 5.20 | 1.40 | 1.33 |
| 7 | O | 1079 | ALA | C-O | -5.20 | 1.17 | 1.24 |
| 7 | O | 1454 | VAL | N-CA | -5.20 | 1.40 | 1.46 |
| 9 | Q | 481 | THR | CA-C | 5.20 | 1.59 | 1.52 |
| 12 | u | 188 | SER | CA-C | -5.20 | 1.46 | 1.52 |
| 13 | w | 1342 | GLN | C-N | 5.20 | 1.40 | 1.33 |
| 15 | i | 156 | GLU | CA-CB | 5.20 | 1.61 | 1.53 |
| 18 | l | 325 | ASP | CA-C | -5.20 | 1.46 | 1.52 |
| 19 | m | 319 | SER | CA-CB | 5.20 | 1.62 | 1.53 |
| 19 | m | 602 | LYS | C-N | 5.20 | 1.39 | 1.33 |
| 20 | n | 167 | ILE | C-N | 5.20 | 1.41 | 1.34 |
| 20 | n | 814 | LEU | C-N | 5.20 | 1.39 | 1.34 |
| 15 | b | 171 | ARG | C-N | 5.20 | 1.41 | 1.34 |
| 19 | f | 165 | ASN | CG-ND2 | 5.20 | 1.44 | 1.33 |
| 4 | A | 698 | GLN | CA-C | 5.20 | 1.59 | 1.52 |
| 17 | d | 40 | GLY | CA-C | -5.20 | 1.44 | 1.51 |
| 14 | a | 173 | PHE | C-N | 5.20 | 1.40 | 1.33 |
| 5 | H | 344 | SER | CA-C | 5.20 | 1.59 | 1.52 |
| 6 | I | 315 | LEU | CA-CB | 5.20 | 1.61 | 1.53 |
| 8 | P | 1505 | LEU | CA-CB | 5.20 | 1.61 | 1.53 |
| 9 | R | 738 | GLN | CA-C | -5.20 | 1.45 | 1.52 |
| 1 | Y | 834 | ILE | CA-C | 5.20 | 1.58 | 1.52 |
| 1 | Y | 968 | LEU | CA-CB | 5.20 | 1.61 | 1.53 |
| 1 | Y | 1212 | GLU | CA-C | -5.20 | 1.45 | 1.52 |
| 15 | i | 294 | GLN | CA-CB | 5.20 | 1.61 | 1.53 |
| 18 | l | 226 | ARG | NE-CZ | 5.20 | 1.38 | 1.33 |
| 17 | d | 175 | THR | N-CA | -5.20 | 1.39 | 1.45 |
| 18 | e | 79 | LYS | CA-C | 5.20 | 1.59 | 1.52 |
| 20 | g | 983 | VAL | N-CA | -5.20 | 1.39 | 1.46 |
| 5 | B | 372 | ALA | C-O | -5.19 | 1.18 | 1.24 |
| 6 | C | 285 | GLN | CA-CB | 5.19 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 995 | VAL | CA-C | -5.19 | 1.46 | 1.52 |
| 7 | O | 188 | ARG | CA-CB | 5.19 | 1.61 | 1.53 |
| 8 | P | 520 | ILE | CA-CB | 5.19 | 1.60 | 1.54 |
| 9 | S | 230 | GLY | N-CA | -5.19 | 1.37 | 1.45 |
| 2 | Z | 148 | ASP | CA-C | -5.19 | 1.45 | 1.52 |
| 18 | l | 22 | ARG | C-N | 5.19 | 1.41 | 1.33 |
| 15 | b | 491 | LEU | CA-CB | -5.19 | 1.46 | 1.53 |
| 16 | c | 425 | TYR | CZ-OH | 5.19 | 1.49 | 1.38 |
| 19 | f | 654 | GLU | C-N | 5.19 | 1.40 | 1.33 |
| 1 | 0 | 1024 | LEU | C-N | 5.19 | 1.41 | 1.33 |
| 2 | 1 | 124 | ASN | CA-C | -5.19 | 1.45 | 1.52 |
| 2 | 1 | 648 | ALA | CA-CB | 5.19 | 1.62 | 1.53 |
| 2 | 1 | 1237 | GLU | N-CA | -5.19 | 1.39 | 1.46 |
| 6 | L | 340 | ILE | CA-CB | -5.19 | 1.47 | 1.54 |
| 7 | M | 1101 | ILE | C-N | -5.19 | 1.27 | 1.33 |
| 7 | M | 1198 | LEU | CA-C | -5.19 | 1.46 | 1.52 |
| 7 | M | 1499 | LEU | CA-C | -5.19 | 1.46 | 1.52 |
| 9 | Q | 147 | ASP | N-CA | -5.19 | 1.39 | 1.45 |
| 9 | R | 587 | THR | N-CA | -5.19 | 1.39 | 1.46 |
| 9 | T | 817 | ALA | C-N | 5.19 | 1.41 | 1.33 |
| 10 | W | 281 | ARG | CA-CB | 5.19 | 1.60 | 1.53 |
| 11 | X | 400 | ILE | CA-C | 5.19 | 1.58 | 1.52 |
| 1 | Y | 422 | LYS | CA-C | -5.19 | 1.46 | 1.52 |
| 13 | x | 1317 | TYR | C-N | 5.19 | 1.41 | 1.33 |
| 4 | y | 765 | LEU | C-N | 5.19 | 1.40 | 1.33 |
| 14 | h | 838 | GLN | CA-C | 5.19 | 1.59 | 1.52 |
| 15 | i | 224 | ILE | N-CA | -5.19 | 1.39 | 1.46 |
| 18 | l | 330 | LEU | N-CA | -5.19 | 1.39 | 1.46 |
| 20 | g | 921 | GLU | CA-CB | 5.19 | 1.61 | 1.53 |
| 1 | 0 | 1232 | ARG | CA-CB | 5.19 | 1.61 | 1.53 |
| 11 | X | 400 | ILE | C-N | 5.19 | 1.41 | 1.33 |
| 1 | Y | 1312 | ALA | CA-C | -5.19 | 1.46 | 1.52 |
| 13 | x | 1285 | ASN | C-N | 5.19 | 1.41 | 1.33 |
| 21 | r | 18 | ASP | CA-CB | 5.19 | 1.61 | 1.53 |
| 20 | g | 591 | PHE | CA-CB | 5.19 | 1.61 | 1.53 |
| 1 | 0 | 678 | ALA | CA-CB | 5.19 | 1.61 | 1.53 |
| 8 | N | 849 | ASN | CG-ND2 | 5.19 | 1.44 | 1.33 |
| 8 | P | 806 | PHE | CA-CB | 5.19 | 1.60 | 1.53 |
| 8 | P | 1097 | LEU | C-N | 5.19 | 1.40 | 1.33 |
| 9 | Q | 477 | TYR | C-N | 5.19 | 1.41 | 1.34 |
| 1 | Y | 775 | LEU | CA-C | -5.19 | 1.45 | 1.52 |
| 2 | Z | 837 | ASP | CA-CB | 5.19 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 946 | GLU | N-CA | -5.19 | 1.40 | 1.46 |
| 12 | u | 60 | SER | C-N | 5.19 | 1.41 | 1.34 |
| 14 | h | 586 | LEU | C-N | 5.19 | 1.39 | 1.33 |
| 17 | k | 13 | HIS | CB-CG | 5.19 | 1.57 | 1.50 |
| 20 | g | 421 | PRO | C-N | 5.19 | 1.41 | 1.33 |
| 4 | D | 671 | LYS | N-CA | -5.19 | 1.40 | 1.46 |
| 5 | H | 473 | ILE | C-O | -5.19 | 1.18 | 1.24 |
| 6 | I | 279 | GLN | CA-CB | 5.19 | 1.61 | 1.53 |
| 4 | J | 805 | ARG | N-CA | -5.19 | 1.40 | 1.46 |
| 9 | R | 210 | GLU | CA-C | -5.19 | 1.46 | 1.52 |
| 2 | Z | 110 | ILE | CA-CB | -5.19 | 1.48 | 1.54 |
| 2 | Z | 1379 | VAL | N-CA | -5.19 | 1.39 | 1.46 |
| 16 | j | 136 | LYS | C-N | 5.19 | 1.40 | 1.33 |
| 19 | m | 191 | GLY | C-N | 5.19 | 1.40 | 1.33 |
| 20 | n | 561 | LYS | CA-CB | 5.19 | 1.61 | 1.53 |
| 15 | b | 275 | SER | CA-C | -5.19 | 1.45 | 1.52 |
| 20 | g | 373 | ASN | CA-C | -5.19 | 1.46 | 1.53 |
| 14 | a | 863 | ASP | C-N | 5.19 | 1.41 | 1.33 |
| 14 | a | 958 | TRP | C-N | 5.19 | 1.39 | 1.33 |
| 14 | a | 969 | MET | CA-CB | 5.19 | 1.61 | 1.53 |
| 1 | 0 | 958 | LYS | C-N | 5.19 | 1.42 | 1.33 |
| 4 | G | 658 | TYR | N-CA | -5.19 | 1.39 | 1.46 |
| 18 | l | 336 | SER | C-N | 5.19 | 1.41 | 1.33 |
| 14 | a | 534 | ASP | N-CA | 5.19 | 1.52 | 1.46 |
| 14 | a | 970 | LEU | C-N | 5.19 | 1.40 | 1.33 |
| 1 | 0 | 1233 | ILE | C-N | 5.18 | 1.41 | 1.33 |
| 2 | 1 | 590 | PHE | CA-C | 5.18 | 1.59 | 1.52 |
| 5 | K | 319 | THR | CA-C | -5.18 | 1.45 | 1.52 |
| 8 | P | 68 | HIS | ND1-CE1 | 5.18 | 1.37 | 1.32 |
| 8 | P | 321 | ILE | N-CA | -5.18 | 1.39 | 1.46 |
| 9 | Q | 681 | SER | CA-C | -5.18 | 1.45 | 1.52 |
| 1 | 0 | 1466 | ILE | N-CA | -5.18 | 1.40 | 1.46 |
| 2 | 1 | 194 | ILE | CA-C | -5.18 | 1.46 | 1.52 |
| 2 | 1 | 483 | LEU | CA-C | 5.18 | 1.59 | 1.52 |
| 5 | H | 394 | THR | CA-C | -5.18 | 1.46 | 1.52 |
| 7 | M | 516 | ARG | CD-NE | 5.18 | 1.53 | 1.46 |
| 8 | P | 885 | VAL | CA-C | 5.18 | 1.59 | 1.52 |
| 8 | P | 967 | LEU | CA-C | -5.18 | 1.46 | 1.52 |
| 9 | Q | 608 | GLN | CA-CB | 5.18 | 1.61 | 1.53 |
| 9 | S | 257 | TRP | CA-CB | 5.18 | 1.61 | 1.53 |
| 9 | S | 416 | GLY | CA-C | -5.18 | 1.44 | 1.51 |
| 9 | T | 151 | HIS | CA-C | -5.18 | 1.45 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | T | 681 | SER | CA-C | 5.18 | 1.59 | 1.52 |
| 2 | Z | 672 | VAL | CA-C | -5.18 | 1.46 | 1.52 |
| 14 | h | 549 | LYS | C-O | 5.18 | 1.30 | 1.24 |
| 15 | i | 536 | LYS | C-N | 5.18 | 1.41 | 1.34 |
| 20 | n | 379 | SER | CA-CB | 5.18 | 1.62 | 1.53 |
| 21 | s | 23 | ASP | C-N | 5.18 | 1.40 | 1.33 |
| 16 | c | 457 | LEU | N-CA | -5.18 | 1.39 | 1.46 |
| 14 | a | 444 | ALA | N-CA | -5.18 | 1.40 | 1.46 |
| 1 | 0 | 1222 | THR | N-CA | -5.18 | 1.40 | 1.46 |
| 2 | 1 | 1325 | LEU | CA-CB | 5.18 | 1.61 | 1.53 |
| 8 | N | 1536 | TRP | N-CA | 5.18 | 1.52 | 1.46 |
| 9 | Q | 278 | LEU | C-N | 5.18 | 1.40 | 1.33 |
| 9 | Q | 417 | ARG | CA-C | -5.18 | 1.46 | 1.53 |
| 9 | Q | 557 | LEU | C-N | -5.18 | 1.28 | 1.33 |
| 19 | f | 165 | ASN | CA-C | -5.18 | 1.46 | 1.52 |
| 8 | N | 696 | GLY | N-CA | -5.18 | 1.37 | 1.45 |
| 7 | O | 1305 | SER | CA-CB | 5.18 | 1.61 | 1.53 |
| 9 | Q | 643 | LEU | N-CA | -5.18 | 1.39 | 1.46 |
| 11 | V | 293 | HIS | ND1-CE1 | 5.18 | 1.37 | 1.32 |
| 12 | v | 571 | ILE | C-N | 5.18 | 1.40 | 1.33 |
| 13 | w | 1365 | ILE | CA-C | -5.18 | 1.45 | 1.52 |
| 14 | h | 410 | ASN | C-N | 5.18 | 1.41 | 1.33 |
| 19 | m | 138 | ASN | C-N | -5.18 | 1.27 | 1.33 |
| 2 | 1 | 986 | ARG | CZ-NH1 | 5.18 | 1.40 | 1.32 |
| 4 | D | 803 | ALA | C-N | 5.18 | 1.40 | 1.33 |
| 7 | M | 224 | ASP | N-CA | 5.18 | 1.52 | 1.45 |
| 7 | M | 754 | ASP | CA-CB | 5.18 | 1.61 | 1.53 |
| 7 | M | 1174 | LYS | CA-C | -5.18 | 1.46 | 1.52 |
| 7 | O | 439 | LEU | C-O | -5.18 | 1.18 | 1.24 |
| 7 | O | 1116 | VAL | N-CA | -5.18 | 1.39 | 1.46 |
| 9 | Q | 277 | TYR | C-O | -5.18 | 1.18 | 1.24 |
| 2 | Z | 153 | GLN | C-N | 5.18 | 1.41 | 1.33 |
| 13 | w | 1214 | ILE | CA-CB | 5.18 | 1.60 | 1.54 |
| 15 | i | 693 | GLU | C-N | 5.18 | 1.39 | 1.34 |
| 19 | m | 536 | ARG | NE-CZ | 5.18 | 1.38 | 1.33 |
| 20 | n | 433 | LEU | C-N | 5.18 | 1.41 | 1.33 |
| 17 | d | 198 | SER | C-O | -5.18 | 1.18 | 1.23 |
| 1 | 0 | 888 | ALA | CA-CB | 5.17 | 1.62 | 1.53 |
| 7 | M | 240 | LEU | CA-CB | 5.17 | 1.61 | 1.53 |
| 7 | O | 1190 | TYR | CA-C | -5.17 | 1.46 | 1.52 |
| 8 | P | 1088 | ASN | C-N | 5.17 | 1.40 | 1.33 |
| 8 | P | 1562 | ASN | N-CA | 5.17 | 1.52 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | R | 330 | GLY | C-N | 5.17 | 1.39 | 1.33 |
| 1 | Y | 529 | GLY | C-N | 5.17 | 1.40 | 1.33 |
| 1 | Y | 584 | GLY | CA-C | -5.17 | 1.46 | 1.51 |
| 1 | Y | 1005 | ARG | CA-C | -5.17 | 1.45 | 1.52 |
| 1 | Y | 1107 | LEU | CA-CB | 5.17 | 1.62 | 1.53 |
| 14 | h | 537 | THR | C-N | 5.17 | 1.40 | 1.33 |
| 15 | i | 533 | GLU | C-N | 5.17 | 1.40 | 1.33 |
| 15 | i | 613 | ASP | N-CA | -5.17 | 1.39 | 1.46 |
| 16 | j | 555 | GLU | N-CA | -5.17 | 1.39 | 1.46 |
| 7 | M | 1317 | GLY | CA-C | -5.17 | 1.45 | 1.52 |
| 8 | P | 1621 | LEU | C-N | 5.17 | 1.40 | 1.33 |
| 9 | R | 652 | ILE | C-N | 5.17 | 1.40 | 1.33 |
| 2 | Z | 1342 | GLU | C-N | 5.17 | 1.41 | 1.34 |
| 18 | l | 195 | GLN | N-CA | -5.17 | 1.39 | 1.46 |
| 2 | 1 | 664 | PHE | N-CA | -5.17 | 1.39 | 1.46 |
| 8 | N | 951 | SER | C-N | 5.17 | 1.41 | 1.33 |
| 8 | P | 1606 | LEU | C-N | 5.17 | 1.41 | 1.33 |
| 9 | R | 604 | ILE | CA-C | -5.17 | 1.45 | 1.52 |
| 9 | T | 555 | GLU | C-N | 5.17 | 1.41 | 1.33 |
| 12 | u | 325 | ILE | C-N | 5.17 | 1.40 | 1.33 |
| 20 | n | 387 | MET | CA-C | -5.17 | 1.46 | 1.52 |
| 20 | n | 986 | ILE | CA-CB | -5.17 | 1.47 | 1.54 |
| 16 | c | 598 | ILE | CB-CG1 | 5.17 | 1.63 | 1.53 |
| 10 | U | 346 | SER | CA-CB | 5.17 | 1.60 | 1.54 |
| 1 | Y | 387 | LEU | CA-CB | 5.17 | 1.60 | 1.53 |
| 1 | 0 | 391 | MET | CA-C | -5.17 | 1.46 | 1.52 |
| 6 | L | 466 | THR | N-CA | -5.17 | 1.40 | 1.46 |
| 7 | O | 1154 | ARG | CZ-NH2 | 5.17 | 1.40 | 1.33 |
| 8 | P | 54 | SER | CA-C | -5.17 | 1.46 | 1.52 |
| 12 | u | 324 | LEU | CA-C | -5.17 | 1.46 | 1.52 |
| 21 | s | 88 | VAL | C-N | 5.17 | 1.39 | 1.33 |
| 4 | A | 696 | SER | C-N | -5.17 | 1.27 | 1.33 |
| 4 | D | 691 | ASN | CA-C | -5.17 | 1.45 | 1.52 |
| 7 | M | 419 | THR | C-N | 5.17 | 1.41 | 1.33 |
| 9 | Q | 415 | ILE | CA-C | -5.17 | 1.46 | 1.53 |
| 9 | S | 470 | GLY | CA-C | -5.17 | 1.44 | 1.51 |
| 2 | Z | 1321 | LEU | C-N | 5.17 | 1.40 | 1.33 |
| 12 | u | 648 | GLN | CA-C | 5.17 | 1.59 | 1.52 |
| 20 | n | 999 | LEU | CA-C | -5.17 | 1.45 | 1.52 |
| 15 | b | 202 | SER | CA-C | -5.17 | 1.45 | 1.52 |
| 20 | g | 141 | THR | C-N | 5.17 | 1.40 | 1.33 |
| 14 | a | 338 | ARG | NE-CZ | 5.17 | 1.38 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 282 | PHE | CA-C | -5.17 | 1.45 | 1.52 |
| 8 | N | 1467 | SER | C-N | 5.17 | 1.40 | 1.34 |
| 9 | S | 219 | VAL | CA-C | -5.17 | 1.45 | 1.52 |
| 1 | Y | 1412 | ILE | CA-CB | 5.17 | 1.60 | 1.54 |
| 2 | Z | 1178 | ARG | CA-C | 5.17 | 1.59 | 1.52 |
| 2 | 1 | 1119 | ALA | CA-CB | 5.16 | 1.62 | 1.53 |
| 4 | D | 799 | SER | CA-C | 5.16 | 1.59 | 1.52 |
| 7 | M | 716 | LEU | C-N | 5.16 | 1.39 | 1.33 |
| 7 | O | 775 | ALA | N-CA | -5.16 | 1.40 | 1.46 |
| 10 | W | 307 | ILE | CA-C | -5.16 | 1.46 | 1.52 |
| 1 | Y | 289 | SER | CA-CB | 5.16 | 1.63 | 1.53 |
| 1 | Y | 1350 | GLU | C-N | 5.16 | 1.40 | 1.33 |
| 12 | u | 233 | MET | CA-C | -5.16 | 1.46 | 1.52 |
| 12 | v | 375 | VAL | C-O | -5.16 | 1.18 | 1.24 |
| 13 | x | 1397 | LYS | CA-C | -5.16 | 1.46 | 1.52 |
| 4 | y | 685 | MET | CA-C | -5.16 | 1.46 | 1.52 |
| 18 | l | 211 | HIS | CE1-NE2 | -5.16 | 1.27 | 1.32 |
| 19 | m | 185 | TYR | CA-CB | 5.16 | 1.61 | 1.53 |
| 19 | m | 378 | ASP | CA-C | -5.16 | 1.45 | 1.52 |
| 19 | m | 651 | ILE | CA-C | -5.16 | 1.47 | 1.53 |
| 21 | t | 40 | ASP | N-CA | -5.16 | 1.40 | 1.46 |
| 15 | b | 389 | ASP | CA-CB | 5.16 | 1.60 | 1.53 |
| 14 | a | 61 | LEU | N-CA | 5.16 | 1.52 | 1.46 |
| 5 | B | 302 | ASN | CA-C | -5.16 | 1.45 | 1.52 |
| 7 | M | 240 | LEU | CA-C | 5.16 | 1.59 | 1.52 |
| 9 | Q | 629 | ARG | CD-NE | 5.16 | 1.53 | 1.46 |
| 9 | S | 736 | LEU | N-CA | -5.16 | 1.40 | 1.46 |
| 11 | V | 297 | ASP | C-N | 5.16 | 1.37 | 1.33 |
| 14 | h | 834 | ARG | CA-C | -5.16 | 1.46 | 1.52 |
| 20 | n | 917 | LEU | CA-CB | 5.16 | 1.61 | 1.53 |
| 20 | g | 590 | LYS | N-CA | -5.16 | 1.39 | 1.46 |
| 7 | M | 351 | HIS | CA-C | -5.16 | 1.45 | 1.52 |
| 7 | M | 1313 | ILE | CA-CB | -5.16 | 1.48 | 1.54 |
| 7 | O | 220 | VAL | C-N | 5.16 | 1.40 | 1.33 |
| 7 | O | 1164 | PHE | CB-CG | 5.16 | 1.62 | 1.50 |
| 7 | O | 1345 | PHE | CA-CB | 5.16 | 1.62 | 1.53 |
| 8 | P | 682 | LEU | N-CA | -5.16 | 1.40 | 1.46 |
| 9 | Q | 86 | PHE | N-CA | -5.16 | 1.40 | 1.46 |
| 9 | T | 552 | VAL | C-O | -5.16 | 1.18 | 1.24 |
| 9 | T | 604 | ILE | C-N | 5.16 | 1.41 | 1.33 |
| 2 | Z | 487 | LYS | CA-C | -5.16 | 1.45 | 1.52 |
| 16 | j | 397 | TYR | CA-C | -5.16 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 18 | e | 226 | ARG | CA-CB | 5.16 | 1.62 | 1.53 |
| 18 | e | 342 | MET | CA-CB | 5.16 | 1.62 | 1.53 |
| 6 | I | 287 | GLN | CA-C | -5.16 | 1.46 | 1.52 |
| 7 | M | 202 | ASP | CA-CB | 5.16 | 1.61 | 1.53 |
| 8 | P | 575 | SER | C-N | 5.16 | 1.41 | 1.33 |
| 9 | Q | 771 | ILE | N-CA | -5.16 | 1.40 | 1.46 |
| 9 | R | 559 | LEU | CA-C | -5.16 | 1.45 | 1.52 |
| 9 | S | 572 | CYS | CA-C | -5.16 | 1.46 | 1.52 |
| 1 | Y | 184 | ILE | CA-CB | 5.16 | 1.61 | 1.54 |
| 1 | Y | 364 | GLN | C-N | 5.16 | 1.41 | 1.33 |
| 2 | Z | 1234 | ILE | N-CA | -5.16 | 1.40 | 1.46 |
| 4 | y | 683 | ALA | C-N | 5.16 | 1.40 | 1.33 |
| 18 | l | 239 | ARG | C-N | 5.16 | 1.40 | 1.33 |
| 19 | m | 483 | VAL | C-O | 5.16 | 1.33 | 1.23 |
| 15 | b | 630 | LEU | CA-CB | 5.16 | 1.61 | 1.53 |
| 1 | 0 | 439 | LEU | CA-C | -5.16 | 1.46 | 1.52 |
| 5 | E | 404 | ARG | NE-CZ | 5.16 | 1.38 | 1.33 |
| 8 | N | 1440 | GLY | N-CA | -5.16 | 1.39 | 1.45 |
| 2 | Z | 229 | ASP | N-CA | -5.16 | 1.39 | 1.46 |
| 21 | p | 79 | PHE | CA-CB | 5.16 | 1.62 | 1.53 |
| 1 | 0 | 141 | GLY | CA-C | 5.16 | 1.59 | 1.52 |
| 6 | L | 437 | ALA | CA-CB | 5.16 | 1.62 | 1.53 |
| 9 | Q | 610 | LEU | N-CA | -5.16 | 1.39 | 1.46 |
| 9 | T | 534 | PHE | N-CA | -5.16 | 1.40 | 1.46 |
| 12 | v | 182 | ILE | C-N | 5.16 | 1.40 | 1.33 |
| 13 | x | 1358 | HIS | C-N | 5.16 | 1.40 | 1.33 |
| 14 | h | 451 | ARG | C-O | -5.16 | 1.18 | 1.24 |
| 14 | h | 929 | HIS | N-CA | -5.16 | 1.39 | 1.46 |
| 15 | b | 226 | GLN | C-N | 5.16 | 1.39 | 1.33 |
| 16 | c | 623 | LEU | CB-CG | 5.16 | 1.63 | 1.53 |
| 16 | c | 633 | THR | N-CA | -5.16 | 1.39 | 1.46 |
| 18 | e | 18 | ASP | C-N | 5.16 | 1.40 | 1.33 |
| 20 | g | 430 | ASN | C-N | 5.16 | 1.39 | 1.33 |
| 20 | g | 1074 | ASN | N-CA | -5.16 | 1.40 | 1.46 |
| 5 | E | 506 | ILE | C-N | 5.15 | 1.41 | 1.33 |
| 8 | P | 338 | SER | C-N | 5.15 | 1.42 | 1.33 |
| 12 | u | 184 | ASP | CA-CB | 5.15 | 1.63 | 1.53 |
| 20 | g | 151 | LEU | CB-CG | 5.15 | 1.63 | 1.53 |
| 5 | B | 363 | GLN | C-N | 5.15 | 1.40 | 1.33 |
| 5 | B | 528 | GLU | C-N | 5.15 | 1.41 | 1.33 |
| 9 | S | 510 | LEU | N-CA | 5.15 | 1.52 | 1.46 |
| 9 | S | 714 | CYS | CA-CB | 5.15 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 1094 | ARG | NE-CZ | 5.15 | 1.38 | 1.33 |
| 12 | u | 198 | ASN | CA-C | -5.15 | 1.46 | 1.52 |
| 13 | w | 1142 | VAL | C-N | 5.15 | 1.40 | 1.33 |
| 4 | z | 667 | GLN | C-N | 5.15 | 1.40 | 1.33 |
| 15 | i | 348 | GLN | CA-CB | 5.15 | 1.62 | 1.53 |
| 16 | c | 495 | CYS | CA-C | 5.15 | 1.59 | 1.52 |
| 6 | F | 328 | GLN | N-CA | -5.15 | 1.39 | 1.46 |
| 7 | O | 423 | LEU | CA-C | -5.15 | 1.45 | 1.53 |
| 8 | P | 962 | SER | CA-C | -5.15 | 1.46 | 1.52 |
| 2 | Z | 550 | ASN | CA-C | -5.15 | 1.45 | 1.52 |
| 19 | m | 255 | GLY | CA-C | -5.15 | 1.43 | 1.51 |
| 21 | p | 64 | ASN | CA-CB | 5.15 | 1.62 | 1.53 |
| 15 | b | 245 | PHE | CA-CB | 5.15 | 1.61 | 1.53 |
| 20 | g | 1114 | TYR | CA-CB | 5.15 | 1.61 | 1.53 |
| 2 | 1 | 908 | GLU | N-CA | -5.15 | 1.40 | 1.46 |
| 2 | 1 | 1113 | ASP | CA-CB | 5.15 | 1.61 | 1.53 |
| 7 | M | 105 | GLN | CA-C | -5.15 | 1.46 | 1.52 |
| 12 | u | 427 | ALA | CA-C | 5.15 | 1.58 | 1.52 |
| 14 | h | 414 | ARG | CD-NE | 5.15 | 1.53 | 1.46 |
| 15 | b | 214 | ARG | CD-NE | 5.15 | 1.53 | 1.46 |
| 19 | f | 535 | ARG | N-CA | -5.15 | 1.39 | 1.46 |
| 20 | g | 1005 | LEU | CA-C | -5.15 | 1.46 | 1.52 |
| 5 | E | 304 | THR | C-N | 5.15 | 1.40 | 1.33 |
| 5 | E | 466 | LEU | CA-CB | 5.15 | 1.61 | 1.53 |
| 7 | M | 219 | HIS | CD2-NE2 | 5.15 | 1.43 | 1.37 |
| 7 | M | 1120 | THR | CA-C | -5.15 | 1.46 | 1.52 |
| 8 | N | 1096 | ILE | C-N | 5.15 | 1.40 | 1.33 |
| 7 | O | 750 | TRP | C-N | -5.15 | 1.27 | 1.33 |
| 8 | P | 713 | LYS | CA-CB | 5.15 | 1.61 | 1.53 |
| 9 | Q | 652 | ILE | N-CA | -5.15 | 1.40 | 1.46 |
| 9 | S | 489 | GLY | CA-C | 5.15 | 1.58 | 1.51 |
| 2 | Z | 192 | HIS | ND1-CE1 | 5.15 | 1.37 | 1.32 |
| 14 | h | 926 | CYS | CA-CB | -5.15 | 1.44 | 1.53 |
| 15 | b | 267 | ARG | N-CA | -5.15 | 1.39 | 1.46 |
| 19 | f | 638 | LEU | N-CA | -5.15 | 1.38 | 1.45 |
| 14 | a | 931 | ASP | CA-CB | 5.15 | 1.61 | 1.53 |
| 14 | a | 950 | SER | CA-CB | 5.15 | 1.61 | 1.53 |
| 14 | a | 959 | GLU | CA-C | -5.15 | 1.46 | 1.53 |
| 1 | Y | 1238 | ARG | NE-CZ | 5.15 | 1.38 | 1.33 |
| 15 | i | 458 | ARG | CD-NE | 5.15 | 1.53 | 1.46 |
| 20 | n | 672 | LEU | CA-C | -5.15 | 1.48 | 1.53 |
| 1 | 0 | 162 | HIS | CG-ND1 | 5.14 | 1.44 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 1155 | ARG | CA-CB | 5.14 | 1.61 | 1.53 |
| 4 | G | 644 | TRP | CA-C | -5.14 | 1.45 | 1.52 |
| 8 | N | 1187 | ILE | CB-CG1 | 5.14 | 1.63 | 1.53 |
| 9 | Q | 24 | GLU | CA-C | 5.14 | 1.59 | 1.52 |
| 9 | S | 134 | LYS | C-O | -5.14 | 1.18 | 1.24 |
| 14 | h | 756 | GLN | CA-C | 5.14 | 1.59 | 1.52 |
| 17 | k | 209 | ASP | CA-C | -5.14 | 1.46 | 1.52 |
| 16 | c | 438 | VAL | C-N | 5.14 | 1.40 | 1.33 |
| 17 | d | 74 | SER | C-N | 5.14 | 1.41 | 1.33 |
| 18 | e | 23 | HIS | ND1-CE1 | 5.14 | 1.37 | 1.32 |
| 19 | f | 221 | PRO | C-N | 5.14 | 1.39 | 1.33 |
| 7 | M | 830 | TYR | N-CA | -5.14 | 1.40 | 1.46 |
| 7 | O | 1357 | ALA | C-N | 5.14 | 1.39 | 1.33 |
| 8 | P | 1515 | LEU | N-CA | 5.14 | 1.51 | 1.46 |
| 2 | Z | 347 | VAL | C-N | 5.14 | 1.41 | 1.33 |
| 19 | f | 334 | ARG | CZ-NH2 | 5.14 | 1.40 | 1.33 |
| 2 | 1 | 204 | VAL | C-N | 5.14 | 1.41 | 1.33 |
| 7 | O | 305 | ASP | CA-C | -5.14 | 1.46 | 1.52 |
| 9 | R | 498 | PHE | N-CA | -5.14 | 1.39 | 1.46 |
| 11 | X | 302 | ARG | C-O | 5.14 | 1.33 | 1.23 |
| 14 | h | 880 | ARG | CD-NE | 5.14 | 1.53 | 1.46 |
| 17 | d | 107 | TRP | NE1-CE2 | -5.14 | 1.31 | 1.37 |
| 14 | a | 228 | LEU | C-N | 5.14 | 1.40 | 1.33 |
| 1 | 0 | 437 | VAL | C-N | 5.14 | 1.40 | 1.33 |
| 1 | 0 | 1158 | HIS | ND1-CE1 | 5.14 | 1.37 | 1.32 |
| 6 | I | 326 | LEU | CA-CB | 5.14 | 1.61 | 1.53 |
| 7 | M | 1200 | PRO | CA-C | -5.14 | 1.46 | 1.52 |
| 8 | P | 1433 | ILE | C-O | -5.14 | 1.18 | 1.24 |
| 9 | Q | 26 | LEU | N-CA | -5.14 | 1.40 | 1.46 |
| 1 | Y | 771 | TYR | N-CA | -5.14 | 1.39 | 1.46 |
| 16 | c | 230 | ASP | CA-CB | 5.14 | 1.61 | 1.53 |
| 16 | c | 366 | PHE | N-CA | 5.14 | 1.52 | 1.46 |
| 18 | e | 6 | SER | CA-C | -5.14 | 1.45 | 1.52 |
| 18 | e | 302 | ASP | CA-C | -5.14 | 1.45 | 1.52 |
| 1 | 0 | 1302 | LEU | N-CA | -5.14 | 1.39 | 1.45 |
| 4 | z | 747 | THR | N-CA | -5.14 | 1.39 | 1.46 |
| 14 | a | 689 | GLY | CA-C | 5.14 | 1.59 | 1.51 |
| 1 | 0 | 368 | ILE | CA-CB | -5.14 | 1.47 | 1.54 |
| 5 | K | 506 | ILE | C-N | 5.14 | 1.40 | 1.33 |
| 8 | P | 1285 | PHE | CA-CB | 5.14 | 1.61 | 1.53 |
| 9 | R | 458 | SER | N-CA | 5.14 | 1.51 | 1.45 |
| 18 | l | 69 | GLY | N-CA | 5.14 | 1.50 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | b | 180 | THR | CA-C | -5.14 | 1.46 | 1.52 |
| 16 | c | 647 | GLN | N-CA | -5.14 | 1.39 | 1.46 |
| 18 | e | 324 | ASP | C-N | 5.14 | 1.40 | 1.33 |
| 20 | g | 581 | PRO | CA-CB | 5.14 | 1.61 | 1.53 |
| 2 | 1 | 216 | SER | CA-CB | 5.13 | 1.60 | 1.52 |
| 15 | i | 96 | PRO | CA-CB | 5.13 | 1.60 | 1.53 |
| 19 | m | 717 | LEU | CA-CB | 5.13 | 1.62 | 1.53 |
| 20 | n | 249 | ASN | CA-C | 5.13 | 1.59 | 1.52 |
| 21 | p | 23 | ASP | CA-C | -5.13 | 1.46 | 1.52 |
| 17 | d | 174 | VAL | N-CA | -5.13 | 1.40 | 1.46 |
| 20 | g | 227 | ARG | CA-C | -5.13 | 1.46 | 1.52 |
| 6 | F | 371 | LYS | N-CA | -5.13 | 1.39 | 1.46 |
| 8 | N | 882 | SER | CA-C | 5.13 | 1.59 | 1.52 |
| 8 | P | 24 | ASP | N-CA | -5.13 | 1.39 | 1.46 |
| 10 | U | 338 | THR | N-CA | -5.13 | 1.39 | 1.46 |
| 12 | v | 693 | ILE | N-CA | -5.13 | 1.40 | 1.46 |
| 20 | g | 230 | PHE | C-N | 5.13 | 1.41 | 1.33 |
| 1 | 0 | 1014 | LYS | N-CA | -5.13 | 1.40 | 1.46 |
| 7 | M | 872 | ILE | C-O | -5.13 | 1.17 | 1.24 |
| 9 | S | 269 | ASN | C-N | 5.13 | 1.40 | 1.33 |
| 9 | S | 474 | PHE | CA-CB | 5.13 | 1.61 | 1.53 |
| 2 | Z | 667 | ALA | CA-C | -5.13 | 1.45 | 1.52 |
| 4 | z | 754 | ASN | C-N | 5.13 | 1.40 | 1.33 |
| 18 | l | 291 | ASN | C-N | 5.13 | 1.40 | 1.33 |
| 19 | m | 398 | ILE | C-N | 5.13 | 1.40 | 1.33 |
| 20 | n | 210 | LEU | CA-CB | 5.13 | 1.62 | 1.53 |
| 20 | g | 868 | HIS | ND1-CE1 | 5.13 | 1.37 | 1.32 |
| 8 | P | 691 | SER | CA-CB | 5.13 | 1.62 | 1.53 |
| 9 | S | 354 | VAL | CA-C | -5.13 | 1.46 | 1.52 |
| 1 | Y | 1103 | LEU | C-N | 5.13 | 1.40 | 1.33 |
| 13 | w | 1272 | ILE | N-CA | -5.13 | 1.40 | 1.46 |
| 1 | 0 | 1400 | GLU | C-N | 5.13 | 1.40 | 1.33 |
| 2 | 1 | 426 | THR | N-CA | 5.13 | 1.52 | 1.45 |
| 7 | M | 206 | ILE | CA-CB | -5.13 | 1.48 | 1.54 |
| 8 | P | 996 | THR | CA-C | -5.13 | 1.47 | 1.52 |
| 8 | P | 1129 | LYS | N-CA | -5.13 | 1.37 | 1.46 |
| 8 | P | 1422 | LEU | N-CA | -5.13 | 1.39 | 1.46 |
| 1 | Y | 973 | ARG | CA-C | -5.13 | 1.46 | 1.52 |
| 12 | u | 149 | ASP | N-CA | -5.13 | 1.39 | 1.46 |
| 15 | b | 319 | SER | CA-CB | 5.13 | 1.61 | 1.53 |
| 1 | 0 | 1069 | ASN | CA-CB | 5.13 | 1.62 | 1.53 |
| 1 | 0 | 1148 | ALA | C-N | 5.13 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 817 | ASN | CA-C | 5.13 | 1.59 | 1.52 |
| 7 | M | 1361 | PHE | C-O | -5.13 | 1.18 | 1.24 |
| 7 | O | 1366 | ARG | N-CA | -5.13 | 1.36 | 1.46 |
| 8 | P | 1335 | GLN | CA-CB | 5.13 | 1.62 | 1.53 |
| 19 | m | 97 | HIS | N-CA | -5.13 | 1.38 | 1.45 |
| 20 | n | 218 | GLY | C-O | -5.13 | 1.19 | 1.23 |
| 16 | c | 279 | GLU | CG-CD | 5.13 | 1.64 | 1.52 |
| 14 | a | 193 | HIS | C-N | 5.13 | 1.40 | 1.33 |
| 9 | S | 826 | ARG | NE-CZ | 5.12 | 1.38 | 1.33 |
| 11 | V | 356 | VAL | N-CA | -5.12 | 1.39 | 1.46 |
| 2 | Z | 850 | HIS | CD2-NE2 | 5.12 | 1.43 | 1.37 |
| 12 | u | 685 | LYS | C-N | -5.12 | 1.27 | 1.33 |
| 1 | 0 | 390 | PRO | CA-C | -5.12 | 1.46 | 1.52 |
| 1 | 0 | 1309 | ASN | C-N | 5.12 | 1.40 | 1.33 |
| 7 | M | 673 | SER | CA-C | 5.12 | 1.59 | 1.52 |
| 8 | P | 1096 | ILE | C-N | 5.12 | 1.40 | 1.33 |
| 12 | v | 275 | GLU | N-CA | -5.12 | 1.40 | 1.46 |
| 14 | h | 257 | TYR | CB-CG | -5.12 | 1.40 | 1.51 |
| 15 | i | 159 | ILE | N-CA | -5.12 | 1.40 | 1.46 |
| 15 | i | 277 | THR | C-N | 5.12 | 1.40 | 1.33 |
| 15 | b | 567 | LEU | C-N | 5.12 | 1.39 | 1.34 |
| 19 | f | 626 | ASP | CA-C | -5.12 | 1.46 | 1.52 |
| 14 | a | 526 | ARG | CZ-NH1 | 5.12 | 1.40 | 1.32 |
| 14 | a | 592 | LYS | CA-CB | 5.12 | 1.59 | 1.53 |
| 2 | Z | 378 | LEU | C-N | 5.12 | 1.40 | 1.33 |
| 14 | h | 375 | ASN | C-N | 5.12 | 1.40 | 1.33 |
| 15 | i | 422 | MET | CA-C | -5.12 | 1.46 | 1.52 |
| 20 | n | 440 | ARG | CA-C | -5.12 | 1.46 | 1.52 |
| 21 | r | 84 | LEU | C-N | 5.12 | 1.40 | 1.33 |
| 15 | b | 531 | LEU | N-CA | -5.12 | 1.41 | 1.46 |
| 8 | N | 322 | HIS | CB-CG | 5.12 | 1.57 | 1.50 |
| 8 | N | 694 | ILE | C-N | 5.12 | 1.40 | 1.33 |
| 8 | P | 1161 | PRO | CA-CB | 5.12 | 1.60 | 1.53 |
| 8 | P | 1176 | PRO | CA-CB | -5.12 | 1.46 | 1.53 |
| 2 | Z | 633 | HIS | ND1-CE1 | 5.12 | 1.37 | 1.32 |
| 13 | w | 1314 | LYS | C-N | 5.12 | 1.40 | 1.33 |
| 19 | m | 35 | PRO | N-CD | -5.12 | 1.40 | 1.47 |
| 14 | a | 1022 | SER | CA-C | 5.12 | 1.59 | 1.52 |
| 4 | D | 761 | ASN | C-O | -5.12 | 1.18 | 1.24 |
| 7 | M | 1545 | ARG | CD-NE | 5.12 | 1.53 | 1.46 |
| 8 | N | 1445 | THR | C-N | 5.12 | 1.40 | 1.33 |
| 9 | R | 665 | LEU | CA-CB | 5.12 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | T | 456 | ARG | CD-NE | 5.12 | 1.53 | 1.46 |
| 9 | T | 625 | GLU | CA-CB | 5.12 | 1.61 | 1.53 |
| 11 | V | 388 | SER | CA-C | 5.12 | 1.59 | 1.52 |
| 12 | v | 135 | LYS | C-N | 5.12 | 1.40 | 1.33 |
| 14 | h | 579 | ILE | CA-C | 5.12 | 1.56 | 1.52 |
| 16 | c | 130 | ASP | C-N | 5.12 | 1.41 | 1.33 |
| 16 | c | 525 | HIS | ND1-CE1 | 5.12 | 1.37 | 1.32 |
| 2 | 1 | 140 | ARG | NE-CZ | 5.12 | 1.38 | 1.33 |
| 4 | G | 769 | ILE | N-CA | 5.12 | 1.52 | 1.46 |
| 21 | q | 30 | ASP | C-N | 5.12 | 1.40 | 1.33 |
| 16 | c | 236 | LEU | CA-C | -5.12 | 1.46 | 1.52 |
| 20 | g | 86 | LEU | N-CA | -5.12 | 1.39 | 1.45 |
| 5 | K | 307 | LYS | C-N | 5.12 | 1.41 | 1.33 |
| 7 | M | 1578 | VAL | C-N | 5.12 | 1.40 | 1.33 |
| 8 | P | 1090 | THR | CB-OG1 | -5.12 | 1.35 | 1.43 |
| 8 | P | 1430 | LEU | N-CA | -5.12 | 1.40 | 1.46 |
| 9 | R | 209 | ARG | CZ-NH1 | 5.12 | 1.40 | 1.32 |
| 1 | Y | 292 | ASN | CA-CB | 5.12 | 1.62 | 1.53 |
| 1 | Y | 1351 | PHE | C-N | 5.12 | 1.40 | 1.33 |
| 4 | y | 643 | LYS | C-N | 5.12 | 1.40 | 1.33 |
| 14 | h | 394 | ASP | N-CA | -5.12 | 1.39 | 1.46 |
| 14 | h | 433 | ILE | C-N | 5.12 | 1.40 | 1.33 |
| 15 | i | 392 | GLN | N-CA | -5.12 | 1.39 | 1.46 |
| 17 | k | 171 | ARG | CZ-NH1 | 5.12 | 1.40 | 1.32 |
| 21 | r | 8 | THR | CA-C | -5.12 | 1.47 | 1.53 |
| 6 | F | 402 | ASP | N-CA | 5.11 | 1.52 | 1.46 |
| 4 | G | 758 | LEU | CA-CB | 5.11 | 1.62 | 1.53 |
| 7 | M | 1548 | ALA | N-CA | -5.11 | 1.40 | 1.46 |
| 7 | O | 435 | PHE | C-N | 5.11 | 1.41 | 1.33 |
| 8 | P | 1312 | LEU | CA-C | -5.11 | 1.46 | 1.52 |
| 9 | T | 540 | ASN | C-N | 5.11 | 1.40 | 1.33 |
| 2 | Z | 654 | SER | C-O | -5.11 | 1.18 | 1.24 |
| 14 | h | 126 | GLY | C-N | 5.11 | 1.40 | 1.33 |
| 14 | h | 661 | GLN | CA-C | -5.11 | 1.45 | 1.52 |
| 18 | l | 198 | LYS | C-N | 5.11 | 1.40 | 1.33 |
| 19 | m | 167 | ASN | C-N | -5.11 | 1.27 | 1.33 |
| 15 | b | 700 | ASP | C-N | 5.11 | 1.40 | 1.33 |
| 14 | a | 821 | HIS | ND1-CE1 | 5.11 | 1.37 | 1.32 |
| 7 | M | 237 | PHE | C-N | 5.11 | 1.40 | 1.33 |
| 9 | T | 551 | ARG | CZ-NH2 | 5.11 | 1.40 | 1.33 |
| 2 | Z | 1363 | PRO | N-CA | -5.11 | 1.41 | 1.47 |
| 20 | g | 373 | ASN | C-N | 5.11 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 543 | VAL | N-CA | -5.11 | 1.40 | 1.46 |
| 9 | Q | 44 | VAL | CA-C | -5.11 | 1.46 | 1.52 |
| 9 | R | 91 | GLN | CA-CB | 5.11 | 1.61 | 1.53 |
| 2 | Z | 1249 | PRO | N-CA | 5.11 | 1.52 | 1.47 |
| 20 | n | 597 | CYS | N-CA | 5.11 | 1.52 | 1.46 |
| 1 | 0 | 946 | LYS | CA-CB | 5.11 | 1.62 | 1.54 |
| 1 | 0 | 1290 | LYS | N-CA | 5.11 | 1.52 | 1.46 |
| 2 | 1 | 457 | SER | C-O | 5.11 | 1.33 | 1.23 |
| 5 | K | 537 | TYR | N-CA | -5.11 | 1.39 | 1.46 |
| 9 | S | 651 | ASP | CA-C | -5.11 | 1.46 | 1.52 |
| 13 | x | 1142 | VAL | CA-C | -5.11 | 1.46 | 1.52 |
| 14 | h | 647 | PHE | CA-CB | 5.11 | 1.61 | 1.53 |
| 19 | m | 189 | LEU | N-CA | -5.11 | 1.40 | 1.46 |
| 2 | 1 | 704 | VAL | CA-CB | 5.11 | 1.60 | 1.54 |
| 4 | A | 669 | LEU | N-CA | -5.11 | 1.40 | 1.46 |
| 5 | B | 323 | LEU | CA-CB | 5.11 | 1.62 | 1.53 |
| 6 | I | 280 | LEU | CA-CB | 5.11 | 1.61 | 1.53 |
| 9 | Q | 97 | GLU | CA-C | -5.11 | 1.46 | 1.52 |
| 11 | X | 389 | LYS | N-CA | -5.11 | 1.40 | 1.46 |
| 2 | Z | 635 | TYR | CA-CB | 5.11 | 1.62 | 1.53 |
| 12 | v | 30 | GLN | C-N | 5.11 | 1.40 | 1.33 |
| 14 | h | 442 | TYR | CA-C | 5.11 | 1.59 | 1.52 |
| 14 | h | 628 | ARG | CZ-NH2 | 5.11 | 1.40 | 1.33 |
| 20 | g | 871 | LEU | CA-C | -5.11 | 1.45 | 1.52 |
| 20 | g | 1014 | SER | N-CA | 5.11 | 1.52 | 1.46 |
| 6 | I | 308 | ILE | N-CA | -5.11 | 1.40 | 1.46 |
| 8 | N | 177 | VAL | CA-C | -5.11 | 1.46 | 1.52 |
| 7 | O | 706 | VAL | C-N | 5.11 | 1.40 | 1.33 |
| 7 | O | 1562 | ASP | CA-C | -5.11 | 1.46 | 1.52 |
| 12 | v | 420 | ILE | C-N | 5.11 | 1.40 | 1.33 |
| 14 | h | 954 | ARG | NE-CZ | 5.11 | 1.38 | 1.33 |
| 16 | j | 492 | PHE | N-CA | 5.11 | 1.52 | 1.46 |
| 20 | n | 1064 | ARG | NE-CZ | 5.11 | 1.38 | 1.33 |
| 16 | c | 142 | ARG | N-CA | 5.11 | 1.52 | 1.46 |
| 14 | a | 548 | GLU | N-CA | -5.11 | 1.40 | 1.46 |
| 5 | E | 309 | ARG | CA-C | -5.10 | 1.46 | 1.52 |
| 5 | K | 355 | PHE | CG-CD2 | 5.10 | 1.49 | 1.38 |
| 5 | K | 444 | LEU | C-N | 5.10 | 1.40 | 1.33 |
| 7 | O | 112 | TYR | CA-CB | 5.10 | 1.61 | 1.53 |
| 9 | R | 571 | LEU | CA-C | 5.10 | 1.59 | 1.52 |
| 20 | n | 218 | GLY | N-CA | -5.10 | 1.38 | 1.44 |
| 20 | n | 520 | ILE | N-CA | -5.10 | 1.41 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | p | 36 | GLN | CA-CB | 5.10 | 1.61 | 1.53 |
| 19 | f | 613 | ILE | CB-CG1 | 5.10 | 1.63 | 1.53 |
| 20 | g | 105 | VAL | N-CA | -5.10 | 1.39 | 1.46 |
| 1 | 0 | 1269 | ALA | N-CA | 5.10 | 1.52 | 1.46 |
| 7 | O | 500 | TRP | NE1-CE2 | 5.10 | 1.43 | 1.37 |
| 9 | S | 209 | ARG | C-N | 5.10 | 1.40 | 1.33 |
| 9 | T | 557 | LEU | C-N | 5.10 | 1.40 | 1.34 |
| 1 | Y | 170 | LYS | C-N | 5.10 | 1.40 | 1.33 |
| 1 | Y | 1233 | ILE | CA-C | 5.10 | 1.59 | 1.52 |
| 4 | z | 745 | TYR | CA-CB | 5.10 | 1.61 | 1.53 |
| 14 | h | 561 | GLN | C-N | 5.10 | 1.40 | 1.33 |
| 15 | i | 674 | ILE | C-N | 5.10 | 1.40 | 1.33 |
| 16 | j | 216 | LEU | CA-C | -5.10 | 1.46 | 1.52 |
| 15 | b | 677 | LEU | N-CA | -5.10 | 1.40 | 1.46 |
| 17 | d | 42 | THR | CA-C | -5.10 | 1.46 | 1.52 |
| 1 | 0 | 616 | ASN | CA-C | -5.10 | 1.46 | 1.52 |
| 14 | h | 658 | HIS | ND1-CE1 | 5.10 | 1.37 | 1.32 |
| 15 | i | 465 | MET | C-N | 5.10 | 1.41 | 1.33 |
| 1 | 0 | 654 | THR | CA-CB | -5.10 | 1.45 | 1.53 |
| 2 | 1 | 676 | LYS | CA-CB | 5.10 | 1.61 | 1.53 |
| 5 | H | 360 | GLN | C-O | -5.10 | 1.17 | 1.24 |
| 9 | Q | 264 | LYS | CA-C | -5.10 | 1.46 | 1.52 |
| 9 | R | 217 | ARG | CZ-NH1 | 5.10 | 1.39 | 1.32 |
| 9 | R | 734 | GLU | N-CA | 5.10 | 1.52 | 1.46 |
| 9 | S | 456 | ARG | CZ-NH2 | 5.10 | 1.40 | 1.33 |
| 1 | Y | 516 | LEU | C-O | -5.10 | 1.19 | 1.23 |
| 1 | Y | 580 | VAL | C-N | 5.10 | 1.39 | 1.33 |
| 12 | u | 544 | THR | CA-CB | 5.10 | 1.61 | 1.53 |
| 14 | h | 448 | THR | C-N | 5.10 | 1.40 | 1.33 |
| 16 | j | 621 | LEU | N-CA | -5.10 | 1.39 | 1.46 |
| 18 | l | 216 | ARG | CD-NE | 5.10 | 1.53 | 1.46 |
| 19 | m | 316 | PRO | CA-C | -5.10 | 1.46 | 1.52 |
| 20 | g | 211 | MET | CA-CB | 5.10 | 1.60 | 1.53 |
| 2 | 1 | 93 | LEU | C-N | 5.10 | 1.41 | 1.33 |
| 5 | K | 345 | PRO | N-CD | 5.10 | 1.54 | 1.47 |
| 8 | N | 558 | LYS | CA-C | -5.10 | 1.45 | 1.52 |
| 8 | N | 770 | HIS | ND1-CE1 | 5.10 | 1.37 | 1.32 |
| 1 | Y | 854 | ILE | CA-C | -5.10 | 1.45 | 1.52 |
| 20 | n | 922 | LEU | CA-CB | 5.10 | 1.61 | 1.53 |
| 21 | s | 14 | SER | CA-CB | 5.10 | 1.62 | 1.53 |
| 19 | f | 589 | HIS | CE1-NE2 | -5.10 | 1.27 | 1.32 |
| 9 | Q | 244 | SER | CA-CB | 5.10 | 1.59 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 1057 | VAL | C-N | 5.10 | 1.40 | 1.33 |
| 20 | n | 234 | ARG | CD-NE | 5.10 | 1.53 | 1.46 |
| 21 | q | 65 | PHE | N-CA | -5.10 | 1.39 | 1.46 |
| 19 | f | 57 | GLY | CA-C | -5.10 | 1.46 | 1.52 |
| 14 | a | 625 | ILE | CA-C | -5.10 | 1.46 | 1.52 |
| 14 | a | 921 | THR | CA-C | 5.10 | 1.59 | 1.52 |
| 2 | 1 | 842 | GLU | C-N | 5.09 | 1.41 | 1.33 |
| 5 | B | 316 | VAL | C-N | 5.09 | 1.40 | 1.33 |
| 6 | F | 274 | ARG | CA-CB | 5.09 | 1.61 | 1.53 |
| 6 | F | 348 | GLN | N-CA | -5.09 | 1.40 | 1.46 |
| 7 | M | 771 | ARG | CD-NE | 5.09 | 1.53 | 1.46 |
| 8 | N | 468 | SER | N-CA | -5.09 | 1.39 | 1.45 |
| 8 | N | 1045 | ALA | N-CA | -5.09 | 1.39 | 1.46 |
| 8 | P | 803 | LEU | CA-CB | 5.09 | 1.61 | 1.53 |
| 10 | W | 250 | ASP | C-N | 5.09 | 1.40 | 1.33 |
| 1 | Y | 1104 | VAL | C-O | -5.09 | 1.18 | 1.24 |
| 15 | i | 682 | LEU | C-N | 5.09 | 1.39 | 1.33 |
| 19 | m | 79 | GLU | CA-CB | 5.09 | 1.61 | 1.53 |
| 20 | n | 83 | ASP | CA-CB | 5.09 | 1.63 | 1.54 |
| 15 | b | 108 | VAL | N-CA | -5.09 | 1.40 | 1.46 |
| 19 | f | 120 | TRP | C-N | 5.09 | 1.40 | 1.33 |
| 20 | g | 99 | VAL | N-CA | -5.09 | 1.40 | 1.46 |
| 8 | P | 1565 | ASN | C-N | 5.09 | 1.40 | 1.33 |
| 14 | h | 883 | GLU | C-N | 5.09 | 1.40 | 1.33 |
| 15 | i | 165 | GLN | CA-C | -5.09 | 1.46 | 1.52 |
| 17 | d | 86 | ASN | C-N | 5.09 | 1.40 | 1.33 |
| 1 | 0 | 1067 | LEU | CA-CB | 5.09 | 1.61 | 1.53 |
| 2 | 1 | 1346 | LEU | CA-C | -5.09 | 1.45 | 1.52 |
| 5 | E | 357 | GLY | C-N | -5.09 | 1.27 | 1.33 |
| 4 | G | 669 | LEU | CA-C | -5.09 | 1.46 | 1.52 |
| 4 | J | 818 | ILE | CA-CB | 5.09 | 1.60 | 1.54 |
| 7 | M | 933 | ASP | CA-CB | 5.09 | 1.61 | 1.53 |
| 7 | M | 1424 | GLU | CA-CB | 5.09 | 1.61 | 1.53 |
| 8 | P | 162 | HIS | CA-C | -5.09 | 1.46 | 1.52 |
| 8 | P | 780 | HIS | CB-CG | 5.09 | 1.57 | 1.50 |
| 9 | Q | 685 | PRO | N-CA | -5.09 | 1.40 | 1.47 |
| 9 | R | 744 | LEU | C-N | 5.09 | 1.41 | 1.33 |
| 9 | R | 821 | GLN | CA-CB | 5.09 | 1.61 | 1.53 |
| 2 | Z | 491 | THR | CA-C | -5.09 | 1.45 | 1.52 |
| 4 | z | 799 | SER | CA-C | -5.09 | 1.46 | 1.52 |
| 14 | h | 222 | SER | CA-CB | 5.09 | 1.61 | 1.53 |
| 16 | j | 627 | ASN | CA-CB | 5.09 | 1.62 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 18 | l | 61 | ILE | N-CA | 5.09 | 1.51 | 1.46 |
| 14 | a | 404 | VAL | CA-C | -5.09 | 1.46 | 1.52 |
| 1 | 0 | 1330 | PHE | CA-C | -5.09 | 1.46 | 1.52 |
| 2 | 1 | 286 | LEU | CB-CG | 5.09 | 1.63 | 1.53 |
| 2 | 1 | 515 | ALA | C-O | 5.09 | 1.33 | 1.23 |
| 2 | 1 | 1114 | VAL | N-CA | -5.09 | 1.40 | 1.46 |
| 8 | N | 148 | VAL | C-N | 5.09 | 1.40 | 1.33 |
| 7 | O | 511 | ILE | CA-C | -5.09 | 1.45 | 1.52 |
| 7 | O | 1030 | ASN | CA-CB | 5.09 | 1.62 | 1.53 |
| 9 | S | 515 | LEU | C-O | 5.09 | 1.33 | 1.23 |
| 1 | Y | 1473 | HIS | ND1-CE1 | 5.09 | 1.37 | 1.32 |
| 15 | b | 270 | LEU | CA-C | -5.09 | 1.46 | 1.52 |
| 20 | g | 253 | LYS | C-N | 5.09 | 1.40 | 1.33 |
| 14 | a | 757 | GLU | CA-C | -5.09 | 1.46 | 1.52 |
| 12 | v | 250 | ILE | CA-C | 5.09 | 1.59 | 1.52 |
| 12 | v | 435 | SER | C-N | 5.09 | 1.40 | 1.33 |
| 17 | k | 264 | LEU | CA-C | -5.09 | 1.46 | 1.52 |
| 16 | c | 174 | ARG | CZ-NH1 | 5.09 | 1.39 | 1.32 |
| 19 | f | 163 | ARG | CA-CB | 5.09 | 1.61 | 1.53 |
| 2 | 1 | 1330 | GLU | N-CA | -5.09 | 1.40 | 1.46 |
| 7 | O | 1505 | HIS | CA-C | 5.09 | 1.59 | 1.52 |
| 8 | P | 777 | ASP | CA-C | -5.09 | 1.46 | 1.52 |
| 8 | P | 979 | ASN | CA-CB | 5.09 | 1.60 | 1.54 |
| 8 | P | 1093 | ASN | CA-CB | 5.09 | 1.60 | 1.53 |
| 9 | Q | 653 | VAL | N-CA | -5.09 | 1.40 | 1.46 |
| 11 | X | 286 | GLU | CA-C | -5.09 | 1.46 | 1.52 |
| 1 | Y | 591 | LYS | C-O | -5.09 | 1.17 | 1.23 |
| 1 | Y | 1480 | ASP | N-CA | -5.09 | 1.39 | 1.46 |
| 12 | v | 381 | ILE | CA-C | 5.09 | 1.59 | 1.52 |
| 14 | h | 55 | GLU | N-CA | 5.09 | 1.52 | 1.46 |
| 18 | l | 224 | ILE | N-CA | -5.09 | 1.39 | 1.46 |
| 20 | n | 936 | LYS | CA-CB | 5.09 | 1.63 | 1.54 |
| 21 | p | 22 | GLU | N-CA | 5.09 | 1.52 | 1.46 |
| 20 | g | 84 | ASP | CA-CB | 5.09 | 1.61 | 1.53 |
| 1 | 0 | 355 | THR | C-N | 5.08 | 1.39 | 1.33 |
| 9 | Q | 273 | VAL | CA-CB | 5.08 | 1.60 | 1.54 |
| 1 | Y | 423 | ILE | CA-CB | -5.08 | 1.48 | 1.54 |
| 1 | Y | 1322 | LEU | N-CA | -5.08 | 1.40 | 1.46 |
| 12 | v | 61 | ARG | CA-CB | 5.08 | 1.61 | 1.53 |
| 18 | l | 164 | HIS | CA-CB | 5.08 | 1.60 | 1.53 |
| 19 | m | 474 | ASN | N-CA | -5.08 | 1.39 | 1.46 |
| 21 | s | 75 | HIS | CG-ND1 | 5.08 | 1.43 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | b | 117 | ASP | C-O | -5.08 | 1.18 | 1.24 |
| 2 | 1 | 273 | PHE | CA-C | -5.08 | 1.46 | 1.52 |
| 7 | M | 23 | ASP | CA-CB | 5.08 | 1.62 | 1.53 |
| 7 | O | 225 | SER | CA-CB | 5.08 | 1.60 | 1.53 |
| 9 | R | 134 | LYS | N-CA | -5.08 | 1.40 | 1.46 |
| 9 | T | 277 | TYR | N-CA | -5.08 | 1.40 | 1.46 |
| 11 | X | 377 | PHE | CA-CB | 5.08 | 1.62 | 1.53 |
| 1 | Y | 1090 | GLU | C-N | 5.08 | 1.40 | 1.33 |
| 2 | Z | 236 | SER | CA-C | -5.08 | 1.46 | 1.52 |
| 13 | w | 1303 | ILE | C-N | 5.08 | 1.40 | 1.33 |
| 13 | w | 1352 | VAL | C-N | 5.08 | 1.40 | 1.33 |
| 20 | n | 293 | GLN | CA-C | -5.08 | 1.46 | 1.52 |
| 20 | n | 708 | TRP | CA-C | -5.08 | 1.46 | 1.52 |
| 19 | f | 284 | SER | CA-C | -5.08 | 1.45 | 1.52 |
| 1 | 0 | 599 | LEU | CA-C | -5.08 | 1.46 | 1.52 |
| 1 | 0 | 1313 | VAL | N-CA | -5.08 | 1.40 | 1.46 |
| 8 | N | 756 | TRP | NE1-CE2 | 5.08 | 1.43 | 1.37 |
| 7 | O | 1552 | PHE | CA-CB | 5.08 | 1.60 | 1.53 |
| 8 | P | 453 | ALA | CA-C | -5.08 | 1.45 | 1.52 |
| 8 | P | 748 | HIS | CB-CG | 5.08 | 1.57 | 1.50 |
| 8 | P | 1026 | THR | N-CA | -5.08 | 1.39 | 1.46 |
| 9 | R | 62 | ALA | C-N | 5.08 | 1.40 | 1.33 |
| 9 | R | 108 | GLU | N-CA | 5.08 | 1.54 | 1.46 |
| 9 | S | 729 | ASN | CA-C | -5.08 | 1.46 | 1.52 |
| 9 | S | 746 | PRO | CA-CB | -5.08 | 1.46 | 1.53 |
| 9 | T | 727 | TYR | C-N | 5.08 | 1.40 | 1.33 |
| 2 | Z | 1116 | TYR | CZ-OH | 5.08 | 1.48 | 1.38 |
| 14 | h | 405 | GLU | CA-C | 5.08 | 1.59 | 1.52 |
| 20 | n | 570 | PHE | C-O | 5.08 | 1.29 | 1.24 |
| 8 | P | 1131 | LYS | CA-C | -5.08 | 1.46 | 1.52 |
| 2 | Z | 1308 | CYS | N-CA | 5.08 | 1.52 | 1.46 |
| 19 | f | 270 | ALA | N-CA | -5.08 | 1.40 | 1.46 |
| 1 | 0 | 1170 | ARG | NE-CZ | 5.08 | 1.38 | 1.33 |
| 7 | M | 9 | GLN | C-O | -5.08 | 1.17 | 1.24 |
| 12 | u | 117 | ASP | C-N | 5.08 | 1.41 | 1.33 |
| 21 | s | 62 | GLY | N-CA | 5.08 | 1.51 | 1.45 |
| 20 | g | 117 | THR | N-CA | -5.08 | 1.38 | 1.46 |
| 14 | a | 258 | ASP | CA-C | -5.08 | 1.46 | 1.52 |
| 14 | a | 801 | ASN | C-N | 5.08 | 1.40 | 1.33 |
| 14 | a | 916 | ARG | CZ-NH1 | 5.08 | 1.39 | 1.32 |
| 5 | H | 342 | LYS | C-N | 5.08 | 1.39 | 1.34 |
| 8 | N | 1515 | LEU | N-CA | 5.08 | 1.51 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | O | 353 | PRO | CA-CB | -5.08 | 1.46 | 1.53 |
| 2 | Z | 264 | ILE | CA-CB | -5.08 | 1.46 | 1.55 |
| 12 | v | 576 | ASP | C-N | 5.08 | 1.40 | 1.33 |
| 14 | h | 205 | LEU | CA-C | -5.08 | 1.46 | 1.52 |
| 19 | m | 548 | GLN | CA-CB | 5.08 | 1.62 | 1.53 |
| 21 | o | 51 | VAL | CA-C | -5.08 | 1.46 | 1.52 |
| 21 | s | 69 | VAL | CA-C | 5.08 | 1.58 | 1.52 |
| 1 | 0 | 433 | ASN | C-N | 5.08 | 1.40 | 1.33 |
| 2 | 1 | 1354 | ASP | CA-C | -5.08 | 1.46 | 1.52 |
| 7 | M | 217 | LEU | N-CA | 5.08 | 1.52 | 1.46 |
| 7 | M | 295 | ARG | C-N | 5.08 | 1.39 | 1.33 |
| 8 | N | 937 | SER | C-N | 5.08 | 1.40 | 1.33 |
| 7 | O | 779 | PRO | N-CD | -5.08 | 1.40 | 1.47 |
| 7 | O | 1465 | GLN | C-N | 5.08 | 1.40 | 1.33 |
| 8 | P | 377 | THR | C-N | 5.08 | 1.40 | 1.33 |
| 8 | P | 1500 | LEU | C-N | 5.08 | 1.40 | 1.33 |
| 9 | S | 507 | ALA | N-CA | -5.08 | 1.40 | 1.46 |
| 4 | y | 812 | THR | C-O | 5.08 | 1.30 | 1.24 |
| 17 | k | 53 | GLU | C-N | 5.08 | 1.41 | 1.33 |
| 18 | l | 26 | THR | CB-OG1 | -5.08 | 1.35 | 1.43 |
| 20 | g | 217 | ALA | N-CA | 5.08 | 1.52 | 1.46 |
| 14 | a | 176 | VAL | N-CA | 5.08 | 1.52 | 1.46 |
| 1 | 0 | 782 | ARG | NE-CZ | 5.07 | 1.38 | 1.33 |
| 4 | A | 702 | ARG | CZ-NH2 | 5.07 | 1.40 | 1.33 |
| 4 | A | 708 | GLU | N-CA | 5.07 | 1.52 | 1.46 |
| 7 | O | 555 | TRP | CA-CB | 5.07 | 1.61 | 1.53 |
| 7 | O | 660 | LEU | CA-CB | 5.07 | 1.62 | 1.53 |
| 8 | P | 186 | LYS | C-N | 5.07 | 1.40 | 1.34 |
| 9 | Q | 224 | ASN | N-CA | 5.07 | 1.52 | 1.46 |
| 9 | Q | 687 | LEU | CA-CB | 5.07 | 1.61 | 1.53 |
| 9 | R | 758 | GLN | N-CA | -5.07 | 1.39 | 1.46 |
| 10 | W | 330 | GLU | CA-C | 5.07 | 1.59 | 1.52 |
| 12 | v | 295 | TYR | C-N | 5.07 | 1.44 | 1.34 |
| 4 | y | 719 | GLU | C-N | 5.07 | 1.40 | 1.33 |
| 14 | h | 464 | THR | CA-C | -5.07 | 1.46 | 1.52 |
| 14 | h | 988 | GLN | C-N | 5.07 | 1.39 | 1.33 |
| 16 | j | 234 | TRP | C-N | 5.07 | 1.40 | 1.33 |
| 20 | n | 1153 | ASN | CA-C | -5.07 | 1.46 | 1.52 |
| 20 | g | 1078 | LEU | CA-CB | 5.07 | 1.61 | 1.53 |
| 14 | a | 692 | PHE | CA-CB | 5.07 | 1.60 | 1.53 |
| 6 | I | 383 | LYS | C-N | 5.07 | 1.40 | 1.33 |
| 8 | N | 1602 | LEU | N-CA | 5.07 | 1.52 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 889 | GLU | C-N | 5.07 | 1.40 | 1.33 |
| 2 | Z | 494 | ASN | CA-CB | 5.07 | 1.62 | 1.53 |
| 14 | h | 996 | LYS | N-CA | -5.07 | 1.39 | 1.46 |
| 19 | m | 656 | ARG | CZ-NH2 | 5.07 | 1.40 | 1.33 |
| 15 | b | 316 | ALA | CA-C | -5.07 | 1.47 | 1.52 |
| 15 | b | 602 | GLU | C-N | 5.07 | 1.40 | 1.33 |
| 1 | 0 | 153 | VAL | C-N | 5.07 | 1.40 | 1.33 |
| 7 | M | 1649 | LYS | N-CA | -5.07 | 1.40 | 1.46 |
| 12 | u | 37 | PHE | C-N | 5.07 | 1.40 | 1.33 |
| 14 | h | 334 | LEU | CA-CB | 5.07 | 1.62 | 1.53 |
| 16 | j | 767 | ASN | CA-CB | 5.07 | 1.62 | 1.53 |
| 19 | m | 449 | LEU | C-N | 5.07 | 1.40 | 1.33 |
| 21 | p | 52 | LYS | CA-CB | 5.07 | 1.61 | 1.53 |
| 16 | c | 272 | ILE | C-O | -5.07 | 1.18 | 1.24 |
| 19 | f | 559 | CYS | CA-C | 5.07 | 1.59 | 1.52 |
| 16 | j | 372 | LEU | CA-CB | 5.07 | 1.60 | 1.53 |
| 15 | b | 608 | PRO | CA-C | 5.07 | 1.59 | 1.52 |
| 20 | g | 418 | VAL | C-N | 5.07 | 1.40 | 1.33 |
| 8 | N | 458 | LYS | C-O | 5.07 | 1.29 | 1.23 |
| 7 | O | 320 | GLU | C-N | 5.07 | 1.40 | 1.33 |
| 7 | O | 1390 | GLN | C-O | -5.07 | 1.17 | 1.24 |
| 9 | R | 217 | ARG | C-N | 5.07 | 1.40 | 1.34 |
| 9 | R | 243 | SER | CA-C | -5.07 | 1.46 | 1.52 |
| 1 | Y | 211 | ILE | CA-C | -5.07 | 1.46 | 1.52 |
| 16 | j | 763 | ILE | CA-C | -5.07 | 1.45 | 1.53 |
| 15 | b | 149 | GLU | N-CA | 5.07 | 1.52 | 1.46 |
| 18 | e | 54 | HIS | CA-C | -5.07 | 1.46 | 1.53 |
| 19 | f | 171 | VAL | C-N | 5.07 | 1.40 | 1.34 |
| 4 | D | 638 | ASP | CA-CB | 5.07 | 1.61 | 1.53 |
| 5 | K | 457 | ASN | CA-C | -5.07 | 1.45 | 1.52 |
| 6 | L | 376 | LYS | C-N | 5.07 | 1.40 | 1.33 |
| 7 | M | 80 | GLU | C-N | 5.07 | 1.40 | 1.33 |
| 7 | O | 1154 | ARG | CA-CB | 5.07 | 1.61 | 1.53 |
| 8 | P | 939 | LEU | CA-CB | 5.07 | 1.61 | 1.53 |
| 9 | R | 551 | ARG | CZ-NH2 | 5.07 | 1.40 | 1.33 |
| 9 | S | 70 | HIS | CA-CB | 5.07 | 1.61 | 1.53 |
| 9 | S | 125 | ILE | N-CA | -5.07 | 1.40 | 1.46 |
| 2 | Z | 1384 | LYS | CA-C | -5.07 | 1.46 | 1.52 |
| 12 | v | 540 | VAL | C-N | 5.07 | 1.40 | 1.33 |
| 15 | i | 403 | HIS | CB-CG | 5.07 | 1.57 | 1.50 |
| 16 | j | 167 | LYS | CA-C | -5.07 | 1.46 | 1.52 |
| 20 | n | 330 | THR | N-CA | 5.07 | 1.52 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | b | 575 | LEU | N-CA | -5.07 | 1.39 | 1.46 |
| 19 | f | 534 | SER | C-N | 5.07 | 1.41 | 1.33 |
| 2 | 1 | 1229 | LYS | CA-C | -5.06 | 1.45 | 1.52 |
| 1 | 0 | 218 | ARG | CD-NE | 5.06 | 1.53 | 1.46 |
| 1 | 0 | 462 | LEU | C-N | 5.06 | 1.40 | 1.33 |
| 2 | 1 | 1375 | ASN | CA-CB | 5.06 | 1.62 | 1.53 |
| 5 | K | 443 | LEU | CA-CB | 5.06 | 1.61 | 1.53 |
| 7 | M | 1453 | ARG | CD-NE | 5.06 | 1.53 | 1.46 |
| 7 | O | 1482 | THR | CA-C | -5.06 | 1.46 | 1.52 |
| 8 | P | 105 | GLU | CA-C | 5.06 | 1.59 | 1.52 |
| 14 | h | 300 | MET | CA-CB | 5.06 | 1.60 | 1.53 |
| 15 | i | 201 | ARG | NE-CZ | 5.06 | 1.38 | 1.33 |
| 19 | m | 458 | ARG | CZ-NH2 | 5.06 | 1.40 | 1.33 |
| 15 | b | 310 | VAL | CA-CB | -5.06 | 1.48 | 1.54 |
| 15 | b | 628 | ALA | CA-CB | 5.06 | 1.61 | 1.53 |
| 17 | d | 21 | GLY | C-N | 5.06 | 1.40 | 1.33 |
| 20 | g | 945 | ARG | NE-CZ | 5.06 | 1.38 | 1.33 |
| 14 | a | 190 | ASP | C-N | 5.06 | 1.38 | 1.33 |
| 8 | N | 794 | ILE | CA-C | 5.06 | 1.59 | 1.52 |
| 11 | X | 378 | ARG | CA-C | -5.06 | 1.46 | 1.53 |
| 1 | 0 | 464 | SER | N-CA | -5.06 | 1.40 | 1.46 |
| 2 | 1 | 173 | TRP | NE1-CE2 | -5.06 | 1.31 | 1.37 |
| 8 | N | 1062 | ARG | C-N | 5.06 | 1.40 | 1.34 |
| 8 | P | 855 | CYS | CA-C | -5.06 | 1.47 | 1.53 |
| 9 | Q | 351 | GLN | CA-CB | 5.06 | 1.61 | 1.53 |
| 9 | S | 499 | SER | CA-CB | 5.06 | 1.62 | 1.53 |
| 2 | Z | 923 | ILE | N-CA | -5.06 | 1.39 | 1.46 |
| 12 | v | 635 | ARG | CA-CB | 5.06 | 1.61 | 1.53 |
| 13 | w | 1223 | ALA | C-N | 5.06 | 1.40 | 1.33 |
| 16 | j | 205 | ASN | CA-CB | 5.06 | 1.61 | 1.53 |
| 16 | j | 662 | SER | C-N | 5.06 | 1.40 | 1.33 |
| 18 | l | 316 | GLY | C-N | 5.06 | 1.40 | 1.33 |
| 16 | c | 148 | TYR | C-N | 5.06 | 1.40 | 1.33 |
| 2 | 1 | 1382 | TYR | C-N | 5.06 | 1.40 | 1.33 |
| 7 | M | 1579 | ASN | C-O | -5.06 | 1.18 | 1.24 |
| 9 | Q | 319 | SER | CA-CB | 5.06 | 1.62 | 1.53 |
| 9 | Q | 461 | ASP | C-N | 5.06 | 1.38 | 1.33 |
| 1 | Y | 783 | ASP | CA-CB | 5.06 | 1.61 | 1.53 |
| 2 | Z | 183 | TRP | N-CA | -5.06 | 1.40 | 1.45 |
| 12 | v | 548 | SER | N-CA | 5.06 | 1.52 | 1.46 |
| 14 | h | 510 | LEU | C-N | 5.06 | 1.41 | 1.33 |
| 16 | j | 185 | PHE | N-CA | -5.06 | 1.40 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 21 | q | 25 | LEU | CA-C | 5.06 | 1.59 | 1.52 |
| 16 | c | 312 | GLU | CA-CB | 5.06 | 1.62 | 1.53 |
| 16 | c | 513 | ARG | CA-C | -5.06 | 1.46 | 1.52 |
| 17 | d | 144 | HIS | C-O | 5.06 | 1.30 | 1.24 |
| 14 | a | 508 | LYS | CA-CB | 5.06 | 1.61 | 1.53 |
| 8 | P | 77 | ASN | CA-C | 5.06 | 1.58 | 1.52 |
| 12 | v | 34 | ARG | NE-CZ | 5.06 | 1.38 | 1.33 |
| 12 | v | 599 | MET | CA-CB | 5.06 | 1.61 | 1.53 |
| 14 | a | 752 | HIS | CA-C | 5.06 | 1.59 | 1.52 |
| 1 | 0 | 1386 | PRO | CA-CB | -5.05 | 1.47 | 1.53 |
| 2 | 1 | 877 | SER | C-N | 5.05 | 1.40 | 1.33 |
| 5 | K | 352 | ILE | CA-C | -5.05 | 1.46 | 1.52 |
| 9 | S | 629 | ARG | CD-NE | 5.05 | 1.53 | 1.46 |
| 1 | Y | 171 | THR | C-O | -5.05 | 1.18 | 1.24 |
| 14 | h | 451 | ARG | CZ-NH2 | 5.05 | 1.40 | 1.33 |
| 17 | k | 208 | ARG | NE-CZ | 5.05 | 1.38 | 1.33 |
| 17 | k | 210 | VAL | CA-CB | -5.05 | 1.47 | 1.53 |
| 20 | n | 439 | MET | C-N | 5.05 | 1.40 | 1.33 |
| 21 | t | 15 | ASP | C-O | -5.05 | 1.17 | 1.23 |
| 16 | c | 494 | SER | N-CA | -5.05 | 1.39 | 1.46 |
| 14 | a | 233 | TYR | N-CA | 5.05 | 1.52 | 1.45 |
| 7 | O | 1341 | ASP | C-O | -5.05 | 1.17 | 1.24 |
| 8 | P | 101 | PHE | CA-CB | 5.05 | 1.63 | 1.53 |
| 2 | Z | 500 | THR | C-N | 5.05 | 1.39 | 1.33 |
| 19 | m | 539 | LEU | N-CA | -5.05 | 1.39 | 1.46 |
| 20 | g | 1014 | SER | CA-C | -5.05 | 1.46 | 1.52 |
| 4 | D | 686 | ALA | CA-C | -5.05 | 1.46 | 1.52 |
| 4 | G | 704 | GLN | N-CA | -5.05 | 1.40 | 1.46 |
| 8 | P | 688 | THR | CB-OG1 | -5.05 | 1.35 | 1.43 |
| 9 | S | 317 | ASP | C-O | -5.05 | 1.18 | 1.24 |
| 1 | Y | 1331 | ARG | CZ-NH2 | 5.05 | 1.40 | 1.33 |
| 16 | j | 344 | SER | CA-C | 5.05 | 1.59 | 1.52 |
| 18 | l | 109 | GLY | C-N | 5.05 | 1.40 | 1.33 |
| 20 | n | 1001 | ASP | CA-C | -5.05 | 1.46 | 1.52 |
| 21 | q | 27 | ILE | C-N | 5.05 | 1.40 | 1.33 |
| 15 | b | 613 | ASP | CA-C | -5.05 | 1.46 | 1.52 |
| 19 | f | 528 | HIS | CB-CG | 5.05 | 1.57 | 1.50 |
| 20 | g | 387 | MET | C-N | 5.05 | 1.39 | 1.33 |
| 20 | g | 1134 | HIS | CA-C | -5.05 | 1.46 | 1.52 |
| 14 | a | 302 | THR | N-CA | -5.05 | 1.39 | 1.46 |
| 14 | a | 724 | PHE | CA-CB | 5.05 | 1.61 | 1.53 |
| 5 | E | 296 | LYS | N-CA | -5.05 | 1.39 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | J | 655 | PHE | C-O | -5.05 | 1.18 | 1.24 |
| 7 | M | 216 | LEU | CA-CB | 5.05 | 1.61 | 1.53 |
| 7 | M | 929 | TYR | C-N | 5.05 | 1.39 | 1.33 |
| 8 | N | 704 | ASP | CA-CB | 5.05 | 1.61 | 1.53 |
| 8 | N | 937 | SER | CA-C | -5.05 | 1.46 | 1.53 |
| 9 | R | 607 | ARG | N-CA | -5.05 | 1.39 | 1.46 |
| 9 | R | 801 | GLN | C-N | 5.05 | 1.41 | 1.34 |
| 9 | T | 333 | ILE | CA-CB | -5.05 | 1.48 | 1.54 |
| 9 | T | 820 | ILE | CA-C | 5.05 | 1.57 | 1.52 |
| 1 | Y | 273 | ILE | C-N | 5.05 | 1.40 | 1.33 |
| 2 | Z | 237 | PHE | CA-C | -5.05 | 1.46 | 1.52 |
| 13 | w | 1404 | GLU | N-CA | -5.05 | 1.40 | 1.46 |
| 4 | z | 639 | ASP | C-N | 5.05 | 1.40 | 1.33 |
| 18 | l | 204 | VAL | CA-C | -5.05 | 1.46 | 1.52 |
| 19 | m | 612 | ASN | C-N | 5.05 | 1.41 | 1.33 |
| 2 | 1 | 572 | PRO | N-CD | -5.05 | 1.40 | 1.47 |
| 5 | B | 322 | ILE | N-CA | -5.05 | 1.40 | 1.46 |
| 9 | S | 209 | ARG | CA-CB | 5.05 | 1.61 | 1.53 |
| 15 | i | 86 | ASP | C-N | 5.05 | 1.40 | 1.33 |
| 15 | b | 432 | ASN | C-N | 5.05 | 1.39 | 1.33 |
| 18 | e | 48 | SER | C-N | 5.05 | 1.39 | 1.33 |
| 7 | M | 1532 | ARG | CA-CB | 5.05 | 1.61 | 1.53 |
| 8 | N | 341 | PHE | CA-C | -5.05 | 1.46 | 1.52 |
| 7 | O | 1543 | LEU | C-N | 5.05 | 1.40 | 1.33 |
| 8 | P | 1450 | LEU | CA-C | -5.05 | 1.46 | 1.52 |
| 9 | Q | 300 | THR | C-N | 5.05 | 1.41 | 1.34 |
| 9 | Q | 341 | LEU | CA-CB | 5.05 | 1.61 | 1.53 |
| 9 | R | 663 | ASP | CA-CB | 5.05 | 1.61 | 1.53 |
| 2 | Z | 808 | ALA | CA-CB | 5.05 | 1.61 | 1.53 |
| 14 | h | 845 | ILE | CA-C | -5.05 | 1.46 | 1.52 |
| 14 | h | 877 | ILE | C-N | 5.05 | 1.40 | 1.33 |
| 19 | m | 314 | ILE | C-O | -5.05 | 1.18 | 1.24 |
| 21 | p | 27 | ILE | C-N | 5.05 | 1.40 | 1.33 |
| 15 | b | 642 | TRP | CA-CB | 5.05 | 1.61 | 1.53 |
| 1 | 0 | 1160 | HIS | ND1-CE1 | 5.04 | 1.37 | 1.32 |
| 1 | 0 | 1316 | SER | CA-C | -5.04 | 1.46 | 1.52 |
| 4 | D | 683 | ALA | CA-C | -5.04 | 1.46 | 1.52 |
| 7 | O | 33 | GLN | C-N | 5.04 | 1.40 | 1.33 |
| 9 | R | 368 | LEU | N-CA | -5.04 | 1.39 | 1.46 |
| 14 | h | 878 | HIS | CD2-NE2 | 5.04 | 1.43 | 1.37 |
| 19 | m | 552 | ARG | CD-NE | 5.04 | 1.53 | 1.46 |
| 20 | n | 71 | THR | CB-OG1 | -5.04 | 1.35 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 19 | f | 62 | VAL | CA-CB | 5.04 | 1.60 | 1.54 |
| 1 | 0 | 981 | ILE | CB-CG1 | 5.04 | 1.63 | 1.53 |
| 2 | 1 | 425 | ILE | C-N | 5.04 | 1.40 | 1.33 |
| 7 | M | 446 | CYS | C-N | 5.04 | 1.40 | 1.34 |
| 8 | N | 1503 | VAL | CA-CB | -5.04 | 1.48 | 1.54 |
| 7 | O | 1310 | VAL | C-O | -5.04 | 1.18 | 1.24 |
| 8 | P | 1604 | LYS | CA-C | -5.04 | 1.46 | 1.52 |
| 12 | u | 559 | GLU | C-N | 5.04 | 1.40 | 1.33 |
| 14 | h | 463 | ILE | C-N | 5.04 | 1.40 | 1.33 |
| 14 | h | 810 | ASP | C-N | 5.04 | 1.41 | 1.33 |
| 16 | j | 227 | THR | CA-C | -5.04 | 1.45 | 1.52 |
| 16 | j | 458 | ARG | C-N | 5.04 | 1.41 | 1.34 |
| 16 | j | 459 | PHE | CA-C | 5.04 | 1.59 | 1.52 |
| 17 | k | 43 | HIS | ND1-CE1 | 5.04 | 1.37 | 1.32 |
| 17 | k | 99 | SER | C-N | 5.04 | 1.40 | 1.33 |
| 16 | c | 575 | SER | N-CA | -5.04 | 1.40 | 1.46 |
| 18 | e | 183 | LEU | C-N | 5.04 | 1.40 | 1.33 |
| 20 | g | 317 | LEU | N-CA | -5.04 | 1.40 | 1.46 |
| 5 | B | 351 | GLN | CA-CB | 5.04 | 1.61 | 1.53 |
| 5 | B | 472 | ASN | CA-CB | 5.04 | 1.61 | 1.53 |
| 7 | M | 461 | LEU | CB-CG | 5.04 | 1.63 | 1.53 |
| 8 | P | 109 | ARG | CZ-NH2 | 5.04 | 1.40 | 1.33 |
| 1 | Y | 842 | TYR | CA-C | -5.04 | 1.46 | 1.52 |
| 1 | Y | 1106 | ASP | CA-C | -5.04 | 1.46 | 1.52 |
| 12 | v | 113 | HIS | C-O | -5.04 | 1.17 | 1.24 |
| 17 | k | 242 | PRO | CA-CB | 5.04 | 1.61 | 1.53 |
| 19 | m | 618 | GLU | N-CA | 5.04 | 1.52 | 1.46 |
| 19 | m | 715 | LEU | CA-C | -5.04 | 1.45 | 1.52 |
| 20 | n | 761 | ASN | CA-CB | 5.04 | 1.61 | 1.53 |
| 19 | f | 397 | ASP | C-N | 5.04 | 1.40 | 1.33 |
| 2 | 1 | 441 | ARG | CZ-NH1 | 5.04 | 1.39 | 1.32 |
| 7 | M | 566 | THR | CA-C | -5.04 | 1.46 | 1.52 |
| 8 | N | 645 | SER | CA-C | -5.04 | 1.47 | 1.53 |
| 1 | Y | 777 | ILE | C-N | 5.04 | 1.40 | 1.33 |
| 17 | d | 135 | THR | CA-C | -5.04 | 1.46 | 1.52 |
| 20 | g | 137 | ARG | NE-CZ | 5.04 | 1.38 | 1.33 |
| 1 | 0 | 1063 | SER | C-N | 5.04 | 1.39 | 1.34 |
| 7 | M | 322 | ILE | C-N | 5.04 | 1.40 | 1.33 |
| 7 | M | 1397 | SER | C-N | 5.04 | 1.39 | 1.33 |
| 7 | O | 499 | PHE | CB-CG | 5.04 | 1.62 | 1.50 |
| 9 | Q | 510 | LEU | CA-C | -5.04 | 1.45 | 1.52 |
| 1 | Y | 428 | PRO | C-N | 5.04 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 1382 | GLU | C-N | 5.04 | 1.40 | 1.33 |
| 2 | Z | 540 | VAL | C-N | 5.04 | 1.40 | 1.33 |
| 12 | u | 56 | SER | N-CA | -5.04 | 1.40 | 1.45 |
| 12 | u | 161 | GLU | C-N | 5.04 | 1.41 | 1.33 |
| 15 | i | 403 | HIS | ND1-CE1 | 5.04 | 1.37 | 1.32 |
| 18 | l | 128 | LEU | CA-CB | 5.04 | 1.62 | 1.53 |
| 20 | n | 625 | GLN | C-O | -5.04 | 1.17 | 1.23 |
| 15 | b | 454 | LEU | CA-C | -5.04 | 1.45 | 1.52 |
| 15 | b | 698 | LYS | CA-C | -5.04 | 1.45 | 1.52 |
| 20 | g | 1002 | LEU | CA-C | -5.04 | 1.46 | 1.52 |
| 1 | 0 | 1281 | THR | CA-C | 5.04 | 1.58 | 1.52 |
| 1 | 0 | 1289 | ILE | C-N | 5.04 | 1.40 | 1.33 |
| 6 | F | 342 | GLU | C-N | 5.04 | 1.40 | 1.33 |
| 8 | P | 1189 | ASP | CA-CB | 5.04 | 1.61 | 1.53 |
| 8 | P | 1453 | ILE | CA-C | -5.04 | 1.47 | 1.52 |
| 12 | u | 345 | ASN | CA-CB | 5.04 | 1.59 | 1.53 |
| 12 | u | 581 | PHE | N-CA | -5.04 | 1.39 | 1.46 |
| 19 | m | 623 | PHE | CA-C | -5.04 | 1.46 | 1.52 |
| 20 | n | 352 | TYR | CA-C | -5.04 | 1.46 | 1.52 |
| 20 | n | 527 | ILE | CA-CB | -5.04 | 1.48 | 1.54 |
| 15 | b | 379 | LEU | CA-C | -5.04 | 1.46 | 1.52 |
| 19 | f | 77 | LEU | C-N | 5.04 | 1.40 | 1.33 |
| 2 | 1 | 746 | SER | C-N | 5.04 | 1.39 | 1.33 |
| 5 | K | 447 | SER | CA-C | -5.04 | 1.46 | 1.52 |
| 7 | M | 78 | SER | C-N | 5.04 | 1.41 | 1.33 |
| 7 | O | 173 | ALA | CA-CB | 5.04 | 1.61 | 1.53 |
| 8 | P | 1445 | THR | CA-C | -5.04 | 1.45 | 1.52 |
| 9 | T | 711 | LYS | N-CA | -5.04 | 1.40 | 1.46 |
| 18 | l | 227 | TRP | NE1-CE2 | 5.04 | 1.43 | 1.37 |
| 18 | e | 297 | LEU | C-N | 5.04 | 1.40 | 1.33 |
| 14 | a | 584 | ASN | C-N | 5.04 | 1.40 | 1.33 |
| 4 | J | 727 | SER | C-O | 5.03 | 1.33 | 1.23 |
| 7 | M | 1031 | VAL | N-CA | -5.03 | 1.40 | 1.46 |
| 8 | P | 158 | SER | C-N | 5.03 | 1.40 | 1.33 |
| 8 | P | 716 | LYS | CA-CB | 5.03 | 1.61 | 1.53 |
| 1 | Y | 782 | ARG | CD-NE | 5.03 | 1.53 | 1.46 |
| 12 | v | 326 | LEU | C-N | 5.03 | 1.40 | 1.33 |
| 15 | i | 338 | VAL | CA-CB | -5.03 | 1.48 | 1.54 |
| 20 | n | 127 | ASP | CA-C | -5.03 | 1.46 | 1.52 |
| 16 | c | 343 | TRP | NE1-CE2 | -5.03 | 1.31 | 1.37 |
| 20 | g | 284 | TYR | CA-C | -5.03 | 1.46 | 1.53 |
| 14 | a | 297 | LEU | CA-CB | 5.03 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 1363 | PRO | N-CA | -5.03 | 1.39 | 1.48 |
| 9 | R | 620 | LEU | CB-CG | 5.03 | 1.63 | 1.53 |
| 1 | Y | 578 | VAL | C-O | 5.03 | 1.29 | 1.24 |
| 20 | n | 554 | GLY | C-N | 5.03 | 1.40 | 1.33 |
| 1 | 0 | 220 | LYS | CA-C | 5.03 | 1.58 | 1.52 |
| 5 | B | 334 | GLU | N-CA | -5.03 | 1.40 | 1.46 |
| 6 | F | 292 | HIS | CA-C | -5.03 | 1.46 | 1.52 |
| 5 | K | 303 | THR | CA-CB | 5.03 | 1.62 | 1.53 |
| 7 | M | 1326 | ASN | CA-CB | 5.03 | 1.62 | 1.53 |
| 8 | N | 109 | ARG | CA-CB | 5.03 | 1.61 | 1.53 |
| 7 | O | 489 | TYR | CA-CB | 5.03 | 1.61 | 1.53 |
| 9 | S | 306 | LYS | C-N | 5.03 | 1.40 | 1.34 |
| 1 | Y | 1189 | LYS | CA-C | -5.03 | 1.46 | 1.52 |
| 2 | Z | 927 | HIS | CG-CD2 | 5.03 | 1.41 | 1.35 |
| 2 | Z | 1207 | ASN | CA-C | 5.03 | 1.59 | 1.52 |
| 12 | u | 270 | VAL | C-N | 5.03 | 1.40 | 1.33 |
| 14 | h | 452 | ASP | CA-CB | 5.03 | 1.61 | 1.53 |
| 21 | s | 30 | ASP | CA-CB | 5.03 | 1.61 | 1.53 |
| 17 | d | 97 | VAL | C-N | 5.03 | 1.40 | 1.33 |
| 19 | f | 419 | LEU | CA-C | 5.03 | 1.59 | 1.52 |
| 5 | B | 345 | PRO | C-N | 5.03 | 1.40 | 1.33 |
| 7 | M | 1295 | ALA | CA-C | -5.03 | 1.46 | 1.52 |
| 7 | O | 103 | LYS | CA-C | -5.03 | 1.46 | 1.52 |
| 1 | Y | 892 | ALA | C-N | 5.03 | 1.39 | 1.33 |
| 15 | i | 226 | GLN | C-N | -5.03 | 1.26 | 1.33 |
| 15 | i | 576 | PHE | C-O | 5.03 | 1.29 | 1.24 |
| 16 | j | 334 | ASP | CA-CB | 5.03 | 1.61 | 1.53 |
| 16 | c | 504 | GLU | N-CA | -5.03 | 1.40 | 1.46 |
| 19 | f | 608 | SER | CA-CB | 5.03 | 1.60 | 1.53 |
| 20 | g | 271 | ARG | C-N | 5.03 | 1.41 | 1.33 |
| 7 | M | 763 | HIS | CE1-NE2 | 5.03 | 1.37 | 1.32 |
| 8 | P | 1649 | ASP | CA-CB | 5.03 | 1.61 | 1.53 |
| 9 | T | 467 | ILE | N-CA | -5.03 | 1.40 | 1.46 |
| 10 | W | 343 | VAL | C-N | 5.03 | 1.40 | 1.33 |
| 1 | Y | 291 | LEU | CA-C | -5.03 | 1.46 | 1.52 |
| 1 | Y | 1456 | TYR | C-N | 5.03 | 1.40 | 1.33 |
| 2 | Z | 764 | ASP | CA-C | -5.03 | 1.45 | 1.52 |
| 2 | Z | 1385 | ASP | CA-C | -5.03 | 1.46 | 1.52 |
| 13 | w | 1360 | GLU | C-N | 5.03 | 1.40 | 1.33 |
| 4 | y | 713 | ASN | CA-C | -5.03 | 1.46 | 1.52 |
| 20 | g | 128 | ASP | CA-C | -5.03 | 1.46 | 1.52 |
| 1 | 0 | 1101 | ARG | NE-CZ | 5.03 | 1.38 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 21 | ASP | N-CA | -5.03 | 1.40 | 1.46 |
| 7 | M | 199 | GLY | C-N | 5.03 | 1.40 | 1.33 |
| 8 | N | 1196 | TYR | C-N | 5.03 | 1.40 | 1.33 |
| 8 | N | 1289 | LYS | CA-C | -5.03 | 1.46 | 1.52 |
| 7 | O | 1599 | GLU | CA-CB | 5.03 | 1.61 | 1.53 |
| 8 | P | 762 | LEU | CA-C | -5.03 | 1.46 | 1.52 |
| 9 | R | 99 | ASN | C-N | 5.03 | 1.39 | 1.33 |
| 9 | T | 652 | ILE | CA-C | -5.03 | 1.45 | 1.52 |
| 4 | y | 641 | VAL | N-CA | -5.03 | 1.40 | 1.46 |
| 18 | l | 149 | THR | C-N | 5.03 | 1.40 | 1.33 |
| 19 | m | 107 | LYS | C-O | -5.03 | 1.17 | 1.24 |
| 12 | v | 117 | ASP | C-N | 5.02 | 1.40 | 1.33 |
| 20 | n | 373 | ASN | CA-CB | 5.02 | 1.61 | 1.53 |
| 5 | K | 311 | PHE | N-CA | -5.02 | 1.40 | 1.46 |
| 7 | M | 1077 | THR | C-N | 5.02 | 1.40 | 1.33 |
| 8 | N | 382 | PHE | CA-C | -5.02 | 1.46 | 1.52 |
| 8 | P | 1071 | LYS | N-CA | -5.02 | 1.39 | 1.46 |
| 8 | P | 1197 | VAL | CA-CB | 5.02 | 1.60 | 1.54 |
| 9 | S | 42 | ILE | CA-CB | -5.02 | 1.50 | 1.55 |
| 9 | S | 743 | ASP | N-CA | -5.02 | 1.38 | 1.46 |
| 11 | V | 367 | LEU | N-CA | -5.02 | 1.39 | 1.46 |
| 1 | Y | 204 | VAL | N-CA | -5.02 | 1.39 | 1.46 |
| 12 | u | 186 | GLU | CA-C | -5.02 | 1.46 | 1.52 |
| 12 | u | 193 | THR | CA-C | -5.02 | 1.46 | 1.52 |
| 15 | i | 418 | ALA | C-N | 5.02 | 1.41 | 1.33 |
| 16 | j | 267 | ARG | NE-CZ | 5.02 | 1.38 | 1.33 |
| 16 | j | 565 | TYR | CG-CD2 | 5.02 | 1.49 | 1.39 |
| 18 | l | 148 | TRP | CA-CB | 5.02 | 1.59 | 1.52 |
| 20 | g | 537 | GLU | N-CA | -5.02 | 1.39 | 1.46 |
| 20 | g | 781 | TYR | C-N | 5.02 | 1.40 | 1.33 |
| 5 | B | 457 | ASN | C-N | 5.02 | 1.40 | 1.33 |
| 6 | L | 406 | PHE | C-N | 5.02 | 1.40 | 1.33 |
| 8 | P | 1181 | THR | CB-OG1 | -5.02 | 1.35 | 1.43 |
| 11 | V | 282 | ASN | C-N | 5.02 | 1.40 | 1.33 |
| 14 | h | 467 | GLY | N-CA | -5.02 | 1.38 | 1.45 |
| 19 | m | 403 | SER | CA-C | 5.02 | 1.59 | 1.52 |
| 16 | c | 763 | ILE | CA-CB | -5.02 | 1.49 | 1.54 |
| 19 | f | 652 | LEU | C-N | 5.02 | 1.39 | 1.33 |
| 2 | 1 | 988 | CYS | CA-C | 5.02 | 1.58 | 1.52 |
| 4 | G | 771 | ASN | CB-CG | 5.02 | 1.64 | 1.52 |
| 7 | M | 545 | HIS | CA-CB | 5.02 | 1.62 | 1.53 |
| 7 | M | 739 | ARG | N-CA | 5.02 | 1.52 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | M | 1345 | PHE | CA-CB | 5.02 | 1.61 | 1.53 |
| 8 | N | 1409 | ALA | N-CA | -5.02 | 1.40 | 1.46 |
| 9 | Q | 547 | TYR | N-CA | -5.02 | 1.41 | 1.46 |
| 9 | R | 290 | TYR | N-CA | -5.02 | 1.40 | 1.46 |
| 9 | S | 630 | ARG | CZ-NH2 | 5.02 | 1.40 | 1.33 |
| 2 | Z | 214 | PHE | CA-C | -5.02 | 1.46 | 1.52 |
| 13 | x | 1278 | CYS | CA-CB | 5.02 | 1.62 | 1.53 |
| 20 | n | 753 | PHE | N-CA | 5.02 | 1.52 | 1.46 |
| 15 | b | 257 | LEU | CA-CB | 5.02 | 1.60 | 1.53 |
| 16 | c | 513 | ARG | NE-CZ | 5.02 | 1.38 | 1.33 |
| 19 | f | 466 | ASN | C-N | 5.02 | 1.40 | 1.33 |
| 20 | g | 974 | ARG | NE-CZ | 5.02 | 1.38 | 1.33 |
| 1 | 0 | 976 | THR | C-N | 5.02 | 1.40 | 1.33 |
| 2 | 1 | 758 | SER | CA-CB | 5.02 | 1.61 | 1.53 |
| 4 | G | 743 | GLN | C-N | 5.02 | 1.40 | 1.33 |
| 5 | H | 511 | GLU | CA-CB | 5.02 | 1.61 | 1.53 |
| 7 | M | 161 | GLN | CA-C | -5.02 | 1.46 | 1.52 |
| 8 | N | 1240 | PHE | N-CA | -5.02 | 1.39 | 1.46 |
| 9 | R | 246 | ASN | CA-C | -5.02 | 1.46 | 1.52 |
| 9 | T | 211 | LYS | C-N | 5.02 | 1.40 | 1.33 |
| 1 | Y | 1025 | ASN | CA-CB | 5.02 | 1.60 | 1.53 |
| 14 | h | 239 | GLN | N-CA | -5.02 | 1.40 | 1.46 |
| 14 | h | 240 | ASN | C-N | 5.02 | 1.40 | 1.33 |
| 15 | i | 467 | ASN | N-CA | -5.02 | 1.40 | 1.46 |
| 15 | b | 628 | ALA | C-N | 5.02 | 1.40 | 1.33 |
| 16 | c | 579 | ARG | NE-CZ | 5.02 | 1.38 | 1.33 |
| 9 | R | 79 | SER | N-CA | -5.02 | 1.39 | 1.46 |
| 11 | V | 396 | ALA | N-CA | -5.02 | 1.40 | 1.46 |
| 16 | c | 766 | LYS | CA-C | -5.02 | 1.46 | 1.52 |
| 1 | 0 | 1349 | MET | N-CA | -5.01 | 1.39 | 1.46 |
| 4 | A | 646 | ASN | CA-CB | 5.01 | 1.61 | 1.53 |
| 5 | B | 464 | ALA | N-CA | -5.01 | 1.40 | 1.46 |
| 4 | G | 798 | ASN | CA-CB | 5.01 | 1.61 | 1.53 |
| 7 | O | 997 | ALA | C-O | -5.01 | 1.20 | 1.23 |
| 9 | R | 76 | SER | CA-C | 5.01 | 1.59 | 1.52 |
| 17 | k | 88 | ARG | CD-NE | 5.01 | 1.53 | 1.46 |
| 19 | m | 395 | CYS | C-O | 5.01 | 1.30 | 1.24 |
| 20 | n | 382 | ARG | CD-NE | 5.01 | 1.53 | 1.46 |
| 17 | d | 286 | GLU | N-CA | -5.01 | 1.39 | 1.46 |
| 14 | a | 917 | ASP | CA-CB | 5.01 | 1.61 | 1.53 |
| 7 | O | 190 | TYR | CA-C | -5.01 | 1.45 | 1.52 |
| 20 | g | 557 | LEU | C-N | 5.01 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | g | 650 | LEU | CA-CB | 5.01 | 1.61 | 1.53 |
| 7 | M | 702 | LYS | N-CA | -5.01 | 1.39 | 1.46 |
| 7 | M | 721 | SER | CA-C | -5.01 | 1.46 | 1.52 |
| 8 | N | 422 | GLU | CA-C | -5.01 | 1.46 | 1.52 |
| 8 | N | 557 | TYR | CA-C | -5.01 | 1.46 | 1.53 |
| 7 | O | 784 | ILE | CA-C | -5.01 | 1.47 | 1.52 |
| 7 | O | 1425 | LYS | CA-C | -5.01 | 1.46 | 1.52 |
| 9 | Q | 505 | HIS | CE1-NE2 | -5.01 | 1.27 | 1.32 |
| 9 | T | 601 | PRO | CA-C | -5.01 | 1.46 | 1.52 |
| 12 | u | 571 | ILE | CA-C | -5.01 | 1.46 | 1.52 |
| 12 | u | 663 | THR | C-N | 5.01 | 1.40 | 1.34 |
| 19 | f | 665 | MET | CA-C | -5.01 | 1.46 | 1.52 |
| 20 | g | 665 | PHE | N-CA | 5.01 | 1.52 | 1.46 |
| 14 | a | 906 | GLN | CA-CB | 5.01 | 1.61 | 1.53 |
| 1 | 0 | 383 | THR | CA-C | -5.01 | 1.46 | 1.52 |
| 5 | H | 538 | LYS | C-O | 5.01 | 1.29 | 1.24 |
| 4 | J | 690 | GLN | N-CA | 5.01 | 1.52 | 1.46 |
| 7 | M | 28 | VAL | N-CA | 5.01 | 1.51 | 1.46 |
| 7 | M | 167 | ILE | N-CA | -5.01 | 1.40 | 1.46 |
| 7 | M | 605 | ALA | C-O | -5.01 | 1.18 | 1.24 |
| 8 | P | 1194 | LEU | CA-CB | 5.01 | 1.61 | 1.53 |
| 9 | T | 61 | LYS | N-CA | -5.01 | 1.42 | 1.47 |
| 14 | h | 136 | SER | N-CA | -5.01 | 1.38 | 1.46 |
| 14 | h | 578 | ASP | CA-CB | 5.01 | 1.59 | 1.52 |
| 18 | l | 243 | PHE | CA-CB | 5.01 | 1.59 | 1.53 |
| 15 | b | 361 | LEU | N-CA | -5.01 | 1.39 | 1.46 |
| 15 | b | 546 | MET | C-N | 5.01 | 1.40 | 1.33 |
| 17 | d | 152 | SER | CA-CB | 5.01 | 1.61 | 1.53 |
| 20 | g | 115 | LYS | CA-CB | 5.01 | 1.59 | 1.53 |
| 2 | 1 | 1282 | VAL | CA-CB | -5.01 | 1.49 | 1.54 |
| 5 | H | 434 | GLU | CA-C | -5.01 | 1.46 | 1.52 |
| 8 | N | 275 | LEU | CA-C | -5.01 | 1.46 | 1.52 |
| 8 | N | 999 | GLN | C-O | -5.01 | 1.18 | 1.24 |
| 7 | O | 1676 | LEU | CA-C | -5.01 | 1.46 | 1.52 |
| 9 | T | 769 | LYS | C-N | 5.01 | 1.41 | 1.33 |
| 14 | h | 852 | SER | N-CA | -5.01 | 1.39 | 1.46 |
| 15 | b | 654 | GLU | CA-CB | 5.01 | 1.59 | 1.52 |
| 1 | 0 | 174 | GLY | N-CA | 5.01 | 1.51 | 1.45 |
| 2 | 1 | 1119 | ALA | C-O | 5.01 | 1.30 | 1.24 |
| 8 | P | 690 | LEU | N-CA | -5.01 | 1.39 | 1.46 |
| 8 | P | 1212 | THR | CA-CB | 5.01 | 1.61 | 1.53 |
| 21 | s | 46 | LYS | CA-CB | 5.01 | 1.61 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 17 | d | 86 | ASN | CA-CB | 5.01 | 1.61 | 1.53 |
| 20 | g | 1101 | ARG | CD-NE | 5.01 | 1.53 | 1.46 |
| 1 | 0 | 656 | ASP | C-N | 5.00 | 1.41 | 1.33 |
| 9 | T | 573 | HIS | CG-ND1 | -5.00 | 1.32 | 1.38 |
| 2 | Z | 170 | ASN | CA-C | -5.00 | 1.47 | 1.53 |
| 2 | Z | 761 | VAL | CA-C | -5.00 | 1.45 | 1.52 |
| 12 | v | 84 | ASN | CA-C | -5.00 | 1.46 | 1.52 |
| 13 | x | 1446 | LYS | CA-C | -5.00 | 1.46 | 1.52 |
| 20 | n | 424 | VAL | CA-CB | 5.00 | 1.62 | 1.55 |
| 20 | n | 956 | ALA | N-CA | -5.00 | 1.40 | 1.46 |
| 15 | b | 526 | CYS | CA-CB | 5.00 | 1.60 | 1.53 |
| 15 | b | 661 | HIS | N-CA | -5.00 | 1.39 | 1.46 |
| 16 | c | 168 | SER | CA-C | -5.00 | 1.46 | 1.52 |
| 16 | c | 205 | ASN | C-N | 5.00 | 1.40 | 1.34 |
| 14 | a | 298 | PHE | C-N | 5.00 | 1.40 | 1.33 |
| 5 | H | 369 | VAL | C-N | 5.00 | 1.40 | 1.33 |
| 6 | I | 382 | LYS | CA-C | 5.00 | 1.58 | 1.53 |
| 5 | K | 352 | ILE | C-O | -5.00 | 1.18 | 1.24 |
| 7 | O | 325 | PHE | C-O | -5.00 | 1.18 | 1.24 |
| 9 | S | 698 | ASP | N-CA | -5.00 | 1.39 | 1.46 |
| 11 | X | 269 | SER | CA-C | -5.00 | 1.46 | 1.52 |
| 2 | Z | 287 | GLN | N-CA | -5.00 | 1.40 | 1.46 |
| 19 | f | 334 | ARG | CZ-NH1 | 5.00 | 1.39 | 1.32 |
| 20 | g | 1141 | ALA | CA-C | -5.00 | 1.46 | 1.53 |
| 14 | a | 214 | ARG | NE-CZ | 5.00 | 1.38 | 1.33 |
| 1 | 0 | 960 | LYS | CA-CB | 5.00 | 1.61 | 1.54 |
| 1 | 0 | 1148 | ALA | N-CA | -5.00 | 1.40 | 1.46 |
| 1 | 0 | 1441 | ASN | CA-CB | 5.00 | 1.61 | 1.53 |
| 7 | M | 118 | SER | CA-CB | 5.00 | 1.61 | 1.53 |
| 8 | N | 990 | LYS | N-CA | -5.00 | 1.40 | 1.46 |
| 8 | N | 1434 | ASN | CG-ND2 | 5.00 | 1.43 | 1.33 |
| 8 | P | 106 | ARG | C-N | 5.00 | 1.40 | 1.33 |
| 8 | P | 188 | ILE | CA-CB | 5.00 | 1.60 | 1.54 |
| 1 | Y | 203 | VAL | C-N | 5.00 | 1.39 | 1.33 |
| 1 | Y | 1180 | PRO | CA-CB | -5.00 | 1.50 | 1.53 |
| 1 | Y | 1295 | LYS | CA-CB | 5.00 | 1.61 | 1.53 |
| 2 | Z | 841 | ARG | C-N | 5.00 | 1.40 | 1.33 |
| 14 | h | 314 | THR | N-CA | -5.00 | 1.40 | 1.45 |
| 21 | t | 9 | PRO | CA-C | 5.00 | 1.59 | 1.52 |
| 19 | f | 595 | ARG | C-O | 5.00 | 1.30 | 1.24 |
| 14 | a | 26 | LEU | CA-C | -5.00 | 1.46 | 1.52 |

All (15089) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 309 | LEU | N-CA-CB | 36.30 | 172.21 | 110.50 |
| 8 | N | 794 | ILE | N-CA-CB | 32.75 | 165.27 | 111.23 |
| 11 | V | 402 | ASN | N-CA-CB | 26.18 | 155.00 | 110.50 |
| 5 | B | 324 | TYR | N-CA-CB | 25.82 | 154.12 | 110.49 |
| 2 | 1 | 678 | LYS | N-CA-C | -25.14 | 80.28 | 110.44 |
| 10 | W | 284 | LYS | N-CA-CB | 25.07 | 153.12 | 110.50 |
| 9 | Q | 753 | ALA | CB-CA-C | 24.39 | 147.09 | 110.50 |
| 1 | 0 | 419 | LYS | O-C-N | -23.95 | 90.73 | 122.59 |
| 2 | Z | 456 | THR | N-CA-C | 22.99 | 146.87 | 109.40 |
| 1 | 0 | 832 | VAL | CB-CA-C | 22.51 | 148.20 | 111.29 |
| 11 | V | 302 | ARG | N-CA-CB | 21.65 | 147.31 | 110.50 |
| 1 | Y | 832 | VAL | N-CA-CB | 21.56 | 146.80 | 111.23 |
| 10 | W | 283 | ILE | N-CA-CB | 20.94 | 137.48 | 112.15 |
| 21 | p | 55 | ASN | CB-CA-C | -20.66 | 81.34 | 110.06 |
| 10 | U | 283 | ILE | N-CA-CB | 20.56 | 136.27 | 111.60 |
| 10 | W | 249 | ASP | N-CA-CB | 20.32 | 144.83 | 110.49 |
| 2 | 1 | 745 | ILE | CB-CA-C | 20.26 | 144.51 | 111.29 |
| 8 | P | 1094 | SER | N-CA-CB | 20.11 | 142.34 | 110.77 |
| 21 | s | 55 | ASN | N-CA-C | 20.03 | 139.68 | 110.24 |
| 21 | p | 55 | ASN | N-CA-C | 19.90 | 140.15 | 110.30 |
| 8 | P | 1095 | GLU | N-CA-CB | 19.72 | 143.81 | 110.49 |
| 7 | M | 1189 | MET | CB-CA-C | 19.53 | 149.29 | 110.42 |
| 14 | h | 104 | GLN | CA-C-O | 19.13 | 129.03 | 117.94 |
| 21 | t | 55 | ASN | N-CA-C | 19.12 | 138.34 | 110.42 |
| 2 | 1 | 1301 | SER | CB-CA-C | 19.12 | 148.47 | 110.42 |
| 2 | 1 | 922 | LYS | CB-CA-C | 19.07 | 148.37 | 110.42 |
| 8 | P | 256 | THR | N-CA-CB | 19.05 | 143.89 | 111.50 |
| 10 | U | 249 | ASP | N-CA-CB | 19.00 | 142.61 | 110.49 |
| 1 | 0 | 831 | LYS | CB-CA-C | 18.94 | 146.08 | 110.10 |
| 8 | P | 577 | MET | N-CA-CB | 18.70 | 142.29 | 110.50 |
| 8 | N | 794 | ILE | N-CA-C | -18.60 | 70.65 | 109.34 |
| 10 | W | 305 | TYR | N-CA-CB | 18.50 | 143.30 | 110.37 |
| 9 | Q | 754 | ARG | N-CA-CB | 18.48 | 141.72 | 110.49 |
| 7 | O | 603 | GLU | CB-CA-C | 18.41 | 147.05 | 110.42 |
| 2 | 1 | 309 | LEU | N-CA-C | -18.24 | 59.94 | 111.00 |
| 9 | R | 515 | LEU | CB-CA-C | 17.96 | 144.22 | 110.10 |
| 21 | q | 55 | ASN | N-CA-C | 17.93 | 149.00 | 110.80 |
| 7 | O | 1138 | PHE | CB-CA-C | 17.80 | 145.85 | 110.42 |
| 2 | Z | 457 | SER | N-CA-CB | 17.79 | 140.73 | 110.50 |
| 7 | M | 1138 | PHE | CB-CA-C | 17.70 | 145.65 | 110.42 |
| 9 | Q | 754 | ARG | CA-C-O | -17.69 | 95.21 | 120.51 |
| 9 | T | 515 | LEU | CB-CA-C | 17.65 | 143.63 | 110.10 |
| 21 | p | 55 | ASN | N-CA-CB | 17.52 | 138.01 | 109.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 678 | LYS | CB-CA-C | 17.34 | 151.30 | 111.77 |
| 19 | m | 372 | GLY | N-CA-C | 17.29 | 163.43 | 113.30 |
| 7 | O | 1189 | MET | N-CA-CB | 17.19 | 139.53 | 110.49 |
| 2 | Z | 678 | LYS | N-CA-CB | 17.11 | 139.49 | 110.57 |
| 5 | B | 324 | TYR | N-CA-C | -17.08 | 74.43 | 110.80 |
| 2 | 1 | 1300 | SER | N-CA-CB | 17.02 | 137.50 | 109.60 |
| 1 | Y | 1022 | ASP | CB-CA-C | 17.02 | 144.28 | 110.42 |
| 5 | K | 318 | GLU | N-CA-C | 16.93 | 146.86 | 110.80 |
| 8 | N | 1059 | ASN | N-CA-C | 16.68 | 135.33 | 110.64 |
| 8 | N | 257 | LEU | N-CA-CB | 16.67 | 138.66 | 110.49 |
| 11 | V | 401 | ASP | N-CA-CB | 16.40 | 137.43 | 110.37 |
| 8 | N | 552 | LEU | CB-CA-C | 16.33 | 142.91 | 110.42 |
| 11 | V | 301 | LEU | N-CA-CB | 16.25 | 137.20 | 110.39 |
| 6 | L | 370 | ASP | CA-C-O | -16.21 | 97.34 | 120.51 |
| 2 | Z | 922 | LYS | N-CA-CB | 16.15 | 137.78 | 110.49 |
| 4 | G | 726 | VAL | N-CA-C | 16.14 | 142.91 | 109.34 |
| 5 | B | 319 | THR | N-CA-CB | 16.09 | 137.67 | 110.49 |
| 2 | 1 | 916 | PHE | CB-CA-C | 16.07 | 140.64 | 110.10 |
| 2 | Z | 916 | PHE | CB-CA-C | 16.05 | 140.59 | 110.10 |
| 7 | O | 1137 | ASN | N-CA-C | 15.91 | 155.54 | 111.00 |
| 8 | N | 1059 | ASN | CB-CA-C | -15.88 | 90.26 | 109.80 |
| 11 | X | 402 | ASN | N-CA-CB | 15.82 | 137.39 | 110.50 |
| 21 | q | 56 | THR | CB-CA-C | 15.76 | 141.78 | 110.42 |
| 1 | Y | 1022 | ASP | N-CA-CB | -15.75 | 83.87 | 110.49 |
| 21 | t | 55 | ASN | CB-CA-C | -15.74 | 87.83 | 109.71 |
| 19 | m | 373 | THR | CB-CA-C | 15.69 | 141.65 | 110.42 |
| 8 | P | 257 | LEU | CB-CA-C | 15.63 | 141.52 | 110.42 |
| 6 | F | 370 | ASP | N-CA-CB | 15.60 | 136.85 | 110.49 |
| 14 | h | 579 | ILE | N-CA-CB | 15.56 | 120.30 | 110.50 |
| 8 | N | 1059 | ASN | N-CA-CB | 15.48 | 133.03 | 109.19 |
| 21 | s | 55 | ASN | CB-CA-C | -15.37 | 86.79 | 109.84 |
| 9 | T | 514 | LYS | N-CA-CB | 15.30 | 136.35 | 110.49 |
| 1 | Y | 832 | VAL | N-CA-C | -15.25 | 77.61 | 109.34 |
| 21 | o | 56 | THR | CB-CA-C | 15.18 | 140.62 | 110.42 |
| 11 | X | 401 | ASP | N-CA-CB | 15.11 | 136.03 | 110.49 |
| 2 | Z | 916 | PHE | CA-CB-CG | -15.10 | 98.70 | 113.80 |
| 4 | G | 808 | ASP | CA-CB-CG | 15.07 | 127.67 | 112.60 |
| 4 | G | 726 | VAL | CB-CA-C | -14.98 | 86.71 | 111.29 |
| 5 | K | 319 | THR | N-CA-CB | 14.97 | 135.79 | 110.49 |
| 8 | N | 1060 | LEU | CB-CA-C | 14.95 | 140.16 | 110.42 |
| 7 | O | 1137 | ASN | CB-CA-C | -14.89 | 81.80 | 110.10 |
| 1 | Y | 832 | VAL | CB-CA-C | 14.78 | 135.53 | 111.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | o | 55 | ASN | N-CA-C | 14.72 | 142.16 | 110.80 |
| 8 | N | 576 | TYR | N-CA-CB | 14.61 | 134.48 | 110.37 |
| 2 | 1 | 744 | GLY | N-CA-C | 14.60 | 155.64 | 113.30 |
| 2 | 1 | 1300 | SER | N-CA-C | 14.60 | 130.17 | 109.15 |
| 8 | N | 1094 | SER | N-CA-CB | 14.60 | 134.76 | 110.53 |
| 8 | N | 577 | MET | CB-CA-C | 14.54 | 137.73 | 110.10 |
| 8 | P | 1094 | SER | CB-CA-C | -14.54 | 86.88 | 110.14 |
| 14 | a | 578 | ASP | CA-C-N | 14.44 | 129.34 | 120.24 |
| 14 | a | 578 | ASP | C-N-CA | 14.44 | 129.34 | 120.24 |
| 1 | 0 | 1257 | GLN | CB-CA-C | -14.43 | 82.69 | 110.10 |
| 8 | N | 551 | ASN | CA-CB-CG | 14.42 | 127.02 | 112.60 |
| 21 | t | 55 | ASN | N-CA-CB | 14.37 | 131.32 | 109.34 |
| 7 | M | 1585 | PRO | N-CA-CB | 14.32 | 118.55 | 103.23 |
| 21 | r | 55 | ASN | N-CA-CB | 14.19 | 134.47 | 110.49 |
| 8 | N | 793 | LEU | N-CA-CB | 14.15 | 134.55 | 110.50 |
| 2 | 1 | 916 | PHE | N-CA-CB | 14.11 | 134.48 | 110.50 |
| 9 | R | 514 | LYS | N-CA-CB | 14.10 | 134.31 | 110.49 |
| 9 | T | 754 | ARG | CB-CA-C | 14.03 | 138.34 | 110.42 |
| 1 | 0 | 1021 | TYR | N-CA-CB | 14.02 | 134.34 | 110.50 |
| 2 | Z | 915 | LYS | N-CA-C | 14.00 | 140.62 | 110.80 |
| 1 | 0 | 832 | VAL | N-CA-C | -13.97 | 80.28 | 109.34 |
| 4 | G | 727 | SER | CB-CA-C | 13.97 | 136.64 | 110.10 |
| 8 | P | 257 | LEU | N-CA-CB | 13.91 | 134.00 | 110.49 |
| 2 | Z | 921 | SER | N-CA-CB | 13.90 | 134.12 | 110.50 |
| 2 | Z | 678 | LYS | CB-CA-C | -13.85 | 86.49 | 109.89 |
| 5 | B | 319 | THR | CB-CA-C | 13.80 | 137.88 | 110.42 |
| 2 | Z | 679 | SER | CB-CA-C | 13.79 | 137.86 | 110.42 |
| 10 | W | 249 | ASP | N-CA-C | -13.78 | 81.45 | 110.80 |
| 10 | U | 249 | ASP | N-CA-C | -13.77 | 81.47 | 110.80 |
| 1 | 0 | 1022 | ASP | CA-CB-CG | 13.74 | 126.34 | 112.60 |
| 7 | O | 1188 | THR | N-CA-C | 13.74 | 140.06 | 110.80 |
| 21 | q | 56 | THR | CA-CB-OG1 | 13.71 | 130.17 | 109.60 |
| 9 | R | 600 | ILE | CA-C-O | -13.66 | 110.31 | 119.19 |
| 6 | L | 370 | ASP | N-CA-CB | 13.65 | 133.57 | 110.49 |
| 2 | 1 | 915 | LYS | N-CA-CB | 13.65 | 133.56 | 110.49 |
| 2 | Z | 678 | LYS | N-CA-C | 13.65 | 130.70 | 108.32 |
| 21 | s | 55 | ASN | N-CA-CB | 13.54 | 130.47 | 109.48 |
| 2 | Z | 922 | LYS | CB-CA-C | 13.52 | 137.33 | 110.42 |
| 2 | 1 | 679 | SER | N-CA-CB | 13.50 | 133.30 | 110.49 |
| 8 | N | 256 | THR | N-CA-CB | 13.49 | 134.43 | 111.50 |
| 1 | Y | 1021 | TYR | N-CA-CB | 13.45 | 133.37 | 110.50 |
| 6 | I | 369 | LEU | CB-CA-C | 13.37 | 135.51 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1189 | MET | CB-CA-C | 13.37 | 137.03 | 110.42 |
| 21 | t | 56 | THR | CB-CA-C | 13.28 | 136.85 | 110.42 |
| 8 | P | 1095 | GLU | N-CA-C | -13.28 | 82.51 | 110.80 |
| 2 | 1 | 1300 | SER | CB-CA-C | -13.27 | 90.49 | 110.67 |
| 21 | q | 55 | ASN | CB-CA-C | -13.24 | 84.08 | 110.42 |
| 5 | B | 319 | THR | N-CA-C | -13.20 | 82.69 | 110.80 |
| 5 | H | 324 | TYR | CB-CA-C | 13.18 | 136.66 | 110.42 |
| 8 | N | 323 | TYR | N-CA-CB | 13.17 | 122.94 | 109.51 |
| 20 | g | 316 | ILE | N-CA-C | -13.16 | 100.49 | 111.81 |
| 8 | P | 177 | VAL | N-CA-C | -13.13 | 99.83 | 112.96 |
| 1 | Y | 1110 | ASP | CA-CB-CG | 13.10 | 125.70 | 112.60 |
| 14 | a | 120 | ASN | CA-CB-CG | -13.10 | 99.50 | 112.60 |
| 2 | 1 | 1079 | PHE | N-CA-C | -13.08 | 94.26 | 110.61 |
| 5 | K | 319 | THR | CB-CA-C | 13.02 | 136.32 | 110.42 |
| 7 | O | 828 | PHE | CA-CB-CG | -13.00 | 100.80 | 113.80 |
| 9 | T | 753 | ALA | CB-CA-C | -12.95 | 91.07 | 110.50 |
| 21 | s | 16 | ILE | O-C-N | -12.94 | 111.71 | 122.97 |
| 6 | L | 292 | HIS | CA-CB-CG | 12.94 | 126.74 | 113.80 |
| 7 | O | 1189 | MET | N-CA-C | -12.91 | 83.29 | 110.80 |
| 16 | c | 353 | ASN | N-CA-C | -12.91 | 95.76 | 112.93 |
| 19 | m | 373 | THR | N-CA-CB | -12.91 | 88.68 | 110.49 |
| 1 | Y | 1257 | GLN | N-CA-CB | 12.82 | 132.29 | 110.50 |
| 10 | U | 249 | ASP | CB-CA-C | 12.79 | 135.88 | 110.42 |
| 7 | O | 1188 | THR | N-CA-CB | 12.79 | 132.10 | 110.49 |
| 2 | 1 | 154 | VAL | N-CA-C | -12.78 | 100.93 | 113.20 |
| 21 | s | 56 | THR | CB-CA-C | 12.78 | 135.85 | 110.42 |
| 5 | H | 323 | LEU | N-CA-CB | 12.69 | 131.94 | 110.49 |
| 19 | m | 447 | PHE | CA-CB-CG | -12.64 | 101.16 | 113.80 |
| 7 | M | 1335 | ILE | CA-C-N | 12.60 | 130.41 | 120.33 |
| 7 | M | 1335 | ILE | C-N-CA | 12.60 | 130.41 | 120.33 |
| 6 | I | 370 | ASP | CB-CA-C | 12.59 | 135.48 | 110.42 |
| 7 | M | 231 | ILE | N-CA-C | -12.59 | 101.75 | 113.71 |
| 1 | 0 | 1258 | LEU | CB-CA-C | 12.55 | 135.39 | 110.42 |
| 8 | P | 1094 | SER | N-CA-C | 12.51 | 128.85 | 108.34 |
| 1 | Y | 1258 | LEU | CB-CA-C | 12.49 | 135.28 | 110.42 |
| 8 | P | 257 | LEU | N-CA-C | -12.45 | 84.28 | 110.80 |
| 21 | o | 55 | ASN | N-CA-CB | 12.39 | 131.43 | 110.49 |
| 21 | t | 56 | THR | CA-CB-OG1 | 12.38 | 128.17 | 109.60 |
| 1 | 0 | 1007 | ILE | N-CA-C | -12.37 | 101.41 | 113.53 |
| 2 | Z | 456 | THR | CB-CA-C | -12.34 | 85.81 | 109.37 |
| 21 | o | 55 | ASN | CB-CA-C | -12.31 | 85.92 | 110.42 |
| 2 | Z | 922 | LYS | N-CA-C | -12.31 | 84.59 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 832 | VAL | N-CA-CB | 12.30 | 131.52 | 111.23 |
| 7 | O | 636 | SER | CA-C-N | 12.29 | 137.15 | 120.44 |
| 7 | O | 636 | SER | C-N-CA | 12.29 | 137.15 | 120.44 |
| 11 | V | 402 | ASN | N-CA-C | -12.28 | 76.62 | 111.00 |
| 8 | N | 132 | ASN | CA-C-O | 12.28 | 138.06 | 120.51 |
| 8 | N | 935 | VAL | N-CA-C | -12.28 | 101.92 | 111.62 |
| 9 | R | 515 | LEU | N-CA-CB | 12.27 | 131.36 | 110.50 |
| 10 | W | 284 | LYS | N-CA-C | -12.26 | 76.68 | 111.00 |
| 2 | 1 | 1100 | PHE | N-CA-C | 12.25 | 124.63 | 111.28 |
| 2 | 1 | 922 | LYS | CA-C-O | -12.24 | 103.00 | 120.51 |
| 1 | Y | 1233 | ILE | CA-C-N | 12.15 | 136.56 | 120.28 |
| 1 | Y | 1233 | ILE | C-N-CA | 12.15 | 136.56 | 120.28 |
| 10 | W | 248 | TRP | N-CA-CB | 12.13 | 131.12 | 110.50 |
| 8 | N | 472 | ASP | CA-CB-CG | 12.05 | 124.65 | 112.60 |
| 6 | L | 370 | ASP | CB-CA-C | 12.05 | 134.39 | 110.42 |
| 10 | W | 248 | TRP | CB-CA-C | -12.04 | 87.23 | 110.10 |
| 6 | L | 370 | ASP | CA-CB-CG | 12.03 | 124.63 | 112.60 |
| 18 | e | 221 | ALA | CA-C-O | -12.02 | 109.27 | 119.36 |
| 21 | q | 56 | THR | CA-CB-CG2 | -12.01 | 90.08 | 110.50 |
| 14 | h | 195 | GLU | O-C-N | -11.97 | 113.38 | 121.88 |
| 1 | 0 | 975 | ILE | N-CA-C | -11.97 | 102.17 | 111.62 |
| 10 | U | 284 | LYS | N-CA-CB | 11.95 | 130.82 | 110.50 |
| 9 | S | 732 | TRP | CA-C-N | 11.94 | 136.28 | 120.28 |
| 9 | S | 732 | TRP | C-N-CA | 11.94 | 136.28 | 120.28 |
| 9 | Q | 222 | PHE | CA-CB-CG | 11.94 | 125.74 | 113.80 |
| 8 | N | 551 | ASN | N-CA-CB | 11.93 | 130.78 | 110.50 |
| 1 | Y | 269 | ASP | CA-CB-CG | 11.92 | 124.52 | 112.60 |
| 7 | O | 1438 | VAL | CA-C-O | -11.90 | 108.55 | 121.17 |
| 7 | M | 1188 | THR | N-CA-CB | 11.89 | 130.58 | 110.49 |
| 7 | O | 1602 | VAL | N-CA-CB | 11.87 | 119.71 | 110.45 |
| 9 | Q | 790 | ASN | N-CA-C | -11.85 | 98.82 | 113.28 |
| 5 | B | 323 | LEU | N-CA-CB | 11.81 | 130.45 | 110.49 |
| 1 | Y | 104 | ALA | CA-C-N | 11.80 | 133.04 | 119.94 |
| 1 | Y | 104 | ALA | C-N-CA | 11.80 | 133.04 | 119.94 |
| 1 | 0 | 1257 | GLN | N-CA-C | 11.80 | 144.04 | 111.00 |
| 11 | V | 302 | ARG | CB-CA-C | 11.78 | 132.49 | 110.10 |
| 7 | M | 759 | ASP | CA-CB-CG | -11.78 | 100.82 | 112.60 |
| 5 | B | 323 | LEU | N-CA-C | 11.77 | 135.88 | 110.80 |
| 1 | Y | 791 | MET | CA-C-O | -11.76 | 100.81 | 120.80 |
| 9 | Q | 767 | ILE | N-CA-C | -11.74 | 101.62 | 112.90 |
| 6 | L | 343 | ASP | CA-CB-CG | 11.74 | 124.34 | 112.60 |
| 1 | 0 | 145 | PHE | CA-CB-CG | -11.74 | 102.06 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 11 | X | 402 | ASN | CB-CA-C | 11.74 | 132.40 | 110.10 |
| 21 | t | 55 | ASN | CA-CB-CG | -11.73 | 100.87 | 112.60 |
| 7 | O | 1188 | THR | CB-CA-C | -11.73 | 87.08 | 110.42 |
| 9 | R | 743 | ASP | CA-CB-CG | 11.71 | 124.31 | 112.60 |
| 14 | h | 807 | ILE | N-CA-C | -11.71 | 101.64 | 113.47 |
| 5 | B | 318 | GLU | N-CA-CB | 11.70 | 130.27 | 110.49 |
| 10 | W | 249 | ASP | CB-CA-C | 11.69 | 133.68 | 110.42 |
| 2 | 1 | 921 | SER | N-CA-CB | 11.68 | 130.35 | 110.50 |
| 21 | p | 56 | THR | CB-CA-C | 11.67 | 133.64 | 110.42 |
| 7 | M | 824 | ALA | CA-C-N | 11.66 | 129.66 | 120.33 |
| 7 | M | 824 | ALA | C-N-CA | 11.66 | 129.66 | 120.33 |
| 9 | T | 514 | LYS | N-CA-C | 11.65 | 135.62 | 110.80 |
| 8 | P | 372 | ASP | CA-CB-CG | 11.64 | 124.24 | 112.60 |
| 15 | b | 695 | ILE | N-CA-C | -11.61 | 101.14 | 112.17 |
| 21 | r | 56 | THR | CB-CA-C | 11.61 | 133.52 | 110.42 |
| 8 | N | 896 | PHE | CA-CB-CG | -11.60 | 102.20 | 113.80 |
| 20 | g | 609 | VAL | N-CA-C | -11.59 | 101.36 | 112.83 |
| 4 | G | 726 | VAL | N-CA-CB | 11.55 | 130.28 | 111.23 |
| 8 | N | 1072 | TYR | N-CA-C | -11.55 | 99.30 | 113.50 |
| 14 | a | 343 | ASN | N-CA-C | -11.54 | 97.05 | 113.21 |
| 20 | g | 950 | ASN | CA-CB-CG | -11.54 | 101.06 | 112.60 |
| 9 | Q | 425 | ILE | O-C-N | -11.47 | 111.36 | 121.57 |
| 8 | N | 257 | LEU | CB-CA-C | 11.46 | 133.23 | 110.42 |
| 2 | Z | 679 | SER | N-CA-CB | 11.45 | 129.85 | 110.49 |
| 8 | N | 1420 | VAL | N-CA-C | -11.45 | 102.83 | 113.71 |
| 15 | b | 61 | ASN | CA-CB-CG | -11.41 | 101.19 | 112.60 |
| 21 | o | 56 | THR | CA-CB-OG1 | 11.40 | 126.71 | 109.60 |
| 14 | a | 535 | ILE | N-CA-C | 11.40 | 121.37 | 110.42 |
| 8 | P | 577 | MET | CB-CA-C | 11.38 | 131.73 | 110.10 |
| 7 | O | 1299 | ASN | O-C-N | 11.38 | 133.79 | 122.07 |
| 20 | n | 908 | VAL | N-CA-C | -11.37 | 102.07 | 113.10 |
| 8 | N | 997 | VAL | N-CA-C | -11.37 | 102.91 | 113.71 |
| 8 | P | 1095 | GLU | CB-CA-C | 11.37 | 133.04 | 110.42 |
| 7 | M | 1138 | PHE | N-CA-CB | -11.34 | 91.32 | 110.49 |
| 1 | 0 | 920 | GLU | CA-C-N | 11.32 | 132.45 | 120.00 |
| 1 | 0 | 920 | GLU | C-N-CA | 11.32 | 132.45 | 120.00 |
| 9 | T | 514 | LYS | CB-CA-C | -11.30 | 87.94 | 110.42 |
| 11 | V | 302 | ARG | N-CA-C | -11.29 | 79.38 | 111.00 |
| 20 | g | 753 | PHE | N-CA-C | -11.28 | 98.96 | 113.17 |
| 8 | N | 1487 | PHE | CA-CB-CG | -11.26 | 102.54 | 113.80 |
| 7 | O | 36 | ASN | CA-CB-CG | 11.26 | 123.86 | 112.60 |
| 8 | P | 576 | TYR | N-CA-CB | 11.23 | 129.47 | 110.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | R | 758 | GLN | N-CA-C | -11.22 | 98.01 | 112.93 |
| 8 | N | 132 | ASN | CB-CA-C | 11.22 | 132.74 | 110.42 |
| 20 | n | 634 | VAL | N-CA-C | -11.21 | 101.21 | 113.43 |
| 20 | g | 288 | ASN | CA-CB-CG | -11.20 | 101.40 | 112.60 |
| 7 | M | 1273 | LYS | N-CA-CB | 11.17 | 129.37 | 110.49 |
| 7 | O | 510 | PHE | CA-CB-CG | 11.17 | 124.97 | 113.80 |
| 9 | R | 99 | ASN | CA-C-N | 11.13 | 131.84 | 120.38 |
| 9 | R | 99 | ASN | C-N-CA | 11.13 | 131.84 | 120.38 |
| 8 | N | 1095 | GLU | CB-CA-C | 11.12 | 132.55 | 110.42 |
| 16 | c | 186 | ASP | CA-C-O | 11.12 | 132.26 | 120.36 |
| 2 | 1 | 797 | ALA | CA-C-N | 11.10 | 135.16 | 120.28 |
| 2 | 1 | 797 | ALA | C-N-CA | 11.10 | 135.16 | 120.28 |
| 9 | R | 672 | GLN | OE1-CD-NE2 | -11.09 | 111.51 | 122.60 |
| 9 | Q | 754 | ARG | N-CA-C | -11.09 | 87.19 | 110.80 |
| 6 | I | 439 | ILE | N-CA-C | -11.07 | 102.27 | 112.90 |
| 2 | Z | 922 | LYS | CA-C-O | -11.06 | 104.69 | 120.51 |
| 12 | u | 247 | ARG | CA-C-O | -11.04 | 109.23 | 120.82 |
| 6 | I | 350 | PHE | CA-CB-CG | 11.04 | 124.83 | 113.80 |
| 5 | B | 415 | LEU | N-CA-C | -11.02 | 99.50 | 113.16 |
| 10 | U | 248 | TRP | CB-CA-C | -11.01 | 89.19 | 110.10 |
| 21 | r | 54 | GLY | CA-C-N | 11.00 | 142.55 | 121.54 |
| 21 | r | 54 | GLY | C-N-CA | 11.00 | 142.55 | 121.54 |
| 7 | O | 167 | ILE | N-CA-C | -11.00 | 102.10 | 111.56 |
| 19 | f | 695 | ALA | CA-C-N | 10.99 | 136.32 | 120.71 |
| 19 | f | 695 | ALA | C-N-CA | 10.99 | 136.32 | 120.71 |
| 15 | i | 365 | ILE | CA-C-O | -10.99 | 112.70 | 119.51 |
| 18 | e | 120 | HIS | CA-CB-CG | 10.99 | 124.79 | 113.80 |
| 7 | M | 1657 | ASP | O-C-N | 10.99 | 127.85 | 120.27 |
| 15 | b | 465 | MET | N-CA-C | -10.97 | 99.62 | 113.23 |
| 2 | Z | 891 | ARG | CB-CA-C | 10.96 | 130.93 | 110.10 |
| 2 | 1 | 745 | ILE | CA-CB-CG1 | 10.95 | 129.02 | 110.40 |
| 7 | O | 246 | VAL | N-CA-C | -10.92 | 100.65 | 113.42 |
| 1 | 0 | 1258 | LEU | N-CA-CB | 10.90 | 128.90 | 110.49 |
| 21 | p | 56 | THR | CA-CB-OG1 | 10.88 | 125.93 | 109.60 |
| 18 | l | 30 | ASP | CA-CB-CG | 10.88 | 123.48 | 112.60 |
| 9 | S | 621 | HIS | CA-CB-CG | -10.87 | 102.93 | 113.80 |
| 10 | W | 248 | TRP | N-CA-C | 10.86 | 141.41 | 111.00 |
| 7 | M | 210 | LYS | CA-C-N | 10.84 | 134.53 | 120.44 |
| 7 | M | 210 | LYS | C-N-CA | 10.84 | 134.53 | 120.44 |
| 8 | P | 1594 | ASP | CA-CB-CG | 10.83 | 123.43 | 112.60 |
| 7 | M | 705 | ASP | CA-CB-CG | 10.83 | 123.43 | 112.60 |
| 5 | K | 318 | GLU | CB-CA-C | -10.82 | 88.88 | 110.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | Q | 289 | LEU | N-CA-C | -10.82 | 100.57 | 113.88 |
| 1 | Y | 852 | PHE | CA-CB-CG | 10.80 | 124.60 | 113.80 |
| 2 | Z | 724 | TRP | N-CA-C | -10.80 | 99.94 | 113.55 |
| 12 | u | 379 | ASN | CA-CB-CG | 10.80 | 123.40 | 112.60 |
| 9 | Q | 753 | ALA | N-CA-CB | 10.79 | 126.59 | 110.40 |
| 11 | V | 385 | ILE | N-CA-C | -10.79 | 100.34 | 109.19 |
| 15 | i | 655 | PHE | CA-CB-CG | -10.79 | 103.02 | 113.80 |
| 1 | 0 | 702 | PHE | CA-CB-CG | -10.77 | 103.03 | 113.80 |
| 5 | K | 319 | THR | N-CA-C | -10.76 | 87.88 | 110.80 |
| 8 | N | 1434 | ASN | CA-CB-CG | -10.75 | 101.85 | 112.60 |
| 14 | a | 739 | PHE | CA-CB-CG | -10.75 | 103.05 | 113.80 |
| 19 | f | 222 | VAL | N-CA-C | -10.75 | 103.19 | 111.90 |
| 12 | v | 239 | SER | CA-C-N | 10.75 | 134.68 | 120.28 |
| 12 | v | 239 | SER | C-N-CA | 10.75 | 134.68 | 120.28 |
| 14 | h | 682 | ASP | CA-CB-CG | -10.75 | 101.85 | 112.60 |
| 2 | Z | 970 | PHE | CA-CB-CG | 10.75 | 124.55 | 113.80 |
| 5 | H | 323 | LEU | N-CA-C | 10.73 | 133.65 | 110.80 |
| 6 | I | 369 | LEU | N-CA-CB | 10.72 | 128.73 | 110.50 |
| 7 | O | 1601 | ILE | CA-C-N | 10.72 | 128.90 | 120.33 |
| 7 | O | 1601 | ILE | C-N-CA | 10.72 | 128.90 | 120.33 |
| 9 | S | 742 | LEU | CA-C-N | 10.71 | 137.57 | 122.36 |
| 9 | S | 742 | LEU | C-N-CA | 10.71 | 137.57 | 122.36 |
| 16 | c | 280 | ILE | N-CA-CB | 10.70 | 123.06 | 110.55 |
| 14 | a | 953 | LEU | N-CA-C | 10.70 | 122.94 | 111.28 |
| 7 | M | 1242 | MET | CA-C-N | 10.69 | 135.99 | 120.38 |
| 7 | M | 1242 | MET | C-N-CA | 10.69 | 135.99 | 120.38 |
| 8 | N | 257 | LEU | N-CA-C | -10.68 | 88.06 | 110.80 |
| 6 | I | 386 | ASP | CA-CB-CG | -10.67 | 101.93 | 112.60 |
| 8 | N | 383 | LEU | CA-C-N | 10.67 | 134.58 | 120.28 |
| 8 | N | 383 | LEU | C-N-CA | 10.67 | 134.58 | 120.28 |
| 9 | T | 130 | ASN | CA-C-N | 10.66 | 131.97 | 120.03 |
| 9 | T | 130 | ASN | C-N-CA | 10.66 | 131.97 | 120.03 |
| 9 | T | 234 | ILE | CA-C-O | 10.66 | 128.28 | 118.90 |
| 10 | U | 248 | TRP | N-CA-C | 10.65 | 140.82 | 111.00 |
| 1 | Y | 831 | LYS | N-CA-CB | 10.63 | 128.56 | 110.50 |
| 20 | n | 681 | ILE | N-CA-C | -10.62 | 103.23 | 111.62 |
| 7 | O | 1398 | SER | CA-C-N | 10.60 | 134.66 | 120.77 |
| 7 | O | 1398 | SER | C-N-CA | 10.60 | 134.66 | 120.77 |
| 1 | 0 | 419 | LYS | CA-C-N | 10.59 | 141.03 | 121.97 |
| 1 | 0 | 419 | LYS | C-N-CA | 10.59 | 141.03 | 121.97 |
| 7 | O | 897 | ASP | CA-CB-CG | 10.59 | 123.19 | 112.60 |
| 8 | N | 551 | ASN | CB-CA-C | 10.59 | 130.22 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | v | 55 | HIS | CA-CB-CG | 10.59 | 124.39 | 113.80 |
| 9 | T | 753 | ALA | N-CA-C | 10.56 | 140.56 | 111.00 |
| 8 | N | 1210 | LEU | CA-C-N | 10.55 | 133.86 | 120.56 |
| 8 | N | 1210 | LEU | C-N-CA | 10.55 | 133.86 | 120.56 |
| 6 | I | 370 | ASP | CA-C-O | -10.55 | 105.43 | 120.51 |
| 9 | T | 753 | ALA | N-CA-CB | 10.55 | 126.22 | 110.40 |
| 7 | M | 1137 | ASN | N-CA-CB | 10.53 | 128.40 | 110.50 |
| 10 | W | 304 | LYS | N-CA-C | 10.50 | 140.41 | 111.00 |
| 2 | 1 | 925 | ARG | NE-CZ-NH1 | 10.50 | 132.00 | 121.50 |
| 7 | O | 23 | ASP | CA-CB-CG | 10.49 | 123.09 | 112.60 |
| 2 | Z | 573 | LEU | N-CA-C | -10.45 | 99.28 | 113.18 |
| 15 | i | 480 | GLU | N-CA-C | -10.45 | 99.40 | 112.88 |
| 7 | M | 1272 | LEU | CB-CA-C | -10.45 | 90.25 | 110.10 |
| 8 | P | 997 | VAL | N-CA-C | -10.45 | 103.29 | 113.53 |
| 9 | T | 101 | PRO | N-CA-CB | 10.42 | 113.11 | 102.17 |
| 9 | Q | 601 | PRO | CA-C-N | 10.41 | 131.12 | 120.60 |
| 9 | Q | 601 | PRO | C-N-CA | 10.41 | 131.12 | 120.60 |
| 6 | F | 304 | LEU | CA-C-N | 10.39 | 133.65 | 120.56 |
| 6 | F | 304 | LEU | C-N-CA | 10.39 | 133.65 | 120.56 |
| 15 | b | 142 | ALA | CA-C-O | -10.38 | 113.85 | 119.77 |
| 2 | 1 | 728 | VAL | N-CA-C | -10.38 | 102.94 | 112.90 |
| 9 | S | 743 | ASP | CA-CB-CG | 10.38 | 122.98 | 112.60 |
| 8 | N | 257 | LEU | CA-C-O | -10.37 | 105.69 | 120.51 |
| 15 | i | 576 | PHE | CA-CB-CG | -10.37 | 103.44 | 113.80 |
| 16 | j | 133 | ASP | CA-CB-CG | -10.36 | 102.24 | 112.60 |
| 17 | d | 144 | HIS | CA-CB-CG | -10.36 | 103.44 | 113.80 |
| 8 | N | 132 | ASN | CA-CB-CG | 10.33 | 122.93 | 112.60 |
| 19 | f | 660 | THR | O-C-N | -10.33 | 111.29 | 120.48 |
| 7 | O | 602 | ASN | N-CA-CB | 10.32 | 128.05 | 110.50 |
| 20 | n | 710 | ILE | N-CA-C | -10.32 | 102.18 | 113.43 |
| 7 | M | 1613 | VAL | N-CA-C | -10.31 | 102.73 | 111.91 |
| 2 | 1 | 308 | ASN | N-CA-CB | 10.29 | 127.86 | 110.46 |
| 2 | Z | 657 | ILE | N-CA-C | -10.28 | 103.48 | 112.12 |
| 20 | g | 668 | ASN | CA-CB-CG | -10.28 | 102.32 | 112.60 |
| 7 | O | 602 | ASN | N-CA-C | 10.27 | 139.77 | 111.00 |
| 8 | N | 1534 | TYR | N-CA-C | 10.26 | 122.22 | 111.14 |
| 5 | B | 355 | PHE | N-CA-C | -10.24 | 98.74 | 112.26 |
| 1 | Y | 1257 | GLN | CB-CA-C | -10.23 | 90.66 | 110.10 |
| 10 | W | 249 | ASP | CA-CB-CG | 10.23 | 122.83 | 112.60 |
| 15 | i | 102 | LYS | N-CA-C | -10.21 | 101.38 | 114.04 |
| 12 | u | 266 | ARG | NE-CZ-NH1 | 10.21 | 131.71 | 121.50 |
| 14 | a | 442 | TYR | CA-C-N | 10.20 | 133.71 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | a | 442 | TYR | C-N-CA | 10.20 | 133.71 | 120.44 |
| 14 | h | 578 | ASP | CA-CB-CG | 10.19 | 122.79 | 112.60 |
| 4 | A | 808 | ASP | CA-CB-CG | 10.19 | 122.79 | 112.60 |
| 20 | n | 609 | VAL | N-CA-C | -10.19 | 102.75 | 112.83 |
| 7 | M | 1587 | LEU | CA-C-N | 10.18 | 133.39 | 120.56 |
| 7 | M | 1587 | LEU | C-N-CA | 10.18 | 133.39 | 120.56 |
| 14 | h | 695 | TYR | N-CA-C | -10.18 | 98.33 | 113.61 |
| 2 | 1 | 404 | PHE | CA-CB-CG | 10.18 | 123.98 | 113.80 |
| 7 | O | 1603 | PRO | N-CA-CB | 10.18 | 113.94 | 103.25 |
| 2 | 1 | 921 | SER | CB-CA-C | -10.17 | 90.77 | 110.10 |
| 16 | j | 441 | ARG | N-CA-C | -10.17 | 98.99 | 108.75 |
| 20 | n | 142 | PHE | CA-CB-CG | -10.17 | 103.63 | 113.80 |
| 7 | M | 1189 | MET | N-CA-C | -10.16 | 89.15 | 110.80 |
| 10 | W | 305 | TYR | N-CA-C | -10.16 | 87.35 | 109.81 |
| 16 | c | 583 | SER | N-CA-CB | 10.16 | 127.65 | 110.49 |
| 9 | S | 560 | ILE | N-CA-C | -10.15 | 102.53 | 112.17 |
| 8 | P | 940 | SER | N-CA-C | -10.14 | 99.15 | 114.16 |
| 20 | n | 1055 | ASP | N-CA-CB | 10.14 | 127.62 | 110.49 |
| 9 | R | 771 | ILE | CA-C-O | -10.13 | 110.24 | 118.85 |
| 14 | a | 284 | ASN | CA-CB-CG | -10.12 | 102.47 | 112.60 |
| 4 | G | 790 | ASN | CA-CB-CG | 10.12 | 122.72 | 112.60 |
| 15 | i | 218 | GLU | CA-C-O | -10.11 | 109.75 | 120.87 |
| 15 | b | 713 | ILE | N-CA-C | -10.11 | 101.26 | 111.77 |
| 8 | N | 131 | ASP | N-CA-CB | 10.11 | 127.68 | 110.50 |
| 7 | M | 1272 | LEU | N-CA-C | -10.11 | 82.70 | 111.00 |
| 20 | n | 874 | PHE | CA-CB-CG | 10.10 | 123.90 | 113.80 |
| 8 | N | 576 | TYR | N-CA-C | 10.09 | 125.46 | 108.20 |
| 8 | P | 889 | THR | N-CA-C | -10.09 | 101.52 | 114.04 |
| 1 | Y | 831 | LYS | N-CA-C | 10.09 | 139.26 | 111.00 |
| 8 | N | 935 | VAL | N-CA-CB | 10.09 | 119.91 | 111.64 |
| 2 | Z | 650 | LYS | N-CA-CB | 10.08 | 127.52 | 110.49 |
| 2 | Z | 656 | HIS | N-CA-C | -10.08 | 99.25 | 114.16 |
| 16 | j | 322 | ILE | N-CA-C | -10.08 | 92.86 | 107.77 |
| 8 | P | 50 | ASN | CA-CB-CG | -10.07 | 102.53 | 112.60 |
| 12 | v | 545 | LEU | CA-C-N | 10.06 | 131.15 | 119.98 |
| 12 | v | 545 | LEU | C-N-CA | 10.06 | 131.15 | 119.98 |
| 14 | h | 128 | PHE | N-CA-C | -10.06 | 93.93 | 109.52 |
| 12 | u | 27 | PHE | CA-CB-CG | 10.06 | 123.86 | 113.80 |
| 2 | Z | 589 | VAL | N-CA-C | -10.05 | 104.16 | 113.71 |
| 7 | O | 668 | ARG | NE-CZ-NH2 | 10.04 | 128.24 | 119.20 |
| 6 | F | 370 | ASP | CA-C-O | -10.04 | 106.15 | 120.51 |
| 9 | Q | 621 | HIS | CE1-NE2-CD2 | -10.03 | 98.97 | 109.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 602 | ASN | CB-CA-C | -10.02 | 91.07 | 110.10 |
| 14 | h | 871 | HIS | CA-CB-CG | 10.00 | 123.80 | 113.80 |
| 19 | m | 42 | PHE | CA-CB-CG | 9.99 | 123.79 | 113.80 |
| 1 | Y | 1335 | VAL | O-C-N | 9.98 | 132.18 | 122.20 |
| 9 | S | 666 | SER | N-CA-C | -9.98 | 103.25 | 114.62 |
| 14 | h | 100 | ALA | CA-C-N | 9.98 | 135.81 | 120.75 |
| 14 | h | 100 | ALA | C-N-CA | 9.98 | 135.81 | 120.75 |
| 5 | B | 324 | TYR | CB-CA-C | 9.97 | 130.27 | 110.42 |
| 2 | 1 | 308 | ASN | CA-CB-CG | 9.96 | 122.56 | 112.60 |
| 2 | 1 | 1186 | ASP | CA-CB-CG | 9.96 | 122.56 | 112.60 |
| 9 | S | 232 | PHE | CA-CB-CG | 9.96 | 123.76 | 113.80 |
| 1 | 0 | 1286 | ASP | CA-C-N | 9.96 | 134.91 | 120.38 |
| 1 | 0 | 1286 | ASP | C-N-CA | 9.96 | 134.91 | 120.38 |
| 8 | P | 1224 | ASP | N-CA-C | -9.95 | 101.70 | 114.04 |
| 8 | P | 477 | LEU | N-CA-C | 9.95 | 122.13 | 111.28 |
| 2 | Z | 126 | SER | CA-C-N | 9.95 | 135.28 | 121.05 |
| 2 | Z | 126 | SER | C-N-CA | 9.95 | 135.28 | 121.05 |
| 15 | i | 366 | PRO | N-CA-CB | 9.95 | 110.12 | 102.36 |
| 20 | g | 237 | MET | N-CA-C | -9.95 | 99.96 | 114.39 |
| 7 | O | 1356 | LEU | CA-C-N | 9.95 | 134.60 | 120.28 |
| 7 | O | 1356 | LEU | C-N-CA | 9.95 | 134.60 | 120.28 |
| 2 | Z | 915 | LYS | N-CA-CB | 9.94 | 127.29 | 110.49 |
| 5 | H | 292 | VAL | N-CA-C | -9.94 | 102.95 | 112.29 |
| 12 | u | 86 | ASN | CA-CB-CG | 9.93 | 122.53 | 112.60 |
| 2 | 1 | 110 | ILE | CA-C-N | 9.92 | 134.59 | 120.79 |
| 2 | 1 | 110 | ILE | C-N-CA | 9.92 | 134.59 | 120.79 |
| 10 | W | 284 | LYS | CB-CA-C | 9.92 | 128.95 | 110.10 |
| 20 | n | 891 | ILE | N-CA-C | -9.92 | 101.72 | 110.74 |
| 8 | N | 895 | HIS | CA-CB-CG | 9.91 | 123.71 | 113.80 |
| 9 | R | 103 | ILE | N-CA-CB | 9.90 | 121.33 | 110.53 |
| 16 | j | 165 | VAL | CA-C-N | 9.90 | 129.42 | 119.92 |
| 16 | j | 165 | VAL | C-N-CA | 9.90 | 129.42 | 119.92 |
| 7 | O | 25 | PHE | CA-CB-CG | 9.87 | 123.67 | 113.80 |
| 1 | Y | 1086 | ASN | CA-C-N | 9.87 | 130.90 | 119.94 |
| 1 | Y | 1086 | ASN | C-N-CA | 9.87 | 130.90 | 119.94 |
| 6 | L | 436 | LEU | N-CA-C | -9.86 | 101.00 | 113.43 |
| 14 | h | 739 | PHE | N-CA-C | -9.85 | 101.49 | 112.72 |
| 15 | i | 502 | MET | N-CA-C | 9.85 | 122.10 | 111.36 |
| 20 | n | 1033 | VAL | CA-C-N | 9.85 | 133.48 | 120.28 |
| 20 | n | 1033 | VAL | C-N-CA | 9.85 | 133.48 | 120.28 |
| 15 | b | 94 | ARG | NE-CZ-NH2 | 9.85 | 128.06 | 119.20 |
| 14 | h | 441 | GLU | N-CA-C | -9.85 | 100.12 | 112.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | A | 654 | HIS | ND1-CE1-NE2 | 9.84 | 118.23 | 108.40 |
| 19 | m | 477 | ARG | NE-CZ-NH2 | -9.83 | 110.35 | 119.20 |
| 10 | U | 249 | ASP | CA-CB-CG | 9.82 | 122.42 | 112.60 |
| 6 | F | 372 | PHE | CA-C-N | 9.81 | 133.43 | 120.28 |
| 6 | F | 372 | PHE | C-N-CA | 9.81 | 133.43 | 120.28 |
| 6 | L | 378 | HIS | CE1-NE2-CD2 | -9.81 | 99.19 | 109.00 |
| 7 | M | 268 | ILE | CB-CA-C | 9.81 | 123.62 | 111.65 |
| 7 | M | 1188 | THR | N-CA-C | 9.81 | 131.69 | 110.80 |
| 7 | M | 1523 | PHE | CA-C-N | 9.81 | 133.43 | 120.28 |
| 7 | M | 1523 | PHE | C-N-CA | 9.81 | 133.43 | 120.28 |
| 7 | M | 25 | PHE | N-CA-C | -9.81 | 100.16 | 113.30 |
| 7 | O | 1138 | PHE | CA-C-O | -9.80 | 106.50 | 120.51 |
| 1 | Y | 250 | ALA | CA-C-N | 9.79 | 136.65 | 122.35 |
| 1 | Y | 250 | ALA | C-N-CA | 9.79 | 136.65 | 122.35 |
| 5 | B | 324 | TYR | CA-C-O | 9.79 | 134.50 | 120.51 |
| 9 | S | 67 | THR | CA-C-N | 9.78 | 133.39 | 120.28 |
| 9 | S | 67 | THR | C-N-CA | 9.78 | 133.39 | 120.28 |
| 21 | t | 91 | THR | N-CA-C | -9.78 | 94.54 | 109.41 |
| 4 | J | 753 | GLU | CA-C-N | 9.78 | 133.38 | 120.28 |
| 4 | J | 753 | GLU | C-N-CA | 9.78 | 133.38 | 120.28 |
| 8 | P | 639 | PHE | CA-CB-CG | 9.78 | 123.58 | 113.80 |
| 21 | o | 11 | VAL | O-C-N | -9.77 | 111.96 | 122.81 |
| 7 | O | 1475 | ILE | N-CA-C | -9.77 | 100.35 | 111.00 |
| 2 | Z | 915 | LYS | CB-CA-C | -9.77 | 90.98 | 110.42 |
| 20 | n | 343 | SER | N-CA-CB | 9.76 | 126.99 | 110.49 |
| 10 | W | 304 | LYS | CB-CA-C | -9.76 | 91.55 | 110.10 |
| 14 | h | 645 | GLU | CB-CG-CD | -9.76 | 96.00 | 112.60 |
| 2 | 1 | 226 | THR | CA-C-O | -9.76 | 109.26 | 121.46 |
| 1 | Y | 1022 | ASP | N-CA-C | 9.75 | 131.56 | 110.80 |
| 12 | v | 681 | ASP | N-CA-C | 9.74 | 121.90 | 111.28 |
| 2 | Z | 547 | ILE | N-CA-C | -9.74 | 103.98 | 113.53 |
| 2 | 1 | 921 | SER | N-CA-C | 9.73 | 138.25 | 111.00 |
| 5 | E | 397 | ARG | N-CA-C | 9.73 | 122.89 | 111.71 |
| 6 | L | 369 | LEU | N-CA-C | 9.72 | 138.22 | 111.00 |
| 19 | m | 37 | ASN | CA-CB-CG | 9.72 | 122.32 | 112.60 |
| 14 | a | 855 | GLU | CA-C-O | 9.72 | 129.11 | 119.97 |
| 1 | Y | 441 | VAL | CA-C-N | 9.72 | 130.77 | 119.98 |
| 1 | Y | 441 | VAL | C-N-CA | 9.72 | 130.77 | 119.98 |
| 9 | T | 459 | LEU | N-CA-C | -9.72 | 99.24 | 112.94 |
| 17 | k | 231 | CYS | N-CA-C | -9.72 | 93.06 | 108.90 |
| 7 | O | 523 | ARG | NE-CZ-NH2 | -9.71 | 110.46 | 119.20 |
| 14 | h | 156 | TYR | O-C-N | -9.70 | 112.37 | 123.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | G | 802 | ASP | CA-CB-CG | 9.70 | 122.30 | 112.60 |
| 1 | 0 | 178 | GLU | N-CA-C | -9.69 | 102.25 | 114.56 |
| 1 | 0 | 1022 | ASP | CB-CA-C | 9.69 | 129.70 | 110.42 |
| 5 | B | 318 | GLU | N-CA-C | 9.67 | 131.41 | 110.80 |
| 13 | w | 1224 | GLU | CA-C-N | 9.67 | 133.24 | 120.28 |
| 13 | w | 1224 | GLU | C-N-CA | 9.67 | 133.24 | 120.28 |
| 9 | R | 100 | PRO | N-CA-CB | 9.67 | 112.46 | 103.08 |
| 10 | W | 305 | TYR | CB-CA-C | 9.66 | 129.21 | 110.17 |
| 1 | 0 | 1386 | PRO | N-CA-CB | 9.66 | 111.44 | 103.32 |
| 6 | F | 288 | VAL | CA-C-N | 9.66 | 133.58 | 120.44 |
| 6 | F | 288 | VAL | C-N-CA | 9.66 | 133.58 | 120.44 |
| 1 | Y | 459 | ALA | O-C-N | 9.66 | 134.69 | 122.81 |
| 2 | 1 | 768 | ILE | N-CA-C | -9.65 | 101.35 | 113.22 |
| 7 | M | 437 | ASP | CA-CB-CG | 9.65 | 122.25 | 112.60 |
| 9 | T | 134 | LYS | N-CA-C | 9.64 | 121.39 | 111.07 |
| 5 | B | 322 | ILE | CA-C-N | 9.64 | 139.96 | 121.54 |
| 5 | B | 322 | ILE | C-N-CA | 9.64 | 139.96 | 121.54 |
| 7 | M | 1175 | SER | N-CA-C | 9.64 | 122.78 | 111.02 |
| 8 | P | 289 | TYR | N-CA-CB | 9.62 | 126.76 | 110.49 |
| 14 | h | 834 | ARG | N-CA-C | 9.62 | 121.85 | 111.36 |
| 1 | Y | 205 | ASP | N-CA-CB | 9.62 | 126.03 | 110.16 |
| 1 | 0 | 846 | ILE | N-CA-C | -9.61 | 104.58 | 113.71 |
| 19 | m | 373 | THR | CA-C-O | 9.61 | 134.25 | 120.51 |
| 7 | M | 1581 | THR | CA-C-N | 9.60 | 132.92 | 120.44 |
| 7 | M | 1581 | THR | C-N-CA | 9.60 | 132.92 | 120.44 |
| 9 | T | 232 | PHE | CA-CB-CG | -9.60 | 104.20 | 113.80 |
| 20 | g | 941 | ILE | N-CA-C | -9.60 | 103.36 | 112.96 |
| 19 | f | 718 | VAL | O-C-N | 9.59 | 131.17 | 121.87 |
| 7 | M | 501 | SER | N-CA-C | -9.58 | 101.26 | 113.72 |
| 21 | q | 55 | ASN | N-CA-CB | 9.58 | 126.67 | 110.49 |
| 6 | I | 372 | PHE | CA-CB-CG | 9.57 | 123.37 | 113.80 |
| 9 | Q | 754 | ARG | CB-CA-C | 9.57 | 129.47 | 110.42 |
| 2 | Z | 140 | ARG | N-CA-C | -9.57 | 99.11 | 110.41 |
| 9 | Q | 97 | GLU | CA-C-O | 9.57 | 128.11 | 118.73 |
| 5 | K | 392 | LEU | CA-C-N | 9.57 | 135.64 | 122.34 |
| 5 | K | 392 | LEU | C-N-CA | 9.57 | 135.64 | 122.34 |
| 8 | N | 1309 | ARG | NE-CZ-NH2 | 9.57 | 127.81 | 119.20 |
| 1 | 0 | 1422 | SER | CA-C-N | 9.56 | 132.87 | 120.44 |
| 1 | 0 | 1422 | SER | C-N-CA | 9.56 | 132.87 | 120.44 |
| 2 | 1 | 277 | ALA | N-CA-C | -9.56 | 99.98 | 112.41 |
| 21 | p | 54 | GLY | CA-C-N | 9.55 | 136.45 | 121.26 |
| 21 | p | 54 | GLY | C-N-CA | 9.55 | 136.45 | 121.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 909 | PHE | CA-CB-CG | -9.55 | 104.25 | 113.80 |
| 9 | Q | 825 | PRO | CA-C-N | 9.54 | 134.02 | 120.28 |
| 9 | Q | 825 | PRO | C-N-CA | 9.54 | 134.02 | 120.28 |
| 1 | Y | 130 | GLY | CA-C-N | 9.53 | 133.28 | 120.50 |
| 1 | Y | 130 | GLY | C-N-CA | 9.53 | 133.28 | 120.50 |
| 2 | Z | 1357 | LEU | N-CA-C | -9.53 | 101.78 | 113.41 |
| 7 | O | 1221 | LEU | N-CA-C | -9.53 | 94.46 | 109.23 |
| 19 | m | 694 | VAL | N-CA-C | -9.53 | 103.12 | 112.17 |
| 9 | T | 98 | PRO | N-CA-CB | 9.53 | 113.81 | 103.33 |
| 9 | Q | 223 | ASN | CA-CB-CG | 9.52 | 122.12 | 112.60 |
| 2 | 1 | 1076 | ASP | CA-CB-CG | 9.52 | 122.12 | 112.60 |
| 14 | h | 71 | HIS | CB-CG-CD2 | -9.52 | 118.83 | 131.20 |
| 21 | r | 34 | LYS | N-CA-C | -9.52 | 103.77 | 114.62 |
| 7 | M | 846 | VAL | CA-C-N | 9.51 | 129.14 | 120.10 |
| 7 | M | 846 | VAL | C-N-CA | 9.51 | 129.14 | 120.10 |
| 9 | R | 543 | LYS | CA-C-N | 9.51 | 133.20 | 120.65 |
| 9 | R | 543 | LYS | C-N-CA | 9.51 | 133.20 | 120.65 |
| 9 | R | 515 | LEU | N-CA-C | -9.51 | 84.38 | 111.00 |
| 17 | d | 57 | TRP | N-CA-C | -9.51 | 99.11 | 112.13 |
| 15 | i | 308 | ASN | OD1-CG-ND2 | -9.50 | 113.10 | 122.60 |
| 1 | 0 | 1257 | GLN | N-CA-CB | 9.50 | 126.64 | 110.50 |
| 7 | M | 39 | THR | N-CA-C | -9.50 | 100.58 | 113.30 |
| 14 | a | 494 | PHE | CA-CB-CG | -9.49 | 104.31 | 113.80 |
| 7 | O | 725 | ASN | CA-CB-CG | 9.49 | 122.09 | 112.60 |
| 16 | j | 338 | LEU | CA-C-N | 9.49 | 133.00 | 120.28 |
| 16 | j | 338 | LEU | C-N-CA | 9.49 | 133.00 | 120.28 |
| 8 | N | 500 | LYS | N-CA-C | -9.49 | 99.60 | 112.03 |
| 20 | n | 656 | VAL | N-CA-C | -9.49 | 93.73 | 107.77 |
| 4 | D | 672 | GLY | CA-C-N | 9.48 | 130.50 | 119.98 |
| 4 | D | 672 | GLY | C-N-CA | 9.48 | 130.50 | 119.98 |
| 10 | U | 335 | MET | CA-C-N | 9.47 | 136.12 | 122.40 |
| 10 | U | 335 | MET | C-N-CA | 9.47 | 136.12 | 122.40 |
| 6 | L | 370 | ASP | N-CA-C | -9.46 | 90.64 | 110.80 |
| 7 | M | 1086 | LEU | N-CA-C | 9.46 | 121.59 | 111.28 |
| 7 | M | 659 | ASN | CA-CB-CG | -9.45 | 103.15 | 112.60 |
| 2 | 1 | 1299 | LYS | CA-C-N | 9.44 | 136.39 | 121.66 |
| 2 | 1 | 1299 | LYS | C-N-CA | 9.44 | 136.39 | 121.66 |
| 8 | N | 903 | LEU | CA-C-N | 9.44 | 132.94 | 120.28 |
| 8 | N | 903 | LEU | C-N-CA | 9.44 | 132.94 | 120.28 |
| 18 | l | 241 | ARG | N-CA-C | -9.44 | 92.86 | 108.34 |
| 8 | P | 299 | ASN | CA-C-N | 9.44 | 133.31 | 120.38 |
| 8 | P | 299 | ASN | C-N-CA | 9.44 | 133.31 | 120.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 831 | LYS | CB-CA-C | -9.44 | 92.17 | 110.10 |
| 7 | M | 750 | TRP | CA-C-O | -9.43 | 109.95 | 118.63 |
| 19 | m | 182 | LYS | O-C-N | 9.43 | 131.90 | 122.09 |
| 7 | M | 610 | SER | CA-C-O | -9.42 | 110.93 | 120.82 |
| 15 | b | 100 | THR | N-CA-C | -9.42 | 99.08 | 111.71 |
| 12 | v | 184 | ASP | CA-CB-CG | 9.42 | 122.02 | 112.60 |
| 9 | Q | 91 | GLN | N-CA-CB | 9.41 | 123.66 | 110.01 |
| 1 | Y | 852 | PHE | CA-C-N | 9.41 | 133.84 | 120.28 |
| 1 | Y | 852 | PHE | C-N-CA | 9.41 | 133.84 | 120.28 |
| 17 | d | 189 | SER | N-CA-C | -9.41 | 99.67 | 112.94 |
| 16 | j | 428 | ASN | N-CA-C | -9.40 | 102.38 | 114.04 |
| 10 | U | 248 | TRP | N-CA-CB | 9.40 | 126.48 | 110.50 |
| 10 | U | 330 | GLU | N-CA-C | -9.40 | 100.19 | 112.41 |
| 12 | u | 88 | ILE | N-CA-CB | 9.40 | 123.74 | 111.90 |
| 2 | 1 | 965 | GLY | O-C-N | 9.39 | 132.52 | 122.28 |
| 2 | 1 | 405 | LYS | N-CA-C | -9.39 | 90.79 | 110.80 |
| 8 | N | 593 | SER | CB-CA-C | 9.39 | 125.62 | 110.88 |
| 8 | P | 182 | PHE | CA-C-N | 9.38 | 139.47 | 121.54 |
| 8 | P | 182 | PHE | C-N-CA | 9.38 | 139.47 | 121.54 |
| 15 | i | 419 | PHE | CA-CB-CG | -9.39 | 104.41 | 113.80 |
| 1 | Y | 1158 | HIS | CA-CB-CG | 9.38 | 123.18 | 113.80 |
| 7 | M | 344 | ILE | N-CA-C | -9.38 | 103.55 | 112.83 |
| 9 | R | 504 | VAL | N-CA-C | 9.38 | 119.42 | 110.42 |
| 14 | a | 884 | GLU | N-CA-CB | 9.38 | 126.33 | 110.49 |
| 9 | T | 767 | ILE | N-CA-C | -9.37 | 104.01 | 113.10 |
| 2 | Z | 1188 | ARG | N-CA-C | -9.37 | 101.62 | 113.43 |
| 8 | N | 574 | HIS | CE1-NE2-CD2 | -9.36 | 99.64 | 109.00 |
| 1 | Y | 1274 | ASP | CA-CB-CG | 9.36 | 121.96 | 112.60 |
| 8 | N | 1224 | ASP | N-CA-C | -9.35 | 102.25 | 114.31 |
| 16 | j | 638 | ILE | N-CA-C | -9.34 | 101.67 | 111.58 |
| 8 | P | 1001 | ASN | CA-CB-CG | -9.34 | 103.26 | 112.60 |
| 2 | 1 | 916 | PHE | N-CA-C | -9.34 | 84.85 | 111.00 |
| 7 | M | 1362 | ASP | CA-CB-CG | 9.34 | 121.94 | 112.60 |
| 9 | T | 144 | LEU | CA-C-N | 9.34 | 132.57 | 120.44 |
| 9 | T | 144 | LEU | C-N-CA | 9.34 | 132.57 | 120.44 |
| 16 | c | 460 | ASN | N-CA-C | -9.33 | 101.19 | 111.36 |
| 1 | 0 | 1022 | ASP | N-CA-CB | 9.33 | 126.26 | 110.49 |
| 8 | N | 389 | PHE | CA-C-N | 9.33 | 134.10 | 121.23 |
| 8 | N | 389 | PHE | C-N-CA | 9.33 | 134.10 | 121.23 |
| 16 | c | 616 | VAL | CB-CA-C | -9.33 | 99.55 | 112.14 |
| 1 | 0 | 905 | GLU | CA-C-N | 9.32 | 130.25 | 120.00 |
| 1 | 0 | 905 | GLU | C-N-CA | 9.32 | 130.25 | 120.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 1440 | ASP | CA-C-N | 9.32 | 133.15 | 120.38 |
| 1 | 0 | 1440 | ASP | C-N-CA | 9.32 | 133.15 | 120.38 |
| 12 | v | 694 | ILE | CA-C-O | -9.32 | 111.29 | 121.17 |
| 1 | 0 | 1471 | ILE | CA-C-N | 9.31 | 132.61 | 120.60 |
| 1 | 0 | 1471 | ILE | C-N-CA | 9.31 | 132.61 | 120.60 |
| 20 | n | 1150 | TYR | N-CA-C | -9.31 | 99.66 | 114.09 |
| 15 | b | 569 | LYS | N-CA-C | -9.30 | 100.71 | 112.90 |
| 8 | P | 257 | LEU | CA-C-O | -9.30 | 107.22 | 120.51 |
| 20 | n | 776 | ASN | CA-CB-CG | 9.30 | 121.90 | 112.60 |
| 6 | I | 278 | GLU | CA-C-O | -9.29 | 111.13 | 120.70 |
| 14 | h | 734 | HIS | CA-CB-CG | -9.29 | 104.50 | 113.80 |
| 9 | R | 492 | ILE | CA-C-N | 9.29 | 132.73 | 120.28 |
| 9 | R | 492 | ILE | C-N-CA | 9.29 | 132.73 | 120.28 |
| 11 | V | 402 | ASN | CB-CA-C | 9.29 | 127.75 | 110.10 |
| 2 | 1 | 427 | THR | N-CA-C | -9.29 | 102.13 | 112.72 |
| 20 | n | 149 | SER | CA-C-N | 9.29 | 129.36 | 119.89 |
| 20 | n | 149 | SER | C-N-CA | 9.29 | 129.36 | 119.89 |
| 1 | 0 | 452 | MET | CA-C-N | 9.28 | 130.91 | 121.35 |
| 1 | 0 | 452 | MET | C-N-CA | 9.28 | 130.91 | 121.35 |
| 20 | g | 215 | GLU | CA-C-N | 9.28 | 128.93 | 119.56 |
| 20 | g | 215 | GLU | C-N-CA | 9.28 | 128.93 | 119.56 |
| 7 | O | 561 | CYS | CA-C-O | -9.28 | 111.08 | 120.82 |
| 8 | N | 1413 | ASN | CA-CB-CG | -9.28 | 103.33 | 112.60 |
| 12 | v | 642 | ASN | CA-C-N | 9.28 | 132.50 | 120.44 |
| 12 | v | 642 | ASN | C-N-CA | 9.28 | 132.50 | 120.44 |
| 21 | s | 16 | ILE | CA-C-O | 9.28 | 128.75 | 120.96 |
| 12 | u | 562 | ARG | CA-C-N | 9.27 | 132.50 | 120.44 |
| 12 | u | 562 | ARG | C-N-CA | 9.27 | 132.50 | 120.44 |
| 12 | u | 288 | ASN | CB-CA-C | 9.27 | 128.43 | 110.17 |
| 1 | 0 | 1209 | LYS | N-CA-C | 9.27 | 123.32 | 110.35 |
| 7 | O | 298 | ASP | CA-CB-CG | 9.27 | 121.86 | 112.60 |
| 5 | B | 390 | HIS | CG-CD2-NE2 | 9.26 | 116.46 | 107.20 |
| 7 | O | 66 | VAL | CA-C-N | 9.26 | 134.43 | 120.82 |
| 7 | O | 66 | VAL | C-N-CA | 9.26 | 134.43 | 120.82 |
| 7 | O | 21 | ASP | CA-CB-CG | 9.25 | 121.85 | 112.60 |
| 1 | Y | 1272 | GLN | N-CA-C | 9.25 | 122.35 | 111.71 |
| 16 | c | 187 | ASP | CA-C-N | 9.25 | 133.56 | 120.42 |
| 16 | c | 187 | ASP | C-N-CA | 9.25 | 133.56 | 120.42 |
| 2 | 1 | 853 | PHE | CA-CB-CG | 9.25 | 123.05 | 113.80 |
| 7 | M | 827 | ILE | N-CA-C | -9.24 | 102.79 | 111.48 |
| 9 | R | 242 | LEU | N-CA-C | -9.24 | 101.70 | 113.16 |
| 1 | Y | 772 | GLY | CA-C-N | 9.23 | 135.44 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 772 | GLY | C-N-CA | 9.23 | 135.44 | 120.30 |
| 7 | M | 1651 | ASP | CA-C-N | 9.23 | 132.65 | 120.28 |
| 7 | M | 1651 | ASP | C-N-CA | 9.23 | 132.65 | 120.28 |
| 7 | O | 1438 | VAL | CA-C-N | 9.23 | 133.02 | 120.38 |
| 7 | O | 1438 | VAL | C-N-CA | 9.23 | 133.02 | 120.38 |
| 1 | Y | 1329 | ASP | CA-CB-CG | 9.23 | 121.83 | 112.60 |
| 8 | N | 1545 | SER | CA-C-N | 9.23 | 132.64 | 120.28 |
| 8 | N | 1545 | SER | C-N-CA | 9.23 | 132.64 | 120.28 |
| 9 | Q | 263 | MET | N-CA-C | -9.23 | 102.16 | 113.97 |
| 8 | N | 152 | TYR | N-CA-C | -9.22 | 101.34 | 112.59 |
| 7 | O | 1349 | PHE | CA-CB-CG | -9.22 | 104.58 | 113.80 |
| 12 | v | 530 | ASP | CB-CA-C | -9.22 | 96.41 | 110.88 |
| 1 | 0 | 1316 | SER | N-CA-CB | 9.22 | 126.06 | 110.49 |
| 9 | S | 98 | PRO | N-CA-CB | 9.21 | 113.76 | 103.44 |
| 8 | N | 1095 | GLU | N-CA-C | 9.21 | 130.41 | 110.80 |
| 9 | T | 754 | ARG | N-CA-CB | 9.21 | 126.05 | 110.49 |
| 15 | b | 140 | HIS | CA-CB-CG | 9.20 | 123.00 | 113.80 |
| 1 | 0 | 645 | THR | N-CA-C | -9.20 | 101.76 | 113.72 |
| 7 | O | 435 | PHE | CA-CB-CG | 9.20 | 123.00 | 113.80 |
| 16 | j | 657 | CYS | CA-C-N | 9.19 | 132.97 | 120.38 |
| 16 | j | 657 | CYS | C-N-CA | 9.19 | 132.97 | 120.38 |
| 20 | g | 951 | LEU | CA-C-N | 9.19 | 132.59 | 120.28 |
| 20 | g | 951 | LEU | C-N-CA | 9.19 | 132.59 | 120.28 |
| 1 | Y | 1406 | HIS | N-CA-C | -9.18 | 99.39 | 111.24 |
| 9 | R | 352 | VAL | N-CA-C | -9.18 | 103.45 | 112.17 |
| 4 | A | 654 | HIS | CE1-NE2-CD2 | -9.18 | 99.82 | 109.00 |
| 21 | s | 56 | THR | CA-CB-OG1 | 9.18 | 123.36 | 109.60 |
| 2 | Z | 679 | SER | N-CA-C | -9.17 | 91.26 | 110.80 |
| 14 | a | 904 | PHE | CA-CB-CG | -9.17 | 104.63 | 113.80 |
| 9 | T | 250 | ASN | CA-C-N | 9.16 | 132.35 | 120.44 |
| 9 | T | 250 | ASN | C-N-CA | 9.16 | 132.35 | 120.44 |
| 1 | Y | 1161 | MET | CA-C-O | -9.16 | 111.20 | 120.82 |
| 9 | Q | 753 | ALA | N-CA-C | -9.15 | 85.38 | 111.00 |
| 9 | S | 596 | ASP | CA-CB-CG | 9.15 | 121.75 | 112.60 |
| 14 | h | 1035 | ARG | NE-CZ-NH2 | -9.15 | 110.97 | 119.20 |
| 2 | Z | 627 | ASN | CA-CB-CG | 9.14 | 121.74 | 112.60 |
| 14 | h | 968 | ARG | CA-C-N | 9.14 | 133.45 | 120.28 |
| 14 | h | 968 | ARG | C-N-CA | 9.14 | 133.45 | 120.28 |
| 1 | Y | 1257 | GLN | N-CA-C | 9.14 | 136.59 | 111.00 |
| 14 | a | 977 | ALA | CA-C-N | 9.14 | 133.27 | 120.29 |
| 14 | a | 977 | ALA | C-N-CA | 9.14 | 133.27 | 120.29 |
| 2 | 1 | 158 | GLU | N-CA-C | -9.14 | 95.52 | 109.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 1448 | SER | N-CA-CB | 9.14 | 123.26 | 110.01 |
| 16 | c | 430 | ASN | OD1-CG-ND2 | 9.13 | 131.74 | 122.60 |
| 15 | i | 212 | ILE | N-CA-C | -9.13 | 103.96 | 111.81 |
| 14 | h | 15 | TYR | N-CA-C | -9.13 | 95.99 | 108.86 |
| 12 | v | 587 | LYS | CA-C-N | 9.12 | 132.30 | 120.44 |
| 12 | v | 587 | LYS | C-N-CA | 9.12 | 132.30 | 120.44 |
| 2 | 1 | 953 | ILE | CA-C-O | -9.11 | 111.74 | 120.30 |
| 8 | N | 1516 | PRO | N-CA-CB | 9.11 | 113.64 | 103.44 |
| 6 | C | 440 | VAL | N-CA-C | -9.11 | 100.59 | 113.07 |
| 1 | Y | 509 | PHE | CA-CB-CG | -9.11 | 104.69 | 113.80 |
| 20 | n | 326 | PHE | CA-CB-CG | 9.10 | 122.90 | 113.80 |
| 7 | O | 893 | HIS | CA-CB-CG | -9.10 | 104.70 | 113.80 |
| 16 | j | 134 | ASN | CA-CB-CG | 9.10 | 121.70 | 112.60 |
| 14 | a | 476 | PHE | CA-CB-CG | -9.10 | 104.70 | 113.80 |
| 6 | L | 369 | LEU | N-CA-CB | 9.10 | 125.96 | 110.50 |
| 17 | d | 130 | PHE | CA-CB-CG | -9.10 | 104.70 | 113.80 |
| 7 | M | 1409 | ALA | CA-C-N | 9.09 | 132.26 | 120.44 |
| 7 | M | 1409 | ALA | C-N-CA | 9.09 | 132.26 | 120.44 |
| 7 | M | 459 | ASP | N-CA-C | -9.09 | 100.84 | 112.93 |
| 20 | n | 789 | ASN | OD1-CG-ND2 | -9.09 | 113.51 | 122.60 |
| 2 | 1 | 501 | ILE | CA-C-N | 9.09 | 132.71 | 120.63 |
| 2 | 1 | 501 | ILE | C-N-CA | 9.09 | 132.71 | 120.63 |
| 7 | O | 426 | GLN | OE1-CD-NE2 | 9.09 | 131.69 | 122.60 |
| 9 | R | 570 | GLU | CA-C-N | 9.09 | 132.46 | 120.28 |
| 9 | R | 570 | GLU | C-N-CA | 9.09 | 132.46 | 120.28 |
| 1 | 0 | 394 | GLU | CA-C-N | -9.08 | 108.49 | 119.84 |
| 1 | 0 | 394 | GLU | C-N-CA | -9.08 | 108.49 | 119.84 |
| 11 | X | 402 | ASN | CA-C-O | -9.07 | 105.38 | 120.80 |
| 2 | Z | 187 | ASN | CA-CB-CG | -9.07 | 103.53 | 112.60 |
| 8 | P | 1453 | ILE | CA-C-N | 9.07 | 131.43 | 120.09 |
| 8 | P | 1453 | ILE | C-N-CA | 9.07 | 131.43 | 120.09 |
| 7 | O | 934 | ASP | N-CA-CB | 9.06 | 125.00 | 110.77 |
| 8 | P | 1534 | TYR | CA-C-N | 9.06 | 132.80 | 120.38 |
| 8 | P | 1534 | TYR | C-N-CA | 9.06 | 132.80 | 120.38 |
| 12 | u | 533 | LYS | CA-C-N | 9.05 | 132.21 | 120.44 |
| 12 | u | 533 | LYS | C-N-CA | 9.05 | 132.21 | 120.44 |
| 9 | R | 155 | VAL | CA-C-N | 9.05 | 133.37 | 120.79 |
| 9 | R | 155 | VAL | C-N-CA | 9.05 | 133.37 | 120.79 |
| 12 | v | 247 | ARG | CA-C-N | 9.05 | 132.21 | 120.44 |
| 12 | v | 247 | ARG | C-N-CA | 9.05 | 132.21 | 120.44 |
| 8 | P | 577 | MET | N-CA-C | -9.05 | 85.66 | 111.00 |
| 1 | Y | 951 | ASP | N-CA-C | -9.05 | 103.07 | 114.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 727 | GLU | CA-C-O | 9.05 | 129.16 | 121.02 |
| 14 | h | 325 | ALA | CA-C-N | 9.04 | 138.81 | 121.54 |
| 14 | h | 325 | ALA | C-N-CA | 9.04 | 138.81 | 121.54 |
| 5 | B | 323 | LEU | CB-CA-C | -9.04 | 92.43 | 110.42 |
| 1 | 0 | 1025 | ASN | CA-CB-CG | -9.04 | 103.56 | 112.60 |
| 1 | 0 | 639 | VAL | N-CA-C | -9.03 | 95.43 | 108.53 |
| 5 | E | 527 | LEU | CA-C-N | 9.03 | 132.18 | 120.44 |
| 5 | E | 527 | LEU | C-N-CA | 9.03 | 132.18 | 120.44 |
| 7 | M | 1281 | LYS | N-CA-C | 9.03 | 120.73 | 111.07 |
| 14 | h | 864 | PHE | N-CA-CB | -9.03 | 97.25 | 110.70 |
| 18 | l | 116 | PHE | CA-CB-CG | -9.03 | 104.77 | 113.80 |
| 2 | Z | 906 | ALA | CA-C-N | 9.02 | 129.78 | 119.94 |
| 2 | Z | 906 | ALA | C-N-CA | 9.02 | 129.78 | 119.94 |
| 8 | N | 1520 | LEU | O-C-N | 9.02 | 131.68 | 122.12 |
| 14 | a | 978 | ALA | CA-C-N | 9.01 | 132.36 | 120.28 |
| 14 | a | 978 | ALA | C-N-CA | 9.01 | 132.36 | 120.28 |
| 7 | M | 1308 | GLN | N-CA-C | 9.01 | 121.10 | 111.28 |
| 7 | M | 975 | SER | CA-C-N | 9.01 | 132.15 | 120.44 |
| 7 | M | 975 | SER | C-N-CA | 9.01 | 132.15 | 120.44 |
| 11 | V | 298 | PHE | N-CA-CB | 9.01 | 118.70 | 109.51 |
| 20 | g | 142 | PHE | CA-CB-CG | -9.01 | 104.79 | 113.80 |
| 8 | P | 1416 | GLY | CA-C-O | -9.00 | 111.48 | 120.75 |
| 20 | n | 517 | PRO | CA-C-O | -9.00 | 107.51 | 120.56 |
| 1 | 0 | 955 | PRO | N-CA-C | -8.99 | 104.22 | 114.92 |
| 8 | N | 1287 | ILE | N-CA-C | 8.99 | 119.81 | 111.45 |
| 1 | Y | 1414 | SER | N-CA-C | 8.99 | 121.08 | 111.28 |
| 12 | u | 47 | ASN | CA-CB-CG | -8.99 | 103.61 | 112.60 |
| 20 | n | 647 | LYS | N-CA-C | 8.98 | 122.04 | 111.71 |
| 14 | a | 350 | ASN | CA-CB-CG | -8.98 | 103.62 | 112.60 |
| 8 | N | 343 | ASP | N-CA-C | -8.98 | 103.16 | 114.56 |
| 9 | S | 418 | CYS | N-CA-C | -8.98 | 102.24 | 113.55 |
| 8 | P | 745 | HIS | ND1-CE1-NE2 | 8.97 | 117.38 | 108.40 |
| 9 | S | 161 | ILE | CA-C-N | 8.97 | 132.10 | 120.44 |
| 9 | S | 161 | ILE | C-N-CA | 8.97 | 132.10 | 120.44 |
| 8 | N | 1346 | LYS | N-CA-C | -8.96 | 102.07 | 113.72 |
| 19 | m | 105 | PHE | CA-CB-CG | -8.96 | 104.84 | 113.80 |
| 2 | Z | 1274 | LYS | N-CA-C | -8.96 | 102.48 | 113.50 |
| 5 | E | 532 | ALA | N-CA-C | 8.96 | 121.04 | 111.28 |
| 4 | A | 709 | ASN | CA-CB-CG | -8.95 | 103.65 | 112.60 |
| 15 | i | 133 | ASN | OD1-CG-ND2 | -8.96 | 113.64 | 122.60 |
| 19 | m | 612 | ASN | CA-C-N | 8.95 | 127.49 | 120.33 |
| 19 | m | 612 | ASN | C-N-CA | 8.95 | 127.49 | 120.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 183 | ARG | N-CA-C | 8.95 | 120.65 | 111.07 |
| 8 | P | 571 | ASN | N-CA-C | -8.95 | 104.41 | 114.62 |
| 7 | M | 571 | ASN | CA-C-N | 8.95 | 132.27 | 120.28 |
| 7 | M | 571 | ASN | C-N-CA | 8.95 | 132.27 | 120.28 |
| 21 | s | 24 | ILE | O-C-N | 8.95 | 130.55 | 121.87 |
| 2 | 1 | 146 | ILE | CA-C-N | 8.94 | 129.02 | 119.90 |
| 2 | 1 | 146 | ILE | C-N-CA | 8.94 | 129.02 | 119.90 |
| 2 | 1 | 185 | ILE | O-C-N | 8.94 | 130.67 | 121.91 |
| 8 | P | 799 | ALA | CA-C-N | 8.94 | 132.63 | 120.38 |
| 8 | P | 799 | ALA | C-N-CA | 8.94 | 132.63 | 120.38 |
| 9 | R | 332 | PRO | N-CA-CB | 8.94 | 112.64 | 103.25 |
| 6 | C | 471 | SER | N-CA-C | -8.94 | 101.70 | 114.12 |
| 1 | Y | 523 | SER | N-CA-CB | 8.94 | 125.59 | 110.49 |
| 8 | N | 981 | LYS | CA-C-O | 8.93 | 128.21 | 118.65 |
| 7 | O | 326 | ALA | N-CA-CB | 8.93 | 123.98 | 110.22 |
| 8 | P | 1617 | ILE | CA-C-N | 8.93 | 128.69 | 119.76 |
| 8 | P | 1617 | ILE | C-N-CA | 8.93 | 128.69 | 119.76 |
| 1 | 0 | 1155 | ARG | N-CA-C | -8.93 | 103.50 | 114.75 |
| 8 | N | 860 | ALA | N-CA-C | 8.93 | 121.01 | 111.28 |
| 6 | F | 341 | ASP | CA-CB-CG | -8.93 | 103.67 | 112.60 |
| 1 | 0 | 1073 | SER | N-CA-C | -8.93 | 103.51 | 112.97 |
| 7 | M | 1138 | PHE | CA-C-O | -8.92 | 107.75 | 120.51 |
| 9 | T | 762 | ASN | N-CA-C | -8.92 | 94.19 | 108.73 |
| 1 | 0 | 234 | ILE | N-CA-C | -8.92 | 95.64 | 108.48 |
| 7 | O | 1581 | THR | CA-C-O | 8.92 | 130.00 | 120.55 |
| 9 | T | 140 | ILE | CB-CA-C | -8.91 | 100.56 | 111.97 |
| 9 | T | 811 | ARG | N-CA-C | -8.91 | 101.23 | 112.90 |
| 20 | n | 477 | PHE | CA-CB-CG | 8.90 | 122.70 | 113.80 |
| 7 | O | 1185 | ILE | N-CA-C | -8.90 | 104.02 | 112.83 |
| 2 | 1 | 916 | PHE | CA-C-O | -8.90 | 105.68 | 120.80 |
| 7 | O | 1290 | ILE | CA-C-N | 8.90 | 132.01 | 120.44 |
| 7 | O | 1290 | ILE | C-N-CA | 8.90 | 132.01 | 120.44 |
| 9 | S | 135 | ASP | CA-C-N | 8.90 | 132.01 | 120.44 |
| 9 | S | 135 | ASP | C-N-CA | 8.90 | 132.01 | 120.44 |
| 14 | a | 99 | ASN | N-CA-C | -8.90 | 95.55 | 109.07 |
| 14 | h | 650 | HIS | N-CA-C | 8.89 | 120.97 | 111.28 |
| 5 | H | 522 | TYR | N-CA-C | 8.89 | 120.97 | 111.28 |
| 2 | 1 | 1354 | ASP | CA-CB-CG | 8.89 | 121.49 | 112.60 |
| 20 | n | 938 | ASN | CA-CB-CG | 8.89 | 121.49 | 112.60 |
| 20 | g | 1070 | LEU | CA-C-O | -8.88 | 109.73 | 118.34 |
| 20 | n | 249 | ASN | N-CA-C | -8.88 | 101.78 | 114.12 |
| 7 | O | 245 | ARG | NE-CZ-NH1 | 8.87 | 130.37 | 121.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 587 | GLN | CA-C-O | -8.87 | 111.43 | 121.19 |
| 8 | N | 64 | SER | N-CA-C | -8.87 | 100.79 | 113.21 |
| 9 | R | 825 | PRO | CA-C-N | 8.87 | 132.16 | 120.28 |
| 9 | R | 825 | PRO | C-N-CA | 8.87 | 132.16 | 120.28 |
| 7 | O | 1453 | ARG | CA-C-N | 8.86 | 132.03 | 120.60 |
| 7 | O | 1453 | ARG | C-N-CA | 8.86 | 132.03 | 120.60 |
| 14 | a | 919 | PHE | CA-C-N | 8.87 | 132.16 | 120.28 |
| 14 | a | 919 | PHE | C-N-CA | 8.87 | 132.16 | 120.28 |
| 1 | 0 | 1282 | ASP | N-CA-C | -8.86 | 104.52 | 114.62 |
| 8 | N | 755 | ASN | CA-CB-CG | -8.86 | 103.74 | 112.60 |
| 15 | b | 629 | VAL | CA-C-N | 8.86 | 133.10 | 120.79 |
| 15 | b | 629 | VAL | C-N-CA | 8.86 | 133.10 | 120.79 |
| 15 | b | 361 | LEU | N-CA-C | -8.85 | 102.47 | 113.18 |
| 15 | i | 81 | PHE | CA-CB-CG | 8.85 | 122.65 | 113.80 |
| 18 | l | 130 | ASN | N-CA-C | -8.85 | 103.59 | 112.97 |
| 14 | a | 416 | GLY | CA-C-O | -8.85 | 116.12 | 122.23 |
| 7 | O | 1182 | ASN | CA-CB-CG | -8.85 | 103.75 | 112.60 |
| 1 | 0 | 1197 | SER | CA-C-N | 8.84 | 138.43 | 121.54 |
| 1 | 0 | 1197 | SER | C-N-CA | 8.84 | 138.43 | 121.54 |
| 9 | S | 672 | GLN | CA-C-N | 8.84 | 129.39 | 119.93 |
| 9 | S | 672 | GLN | C-N-CA | 8.84 | 129.39 | 119.93 |
| 9 | T | 823 | ARG | N-CA-C | -8.84 | 99.22 | 113.19 |
| 4 | G | 654 | HIS | N-CA-C | 8.84 | 120.92 | 111.28 |
| 1 | Y | 130 | GLY | N-CA-C | -8.84 | 101.78 | 112.48 |
| 7 | O | 635 | PHE | CA-CB-CG | -8.84 | 104.97 | 113.80 |
| 9 | S | 589 | LEU | CA-C-N | 8.83 | 133.25 | 120.71 |
| 9 | S | 589 | LEU | C-N-CA | 8.83 | 133.25 | 120.71 |
| 8 | N | 1519 | CYS | CA-C-N | 8.83 | 132.11 | 120.28 |
| 8 | N | 1519 | CYS | C-N-CA | 8.83 | 132.11 | 120.28 |
| 2 | Z | 916 | PHE | CA-C-O | -8.83 | 105.79 | 120.80 |
| 9 | S | 615 | ASP | N-CA-CB | 8.83 | 125.41 | 110.49 |
| 1 | Y | 1258 | LEU | N-CA-CB | -8.83 | 95.57 | 110.49 |
| 16 | j | 566 | ASP | CA-CB-CG | 8.82 | 121.42 | 112.60 |
| 11 | X | 362 | SER | CA-C-N | 8.82 | 128.54 | 119.19 |
| 11 | X | 362 | SER | C-N-CA | 8.82 | 128.54 | 119.19 |
| 9 | Q | 540 | ASN | CA-CB-CG | 8.82 | 121.42 | 112.60 |
| 12 | v | 66 | ASP | CA-C-N | 8.82 | 132.98 | 120.28 |
| 12 | v | 66 | ASP | C-N-CA | 8.82 | 132.98 | 120.28 |
| 14 | a | 245 | ILE | N-CA-C | -8.82 | 95.82 | 108.17 |
| 1 | 0 | 1233 | ILE | CA-C-N | 8.81 | 132.81 | 120.29 |
| 1 | 0 | 1233 | ILE | C-N-CA | 8.81 | 132.81 | 120.29 |
| 16 | j | 214 | SER | N-CA-C | -8.81 | 101.84 | 112.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | m | 149 | THR | N-CA-C | -8.81 | 102.54 | 113.38 |
| 20 | n | 671 | ASN | CA-CB-CG | -8.81 | 103.79 | 112.60 |
| 15 | b | 222 | GLU | N-CA-C | -8.81 | 100.63 | 112.26 |
| 5 | E | 530 | ASP | N-CA-CB | 8.81 | 123.19 | 110.16 |
| 12 | u | 527 | ILE | CA-C-N | 8.80 | 131.88 | 120.44 |
| 12 | u | 527 | ILE | C-N-CA | 8.80 | 131.88 | 120.44 |
| 9 | T | 156 | MET | CA-C-O | -8.80 | 111.48 | 120.90 |
| 17 | k | 208 | ARG | N-CA-C | -8.80 | 102.46 | 113.55 |
| 2 | 1 | 745 | ILE | CA-CB-CG2 | -8.80 | 95.54 | 110.50 |
| 15 | b | 135 | ASN | CA-CB-CG | -8.79 | 103.81 | 112.60 |
| 8 | N | 593 | SER | CA-C-N | 8.79 | 131.94 | 120.60 |
| 8 | N | 593 | SER | C-N-CA | 8.79 | 131.94 | 120.60 |
| 19 | f | 631 | ILE | N-CA-C | -8.79 | 103.85 | 113.43 |
| 7 | O | 40 | ASP | CA-CB-CG | 8.78 | 121.38 | 112.60 |
| 2 | Z | 114 | PRO | CA-C-O | -8.79 | 111.83 | 121.23 |
| 1 | 0 | 1271 | ILE | O-C-N | 8.77 | 130.38 | 121.87 |
| 2 | 1 | 915 | LYS | N-CA-C | 8.77 | 129.49 | 110.80 |
| 8 | N | 1335 | GLN | OE1-CD-NE2 | -8.77 | 113.83 | 122.60 |
| 7 | M | 218 | HIS | CA-CB-CG | 8.77 | 122.57 | 113.80 |
| 4 | D | 809 | ASP | CA-CB-CG | 8.77 | 121.37 | 112.60 |
| 7 | O | 825 | ILE | CA-C-O | -8.77 | 112.82 | 118.69 |
| 14 | h | 790 | LEU | CA-C-O | -8.77 | 110.46 | 119.49 |
| 8 | P | 1351 | ILE | N-CA-C | -8.76 | 103.17 | 113.42 |
| 20 | g | 735 | LEU | N-CA-C | -8.76 | 101.28 | 112.93 |
| 1 | 0 | 1218 | TYR | N-CA-C | -8.76 | 99.98 | 111.71 |
| 1 | Y | 1161 | MET | O-C-N | 8.76 | 131.09 | 122.07 |
| 4 | A | 663 | ASN | N-CA-C | 8.75 | 120.59 | 111.14 |
| 7 | M | 987 | GLU | CB-CA-C | -8.75 | 95.97 | 110.85 |
| 15 | i | 552 | ILE | CA-C-N | 8.75 | 137.73 | 121.97 |
| 15 | i | 552 | ILE | C-N-CA | 8.75 | 137.73 | 121.97 |
| 9 | R | 784 | ASN | CA-CB-CG | 8.75 | 121.35 | 112.60 |
| 7 | M | 1304 | HIS | CA-CB-CG | 8.75 | 122.55 | 113.80 |
| 16 | c | 323 | SER | N-CA-CB | 8.75 | 125.28 | 110.49 |
| 16 | j | 630 | THR | N-CA-C | -8.75 | 96.76 | 109.18 |
| 10 | W | 304 | LYS | N-CA-CB | 8.74 | 125.37 | 110.50 |
| 1 | 0 | 1101 | ARG | NE-CZ-NH2 | -8.74 | 111.33 | 119.20 |
| 20 | g | 599 | LYS | O-C-N | -8.74 | 111.52 | 122.27 |
| 1 | 0 | 954 | ALA | CA-C-O | -8.74 | 110.84 | 119.49 |
| 2 | Z | 616 | THR | CA-C-N | 8.74 | 129.61 | 119.47 |
| 2 | Z | 616 | THR | C-N-CA | 8.74 | 129.61 | 119.47 |
| 8 | N | 1250 | ILE | CA-CB-CG1 | 8.74 | 125.25 | 110.40 |
| 18 | e | 177 | ARG | NE-CZ-NH2 | -8.74 | 111.34 | 119.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 420 | THR | CA-C-O | 8.73 | 129.93 | 120.58 |
| 7 | O | 1329 | LEU | CA-C-N | 8.73 | 131.99 | 120.28 |
| 7 | O | 1329 | LEU | C-N-CA | 8.73 | 131.99 | 120.28 |
| 16 | j | 631 | GLN | OE1-CD-NE2 | 8.73 | 131.33 | 122.60 |
| 18 | l | 237 | ASP | N-CA-CB | 8.73 | 125.24 | 110.49 |
| 19 | f | 387 | ARG | CA-C-N | 8.72 | 131.73 | 120.56 |
| 19 | f | 387 | ARG | C-N-CA | 8.72 | 131.73 | 120.56 |
| 14 | a | 230 | HIS | ND1-CE1-NE2 | 8.72 | 117.12 | 108.40 |
| 7 | M | 426 | GLN | N-CA-C | -8.72 | 104.68 | 114.62 |
| 17 | d | 94 | VAL | CA-C-O | 8.72 | 130.44 | 120.67 |
| 2 | Z | 454 | PRO | N-CA-C | 8.72 | 121.34 | 110.70 |
| 15 | i | 146 | LEU | N-CA-C | -8.71 | 102.78 | 113.50 |
| 19 | f | 182 | LYS | CA-C-N | 8.71 | 131.77 | 120.44 |
| 19 | f | 182 | LYS | C-N-CA | 8.71 | 131.77 | 120.44 |
| 2 | 1 | 447 | LYS | CA-C-N | 8.71 | 133.24 | 120.87 |
| 2 | 1 | 447 | LYS | C-N-CA | 8.71 | 133.24 | 120.87 |
| 18 | l | 130 | ASN | N-CA-CB | 8.71 | 123.02 | 110.65 |
| 20 | g | 409 | ASP | CA-CB-CG | 8.71 | 121.31 | 112.60 |
| 8 | N | 1645 | LYS | CA-C-N | 8.70 | 131.94 | 120.28 |
| 8 | N | 1645 | LYS | C-N-CA | 8.70 | 131.94 | 120.28 |
| 20 | n | 689 | ILE | N-CA-C | -8.71 | 104.54 | 112.90 |
| 2 | 1 | 1039 | LEU | N-CA-C | 8.70 | 135.36 | 111.00 |
| 7 | M | 1273 | LYS | CB-CA-C | 8.70 | 127.74 | 110.42 |
| 1 | Y | 443 | GLY | N-CA-C | -8.70 | 101.74 | 116.01 |
| 2 | Z | 679 | SER | CA-C-O | -8.70 | 108.06 | 120.51 |
| 19 | f | 622 | GLY | CA-C-N | 8.70 | 132.27 | 120.44 |
| 19 | f | 622 | GLY | C-N-CA | 8.70 | 132.27 | 120.44 |
| 8 | P | 950 | ARG | N-CA-C | 8.69 | 120.75 | 111.28 |
| 4 | G | 724 | ASP | CA-CB-CG | 8.68 | 121.28 | 112.60 |
| 18 | l | 139 | ALA | N-CA-CB | 8.68 | 123.33 | 110.49 |
| 20 | n | 644 | VAL | CA-C-N | 8.68 | 132.74 | 120.42 |
| 20 | n | 644 | VAL | C-N-CA | 8.68 | 132.74 | 120.42 |
| 8 | N | 1565 | ASN | CA-C-N | 8.67 | 138.11 | 121.54 |
| 8 | N | 1565 | ASN | C-N-CA | 8.67 | 138.11 | 121.54 |
| 15 | i | 490 | ALA | N-CA-C | -8.67 | 102.69 | 113.18 |
| 14 | a | 839 | GLU | CA-C-N | 8.67 | 132.77 | 120.28 |
| 14 | a | 839 | GLU | C-N-CA | 8.67 | 132.77 | 120.28 |
| 8 | P | 1199 | TYR | N-CA-C | -8.67 | 100.40 | 112.45 |
| 14 | h | 876 | LEU | N-CA-C | -8.67 | 102.87 | 113.97 |
| 19 | f | 403 | SER | N-CA-C | -8.67 | 102.48 | 113.23 |
| 6 | L | 393 | ASP | CA-C-O | -8.67 | 111.36 | 120.55 |
| 7 | O | 234 | THR | CA-C-O | -8.67 | 108.29 | 120.16 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | i | 544 | ASN | CA-CB-CG | 8.66 | 121.26 | 112.60 |
| 2 | 1 | 880 | SER | N-CA-C | -8.66 | 101.64 | 112.72 |
| 8 | P | 472 | ASP | CA-CB-CG | 8.66 | 121.26 | 112.60 |
| 7 | M | 1009 | ASN | CA-CB-CG | 8.66 | 121.26 | 112.60 |
| 8 | N | 950 | ARG | N-CA-C | -8.66 | 102.89 | 113.97 |
| 14 | a | 600 | ASP | CA-CB-CG | 8.66 | 121.26 | 112.60 |
| 14 | h | 965 | TYR | N-CA-C | -8.65 | 102.53 | 113.43 |
| 17 | d | 224 | SER | CA-C-N | 8.65 | 132.14 | 120.63 |
| 17 | d | 224 | SER | C-N-CA | 8.65 | 132.14 | 120.63 |
| 2 | Z | 704 | VAL | N-CA-C | -8.65 | 94.97 | 107.77 |
| 9 | Q | 69 | ALA | N-CA-C | 8.64 | 120.48 | 111.14 |
| 2 | Z | 606 | SER | N-CA-C | 8.64 | 121.79 | 111.33 |
| 7 | O | 1292 | ARG | CA-C-N | 8.64 | 132.56 | 120.29 |
| 7 | O | 1292 | ARG | C-N-CA | 8.64 | 132.56 | 120.29 |
| 2 | 1 | 1360 | SER | CA-C-O | 8.63 | 128.31 | 118.47 |
| 21 | q | 37 | LEU | CA-C-N | 8.63 | 131.85 | 120.28 |
| 21 | q | 37 | LEU | C-N-CA | 8.63 | 131.85 | 120.28 |
| 1 | Y | 530 | ILE | N-CA-C | -8.63 | 95.39 | 107.99 |
| 12 | v | 148 | ASP | N-CA-C | -8.63 | 102.46 | 113.16 |
| 6 | F | 369 | LEU | N-CA-C | 8.62 | 135.14 | 111.00 |
| 8 | P | 1012 | VAL | N-CA-C | 8.62 | 119.41 | 110.62 |
| 13 | x | 1350 | PHE | CA-C-N | 8.62 | 131.65 | 120.44 |
| 13 | x | 1350 | PHE | C-N-CA | 8.62 | 131.65 | 120.44 |
| 7 | M | 52 | GLU | N-CA-C | 8.62 | 122.58 | 112.93 |
| 1 | 0 | 218 | ARG | CA-C-N | 8.61 | 128.63 | 119.76 |
| 1 | 0 | 218 | ARG | C-N-CA | 8.61 | 128.63 | 119.76 |
| 7 | M | 221 | SER | N-CA-C | -8.61 | 103.84 | 112.97 |
| 1 | Y | 1258 | LEU | N-CA-C | 8.61 | 129.14 | 110.80 |
| 20 | g | 557 | LEU | CA-C-N | 8.61 | 131.82 | 120.28 |
| 20 | g | 557 | LEU | C-N-CA | 8.61 | 131.82 | 120.28 |
| 9 | Q | 214 | ASN | CA-CB-CG | -8.61 | 104.00 | 112.60 |
| 2 | Z | 445 | SER | CA-C-N | -8.61 | 110.68 | 122.30 |
| 2 | Z | 445 | SER | C-N-CA | -8.61 | 110.68 | 122.30 |
| 2 | Z | 355 | HIS | CA-CB-CG | -8.60 | 105.20 | 113.80 |
| 7 | O | 103 | LYS | CA-C-N | 8.60 | 131.69 | 120.60 |
| 7 | O | 103 | LYS | C-N-CA | 8.60 | 131.69 | 120.60 |
| 8 | P | 1640 | ILE | N-CA-C | 8.60 | 119.39 | 110.62 |
| 7 | O | 1474 | PHE | CA-CB-CG | -8.60 | 105.20 | 113.80 |
| 9 | S | 128 | LEU | CA-C-N | 8.60 | 131.61 | 120.44 |
| 9 | S | 128 | LEU | C-N-CA | 8.60 | 131.61 | 120.44 |
| 1 | 0 | 960 | LYS | N-CA-C | -8.59 | 103.23 | 114.31 |
| 5 | B | 317 | ASN | CA-C-N | 8.59 | 137.95 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | B | 317 | ASN | C-N-CA | 8.59 | 137.95 | 121.54 |
| 14 | a | 459 | GLU | CA-C-N | 8.59 | 132.98 | 120.95 |
| 14 | a | 459 | GLU | C-N-CA | 8.59 | 132.98 | 120.95 |
| 1 | 0 | 831 | LYS | N-CA-C | -8.59 | 86.95 | 111.00 |
| 1 | 0 | 1066 | PHE | CA-CB-CG | -8.59 | 105.21 | 113.80 |
| 4 | D | 788 | ASP | CA-CB-CG | 8.59 | 121.19 | 112.60 |
| 8 | N | 1123 | HIS | N-CA-C | -8.59 | 102.93 | 112.72 |
| 15 | i | 391 | GLU | N-CA-C | -8.59 | 102.61 | 113.43 |
| 15 | b | 523 | LEU | N-CA-C | -8.58 | 102.12 | 112.59 |
| 2 | Z | 381 | ALA | CA-C-N | 8.58 | 131.78 | 120.28 |
| 2 | Z | 381 | ALA | C-N-CA | 8.58 | 131.78 | 120.28 |
| 12 | u | 133 | HIS | CE1-NE2-CD2 | -8.58 | 100.42 | 109.00 |
| 1 | 0 | 113 | HIS | CA-C-N | 8.58 | 131.77 | 120.28 |
| 1 | 0 | 113 | HIS | C-N-CA | 8.58 | 131.77 | 120.28 |
| 5 | H | 515 | ASN | CA-CB-CG | -8.58 | 104.02 | 112.60 |
| 7 | M | 1334 | THR | N-CA-C | -8.58 | 100.53 | 112.45 |
| 15 | b | 149 | GLU | CA-C-N | 8.58 | 132.63 | 120.28 |
| 15 | b | 149 | GLU | C-N-CA | 8.58 | 132.63 | 120.28 |
| 9 | Q | 50 | ARG | N-CA-C | -8.57 | 101.26 | 112.41 |
| 7 | O | 35 | LEU | CA-C-N | 8.57 | 137.91 | 121.54 |
| 7 | O | 35 | LEU | C-N-CA | 8.57 | 137.91 | 121.54 |
| 12 | u | 246 | LYS | CA-C-N | 8.57 | 131.59 | 120.44 |
| 12 | u | 246 | LYS | C-N-CA | 8.57 | 131.59 | 120.44 |
| 19 | f | 225 | THR | N-CA-C | -8.57 | 102.21 | 114.12 |
| 1 | 0 | 939 | ASP | N-CA-C | 8.56 | 121.69 | 111.33 |
| 14 | a | 1029 | ASP | CA-CB-CG | 8.56 | 121.16 | 112.60 |
| 9 | S | 727 | TYR | CA-C-O | 8.56 | 129.69 | 119.59 |
| 8 | P | 23 | ASN | CA-CB-CG | 8.55 | 121.15 | 112.60 |
| 2 | Z | 550 | ASN | CA-C-N | 8.55 | 137.88 | 121.54 |
| 2 | Z | 550 | ASN | C-N-CA | 8.55 | 137.88 | 121.54 |
| 6 | I | 282 | GLN | N-CA-C | -8.55 | 102.11 | 112.54 |
| 7 | M | 1120 | THR | N-CA-C | -8.55 | 96.07 | 109.07 |
| 9 | R | 247 | GLY | CA-C-N | 8.55 | 131.73 | 120.28 |
| 9 | R | 247 | GLY | C-N-CA | 8.55 | 131.73 | 120.28 |
| 7 | M | 62 | SER | N-CA-CB | 8.54 | 124.93 | 110.49 |
| 7 | M | 178 | ASN | CA-CB-CG | 8.54 | 121.14 | 112.60 |
| 20 | n | 852 | ILE | N-CA-C | -8.54 | 104.38 | 112.83 |
| 2 | 1 | 962 | LYS | N-CA-C | -8.54 | 100.58 | 112.45 |
| 19 | m | 663 | LEU | CA-C-N | 8.54 | 132.07 | 120.54 |
| 19 | m | 663 | LEU | C-N-CA | 8.54 | 132.07 | 120.54 |
| 8 | P | 444 | ASN | N-CA-C | -8.54 | 101.31 | 112.41 |
| 19 | m | 646 | SER | CA-C-N | 8.54 | 133.29 | 120.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | m | 646 | SER | C-N-CA | 8.54 | 133.29 | 120.31 |
| 2 | 1 | 1074 | ARG | CA-C-N | 8.54 | 133.26 | 121.05 |
| 2 | 1 | 1074 | ARG | C-N-CA | 8.54 | 133.26 | 121.05 |
| 7 | M | 818 | TYR | N-CA-C | -8.53 | 102.43 | 112.92 |
| 9 | T | 691 | ARG | N-CA-C | 8.53 | 120.19 | 111.07 |
| 15 | i | 117 | ASP | CA-CB-CG | 8.52 | 121.12 | 112.60 |
| 7 | O | 1454 | VAL | N-CA-CB | 8.52 | 119.97 | 110.51 |
| 20 | g | 1134 | HIS | CA-CB-CG | 8.52 | 122.32 | 113.80 |
| 14 | a | 840 | PHE | CA-C-N | 8.52 | 131.52 | 120.44 |
| 14 | a | 840 | PHE | C-N-CA | 8.52 | 131.52 | 120.44 |
| 7 | M | 1363 | ILE | N-CA-C | -8.52 | 105.62 | 113.71 |
| 9 | T | 630 | ARG | CA-C-N | 8.52 | 132.04 | 120.54 |
| 9 | T | 630 | ARG | C-N-CA | 8.52 | 132.04 | 120.54 |
| 9 | S | 131 | GLY | CA-C-N | 8.51 | 131.51 | 120.44 |
| 9 | S | 131 | GLY | C-N-CA | 8.51 | 131.51 | 120.44 |
| 8 | N | 777 | ASP | N-CA-C | -8.50 | 99.83 | 111.56 |
| 9 | T | 699 | ASN | CA-C-N | 8.50 | 131.67 | 120.28 |
| 9 | T | 699 | ASN | C-N-CA | 8.50 | 131.67 | 120.28 |
| 18 | e | 2 | GLN | CA-C-O | -8.50 | 111.08 | 119.49 |
| 8 | P | 1161 | PRO | CB-CA-C | 8.49 | 122.42 | 111.46 |
| 8 | P | 1228 | ASP | CA-CB-CG | 8.49 | 121.09 | 112.60 |
| 2 | Z | 427 | THR | N-CA-C | -8.49 | 103.97 | 112.97 |
| 20 | n | 1108 | ALA | CA-C-N | 8.49 | 134.23 | 120.30 |
| 20 | n | 1108 | ALA | C-N-CA | 8.49 | 134.23 | 120.30 |
| 14 | a | 577 | PHE | N-CA-C | -8.49 | 96.08 | 109.50 |
| 8 | P | 844 | TYR | CB-CA-C | -8.49 | 97.55 | 110.88 |
| 9 | S | 408 | ARG | N-CA-C | -8.49 | 103.06 | 113.50 |
| 16 | j | 334 | ASP | CA-C-N | 8.49 | 132.00 | 120.54 |
| 16 | j | 334 | ASP | C-N-CA | 8.49 | 132.00 | 120.54 |
| 9 | R | 553 | ALA | O-C-N | 8.48 | 131.16 | 122.08 |
| 19 | f | 320 | HIS | CG-CD2-NE2 | 8.48 | 115.68 | 107.20 |
| 7 | M | 614 | THR | CA-C-N | 8.48 | 131.47 | 120.44 |
| 7 | M | 614 | THR | C-N-CA | 8.48 | 131.47 | 120.44 |
| 8 | P | 824 | LEU | N-CA-C | -8.48 | 95.08 | 108.90 |
| 16 | c | 328 | ASN | CA-CB-CG | 8.48 | 121.08 | 112.60 |
| 9 | R | 637 | ILE | CB-CA-C | 8.48 | 119.22 | 110.91 |
| 8 | N | 84 | ASP | CA-C-O | 8.47 | 129.86 | 119.78 |
| 8 | P | 1211 | ILE | N-CA-C | 8.47 | 118.55 | 110.42 |
| 7 | M | 454 | LYS | N-CA-CB | 8.47 | 122.57 | 110.12 |
| 8 | N | 1067 | SER | N-CA-C | 8.47 | 121.58 | 111.33 |
| 1 | 0 | 1149 | ALA | CA-C-O | -8.46 | 112.19 | 120.90 |
| 19 | f | 461 | GLN | CA-C-O | -8.46 | 111.58 | 120.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | u | 39 | GLN | N-CA-C | -8.46 | 103.46 | 112.93 |
| 12 | u | 71 | VAL | N-CA-C | -8.45 | 95.95 | 108.12 |
| 6 | C | 397 | ALA | CA-C-O | -8.45 | 111.59 | 120.55 |
| 1 | 0 | 889 | GLU | N-CA-C | -8.45 | 102.74 | 113.72 |
| 7 | M | 1544 | PHE | CA-CB-CG | 8.45 | 122.25 | 113.80 |
| 7 | O | 1482 | THR | N-CA-CB | 8.45 | 124.76 | 110.49 |
| 20 | g | 992 | LYS | N-CA-C | -8.45 | 103.09 | 112.72 |
| 14 | a | 579 | ILE | O-C-N | -8.44 | 114.08 | 120.07 |
| 16 | c | 130 | ASP | CA-CB-CG | -8.44 | 104.16 | 112.60 |
| 16 | c | 619 | VAL | CA-C-N | 8.44 | 131.59 | 120.28 |
| 16 | c | 619 | VAL | C-N-CA | 8.44 | 131.59 | 120.28 |
| 15 | i | 666 | LEU | N-CA-C | -8.44 | 101.92 | 112.72 |
| 19 | m | 634 | PHE | CA-CB-CG | -8.44 | 105.36 | 113.80 |
| 8 | N | 107 | SER | CA-C-N | 8.43 | 132.51 | 120.79 |
| 8 | N | 107 | SER | C-N-CA | 8.43 | 132.51 | 120.79 |
| 8 | P | 737 | ASP | N-CA-C | 8.43 | 120.47 | 111.28 |
| 11 | V | 389 | LYS | N-CA-C | 8.43 | 121.60 | 111.82 |
| 9 | Q | 425 | ILE | N-CA-C | -8.43 | 98.34 | 108.45 |
| 8 | N | 1535 | ASN | CA-CB-CG | 8.42 | 121.02 | 112.60 |
| 1 | Y | 1055 | LEU | N-CA-C | 8.42 | 120.46 | 111.28 |
| 20 | n | 595 | ASN | N-CA-C | -8.42 | 103.52 | 113.88 |
| 21 | q | 16 | ILE | CA-C-N | 8.42 | 132.83 | 120.87 |
| 21 | q | 16 | ILE | C-N-CA | 8.42 | 132.83 | 120.87 |
| 7 | M | 736 | PHE | CA-C-O | -8.42 | 111.08 | 119.08 |
| 9 | R | 406 | PRO | CA-C-N | 8.42 | 131.56 | 120.28 |
| 9 | R | 406 | PRO | C-N-CA | 8.42 | 131.56 | 120.28 |
| 9 | S | 634 | ASP | N-CA-C | -8.42 | 101.87 | 112.90 |
| 1 | Y | 1457 | LYS | N-CA-C | -8.42 | 102.56 | 113.17 |
| 16 | c | 232 | ASN | CA-CB-CG | -8.42 | 104.18 | 112.60 |
| 20 | g | 689 | ILE | CA-C-O | 8.42 | 126.70 | 119.38 |
| 21 | p | 24 | ILE | CA-C-O | -8.41 | 112.25 | 121.17 |
| 1 | 0 | 1263 | GLN | OE1-CD-NE2 | 8.41 | 131.01 | 122.60 |
| 8 | N | 1237 | ASN | N-CA-C | -8.41 | 102.03 | 113.30 |
| 10 | W | 249 | ASP | CA-C-O | 8.41 | 132.53 | 120.51 |
| 8 | N | 365 | LEU | CA-C-N | 8.41 | 131.37 | 120.44 |
| 8 | N | 365 | LEU | C-N-CA | 8.41 | 131.37 | 120.44 |
| 8 | P | 740 | ASN | CA-CB-CG | 8.41 | 121.01 | 112.60 |
| 8 | N | 1510 | PHE | CA-CB-CG | 8.40 | 122.20 | 113.80 |
| 4 | y | 771 | ASN | CA-C-N | 8.40 | 131.15 | 120.56 |
| 4 | y | 771 | ASN | C-N-CA | 8.40 | 131.15 | 120.56 |
| 8 | P | 1044 | LEU | N-CA-C | -8.40 | 100.36 | 110.44 |
| 14 | h | 696 | GLY | CA-C-N | 8.40 | 131.88 | 120.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 696 | GLY | C-N-CA | 8.40 | 131.88 | 120.54 |
| 14 | a | 840 | PHE | CA-CB-CG | -8.40 | 105.40 | 113.80 |
| 1 | Y | 714 | LYS | CA-C-N | 8.40 | 130.34 | 119.84 |
| 1 | Y | 714 | LYS | C-N-CA | 8.40 | 130.34 | 119.84 |
| 1 | Y | 1009 | HIS | CA-CB-CG | 8.40 | 122.20 | 113.80 |
| 2 | 1 | 386 | ARG | NE-CZ-NH2 | 8.39 | 126.75 | 119.20 |
| 8 | P | 214 | LEU | N-CA-C | -8.39 | 103.06 | 113.38 |
| 9 | Q | 161 | ILE | O-C-N | 8.39 | 130.13 | 121.91 |
| 9 | T | 293 | ASN | CA-C-O | 8.39 | 124.67 | 119.55 |
| 7 | M | 1020 | SER | CA-C-N | 8.39 | 131.87 | 120.54 |
| 7 | M | 1020 | SER | C-N-CA | 8.39 | 131.87 | 120.54 |
| 7 | M | 983 | ILE | N-CA-C | 8.39 | 119.18 | 110.62 |
| 20 | g | 406 | ASN | CA-C-O | -8.39 | 112.11 | 121.51 |
| 9 | S | 88 | LYS | CA-C-O | 8.39 | 129.63 | 120.82 |
| 4 | G | 727 | SER | CA-C-O | -8.39 | 106.54 | 120.80 |
| 20 | g | 784 | ASN | CA-CB-CG | 8.38 | 120.98 | 112.60 |
| 7 | O | 893 | HIS | ND1-CE1-NE2 | 8.38 | 116.78 | 108.40 |
| 7 | O | 1110 | MET | CA-C-N | 8.38 | 131.41 | 120.60 |
| 7 | O | 1110 | MET | C-N-CA | 8.38 | 131.41 | 120.60 |
| 20 | n | 923 | HIS | CE1-NE2-CD2 | -8.38 | 100.62 | 109.00 |
| 15 | b | 85 | LYS | N-CA-C | -8.38 | 103.10 | 112.57 |
| 14 | a | 929 | HIS | CE1-NE2-CD2 | -8.38 | 100.62 | 109.00 |
| 7 | M | 352 | ILE | CA-C-N | 8.38 | 130.31 | 119.84 |
| 7 | M | 352 | ILE | C-N-CA | 8.38 | 130.31 | 119.84 |
| 7 | M | 1425 | LYS | CA-C-N | 8.38 | 131.94 | 120.46 |
| 7 | M | 1425 | LYS | C-N-CA | 8.38 | 131.94 | 120.46 |
| 16 | c | 584 | ASN | N-CA-CB | 8.37 | 124.64 | 110.49 |
| 8 | N | 1623 | GLU | CA-C-N | 8.37 | 132.33 | 120.28 |
| 8 | N | 1623 | GLU | C-N-CA | 8.37 | 132.33 | 120.28 |
| 9 | T | 707 | HIS | CA-C-N | 8.36 | 131.92 | 120.46 |
| 9 | T | 707 | HIS | C-N-CA | 8.36 | 131.92 | 120.46 |
| 11 | V | 301 | LEU | N-CA-C | 8.36 | 123.30 | 107.75 |
| 14 | h | 824 | PHE | CA-CB-CG | -8.36 | 105.44 | 113.80 |
| 9 | R | 338 | PHE | CA-CB-CG | -8.36 | 105.44 | 113.80 |
| 14 | a | 260 | VAL | N-CA-C | -8.36 | 105.18 | 113.20 |
| 7 | M | 692 | TYR | N-CA-C | -8.35 | 100.47 | 111.24 |
| 2 | Z | 1138 | ASN | CA-CB-CG | -8.35 | 104.25 | 112.60 |
| 8 | N | 1520 | LEU | CA-C-O | -8.35 | 111.70 | 120.55 |
| 7 | O | 1177 | VAL | N-CA-C | -8.35 | 105.19 | 113.20 |
| 17 | k | 142 | ASP | CA-CB-CG | -8.35 | 104.25 | 112.60 |
| 20 | n | 792 | LEU | N-CA-C | -8.35 | 102.12 | 113.30 |
| 20 | n | 863 | ARG | NE-CZ-NH2 | 8.35 | 126.71 | 119.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 891 | ARG | N-CA-CB | 8.34 | 124.68 | 110.50 |
| 2 | Z | 902 | LEU | N-CA-C | -8.34 | 102.12 | 113.30 |
| 12 | u | 686 | MET | CA-C-N | 8.34 | 131.29 | 120.44 |
| 12 | u | 686 | MET | C-N-CA | 8.34 | 131.29 | 120.44 |
| 20 | g | 529 | HIS | CA-CB-CG | 8.34 | 122.14 | 113.80 |
| 14 | h | 657 | LEU | N-CA-CB | 8.34 | 122.38 | 110.12 |
| 19 | f | 547 | GLU | N-CA-C | -8.34 | 101.18 | 112.94 |
| 4 | A | 693 | ILE | CA-C-N | 8.34 | 132.99 | 120.31 |
| 4 | A | 693 | ILE | C-N-CA | 8.34 | 132.99 | 120.31 |
| 8 | N | 774 | ILE | N-CA-C | -8.34 | 103.04 | 111.88 |
| 14 | h | 264 | ASP | CA-CB-CG | 8.34 | 120.94 | 112.60 |
| 5 | B | 390 | HIS | CA-C-N | 8.34 | 131.97 | 120.63 |
| 5 | B | 390 | HIS | C-N-CA | 8.34 | 131.97 | 120.63 |
| 16 | c | 489 | HIS | CE1-NE2-CD2 | -8.34 | 100.66 | 109.00 |
| 5 | H | 511 | GLU | CA-C-N | 8.33 | 131.88 | 120.46 |
| 5 | H | 511 | GLU | C-N-CA | 8.33 | 131.88 | 120.46 |
| 9 | T | 549 | ASP | CA-C-N | 8.33 | 128.02 | 119.19 |
| 9 | T | 549 | ASP | C-N-CA | 8.33 | 128.02 | 119.19 |
| 9 | T | 574 | GLU | CA-C-N | 8.33 | 131.79 | 120.54 |
| 9 | T | 574 | GLU | C-N-CA | 8.33 | 131.79 | 120.54 |
| 2 | Z | 976 | LYS | N-CA-C | -8.33 | 101.11 | 113.61 |
| 19 | f | 76 | HIS | CA-CB-CG | 8.33 | 122.13 | 113.80 |
| 14 | a | 871 | HIS | ND1-CE1-NE2 | 8.33 | 116.73 | 108.40 |
| 20 | g | 1064 | ARG | NE-CZ-NH2 | 8.33 | 126.70 | 119.20 |
| 2 | Z | 787 | ALA | CB-CA-C | -8.33 | 106.96 | 116.54 |
| 7 | M | 562 | LEU | CA-C-N | 8.33 | 131.26 | 120.44 |
| 7 | M | 562 | LEU | C-N-CA | 8.33 | 131.26 | 120.44 |
| 9 | R | 596 | ASP | CA-CB-CG | 8.33 | 120.93 | 112.60 |
| 7 | O | 196 | ILE | CA-C-N | 8.32 | 132.36 | 120.79 |
| 7 | O | 196 | ILE | C-N-CA | 8.32 | 132.36 | 120.79 |
| 10 | U | 284 | LYS | CB-CA-C | 8.32 | 125.91 | 110.10 |
| 20 | g | 836 | PHE | N-CA-C | -8.32 | 101.85 | 114.16 |
| 15 | b | 95 | ILE | CA-C-N | 8.32 | 128.81 | 119.83 |
| 15 | b | 95 | ILE | C-N-CA | 8.32 | 128.81 | 119.83 |
| 20 | g | 595 | ASN | N-CA-C | -8.32 | 103.07 | 113.55 |
| 2 | 1 | 626 | GLU | N-CA-C | -8.31 | 102.40 | 112.54 |
| 8 | N | 262 | SER | CA-C-O | -8.31 | 111.66 | 120.55 |
| 9 | Q | 806 | LEU | CA-C-O | -8.31 | 112.09 | 120.82 |
| 21 | o | 54 | GLY | CA-C-N | 8.31 | 137.41 | 121.54 |
| 21 | o | 54 | GLY | C-N-CA | 8.31 | 137.41 | 121.54 |
| 8 | N | 339 | GLU | CA-C-N | 8.31 | 131.41 | 120.28 |
| 8 | N | 339 | GLU | C-N-CA | 8.31 | 131.41 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | E | 394 | THR | N-CA-C | -8.30 | 103.08 | 113.55 |
| 15 | i | 571 | TYR | N-CA-C | -8.31 | 104.01 | 114.56 |
| 7 | M | 1002 | LEU | CA-C-N | 8.30 | 131.23 | 120.44 |
| 7 | M | 1002 | LEU | C-N-CA | 8.30 | 131.23 | 120.44 |
| 2 | Z | 1204 | ASP | CA-CB-CG | 8.30 | 120.90 | 112.60 |
| 13 | w | 1235 | MET | CA-C-N | 8.30 | 131.24 | 120.44 |
| 13 | w | 1235 | MET | C-N-CA | 8.30 | 131.24 | 120.44 |
| 14 | a | 291 | LEU | CA-C-O | -8.30 | 113.07 | 119.46 |
| 7 | M | 1122 | TRP | N-CA-C | -8.30 | 104.30 | 114.75 |
| 7 | O | 740 | LEU | N-CA-C | -8.29 | 94.01 | 108.69 |
| 19 | m | 383 | PRO | CA-C-N | 8.30 | 131.22 | 120.44 |
| 19 | m | 383 | PRO | C-N-CA | 8.30 | 131.22 | 120.44 |
| 19 | m | 509 | HIS | CA-C-N | 8.29 | 131.22 | 120.44 |
| 19 | m | 509 | HIS | C-N-CA | 8.29 | 131.22 | 120.44 |
| 14 | a | 929 | HIS | ND1-CE1-NE2 | 8.29 | 116.69 | 108.40 |
| 9 | R | 678 | ASP | CA-C-N | 8.29 | 133.00 | 120.82 |
| 9 | R | 678 | ASP | C-N-CA | 8.29 | 133.00 | 120.82 |
| 2 | Z | 242 | HIS | N-CA-C | 8.29 | 121.38 | 111.02 |
| 20 | n | 445 | ASP | N-CA-C | -8.29 | 95.73 | 109.07 |
| 14 | a | 845 | ILE | N-CA-C | -8.29 | 105.41 | 113.53 |
| 16 | j | 272 | ILE | CA-C-N | 8.28 | 131.81 | 120.46 |
| 16 | j | 272 | ILE | C-N-CA | 8.28 | 131.81 | 120.46 |
| 21 | p | 40 | ASP | CA-C-O | -8.28 | 111.77 | 120.55 |
| 17 | d | 224 | SER | CA-C-O | -8.28 | 111.97 | 121.66 |
| 6 | C | 318 | SER | N-CA-C | 8.28 | 120.39 | 111.36 |
| 1 | Y | 160 | ILE | N-CA-C | -8.28 | 103.75 | 111.45 |
| 7 | M | 1455 | THR | CA-C-N | 8.28 | 129.11 | 120.00 |
| 7 | M | 1455 | THR | C-N-CA | 8.28 | 129.11 | 120.00 |
| 8 | P | 1320 | GLU | CA-C-N | 8.28 | 132.49 | 120.82 |
| 8 | P | 1320 | GLU | C-N-CA | 8.28 | 132.49 | 120.82 |
| 1 | Y | 394 | GLU | CA-C-N | 8.28 | 128.24 | 119.05 |
| 1 | Y | 394 | GLU | C-N-CA | 8.28 | 128.24 | 119.05 |
| 15 | b | 66 | PRO | CA-C-O | -8.28 | 115.18 | 121.31 |
| 8 | N | 695 | LEU | N-CA-C | -8.28 | 103.28 | 112.72 |
| 7 | O | 875 | VAL | CA-C-N | 8.28 | 131.71 | 120.54 |
| 7 | O | 875 | VAL | C-N-CA | 8.28 | 131.71 | 120.54 |
| 2 | Z | 850 | HIS | CE1-NE2-CD2 | -8.28 | 100.72 | 109.00 |
| 9 | S | 71 | TYR | CA-C-N | 8.28 | 131.71 | 120.54 |
| 9 | S | 71 | TYR | C-N-CA | 8.28 | 131.71 | 120.54 |
| 9 | R | 470 | GLY | CA-C-N | 8.27 | 127.92 | 119.56 |
| 9 | R | 470 | GLY | C-N-CA | 8.27 | 127.92 | 119.56 |
| 9 | Q | 787 | HIS | N-CA-C | 8.27 | 121.42 | 111.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 457 | SER | CB-CA-C | 8.27 | 125.82 | 110.10 |
| 15 | b | 327 | GLU | CA-C-N | 8.27 | 131.36 | 120.28 |
| 15 | b | 327 | GLU | C-N-CA | 8.27 | 131.36 | 120.28 |
| 5 | B | 440 | PHE | CA-CB-CG | -8.27 | 105.53 | 113.80 |
| 8 | P | 1086 | ILE | N-CA-C | -8.27 | 102.82 | 111.58 |
| 8 | N | 911 | PRO | N-CA-C | 8.27 | 124.58 | 113.84 |
| 8 | P | 1311 | LEU | N-CA-CB | 8.27 | 122.00 | 110.01 |
| 2 | Z | 575 | ARG | NE-CZ-NH1 | 8.27 | 129.77 | 121.50 |
| 7 | O | 927 | GLY | CA-C-N | 8.26 | 132.18 | 120.28 |
| 7 | O | 927 | GLY | C-N-CA | 8.26 | 132.18 | 120.28 |
| 8 | N | 1239 | ASP | CA-CB-CG | 8.26 | 120.86 | 112.60 |
| 9 | T | 811 | ARG | NE-CZ-NH2 | -8.26 | 111.77 | 119.20 |
| 8 | N | 861 | ILE | O-C-N | 8.26 | 129.88 | 121.87 |
| 7 | O | 1306 | TRP | CA-C-N | 8.26 | 131.02 | 120.70 |
| 7 | O | 1306 | TRP | C-N-CA | 8.26 | 131.02 | 120.70 |
| 16 | c | 558 | ASN | CA-CB-CG | 8.26 | 120.86 | 112.60 |
| 19 | f | 179 | ILE | CA-C-N | 8.26 | 132.87 | 120.31 |
| 19 | f | 179 | ILE | C-N-CA | 8.26 | 132.87 | 120.31 |
| 7 | M | 307 | ASP | N-CA-CB | 8.26 | 124.45 | 110.49 |
| 13 | x | 1439 | VAL | CA-C-N | 8.25 | 129.14 | 119.98 |
| 13 | x | 1439 | VAL | C-N-CA | 8.25 | 129.14 | 119.98 |
| 9 | T | 462 | PHE | CA-CB-CG | 8.24 | 122.05 | 113.80 |
| 20 | g | 782 | ASP | N-CA-CB | 8.24 | 121.96 | 110.01 |
| 1 | 0 | 1353 | ASN | CA-CB-CG | -8.24 | 104.36 | 112.60 |
| 4 | G | 712 | ASP | CA-CB-CG | 8.24 | 120.84 | 112.60 |
| 9 | S | 473 | ARG | N-CA-C | -8.24 | 102.11 | 114.64 |
| 7 | M | 209 | ASN | CA-CB-CG | 8.24 | 120.84 | 112.60 |
| 15 | b | 216 | ASP | N-CA-C | -8.24 | 93.25 | 110.80 |
| 8 | N | 936 | LEU | CA-C-O | -8.24 | 111.82 | 120.55 |
| 9 | T | 123 | MET | CB-CA-C | -8.24 | 97.95 | 110.88 |
| 9 | R | 732 | TRP | N-CA-C | -8.24 | 103.69 | 114.31 |
| 4 | G | 811 | SER | CA-C-N | 8.23 | 131.31 | 120.28 |
| 4 | G | 811 | SER | C-N-CA | 8.23 | 131.31 | 120.28 |
| 1 | 0 | 441 | VAL | CA-C-N | 8.23 | 129.12 | 119.98 |
| 1 | 0 | 441 | VAL | C-N-CA | 8.23 | 129.12 | 119.98 |
| 8 | P | 109 | ARG | NE-CZ-NH2 | -8.23 | 111.79 | 119.20 |
| 8 | P | 1467 | SER | CA-C-N | 8.23 | 131.74 | 120.46 |
| 8 | P | 1467 | SER | C-N-CA | 8.23 | 131.74 | 120.46 |
| 7 | M | 696 | PHE | CA-CB-CG | -8.23 | 105.57 | 113.80 |
| 9 | S | 767 | ILE | N-CA-C | -8.23 | 103.33 | 112.80 |
| 7 | O | 903 | ASN | CA-C-N | 8.23 | 132.50 | 120.90 |
| 7 | O | 903 | ASN | C-N-CA | 8.23 | 132.50 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | r | 55 | ASN | N-CA-C | 8.23 | 128.32 | 110.80 |
| 12 | v | 183 | THR | N-CA-C | 8.22 | 121.05 | 111.02 |
| 21 | t | 40 | ASP | CA-C-N | 8.22 | 131.73 | 120.46 |
| 21 | t | 40 | ASP | C-N-CA | 8.22 | 131.73 | 120.46 |
| 12 | v | 339 | VAL | CA-C-N | 8.22 | 133.64 | 121.72 |
| 12 | v | 339 | VAL | C-N-CA | 8.22 | 133.64 | 121.72 |
| 7 | M | 1276 | ASP | CA-CB-CG | 8.22 | 120.82 | 112.60 |
| 15 | i | 473 | LEU | CA-C-N | 8.22 | 131.29 | 120.28 |
| 15 | i | 473 | LEU | C-N-CA | 8.22 | 131.29 | 120.28 |
| 20 | g | 1001 | ASP | CA-CB-CG | 8.22 | 120.82 | 112.60 |
| 14 | a | 23 | THR | N-CA-C | -8.22 | 103.35 | 112.72 |
| 5 | E | 288 | ILE | CA-C-N | 8.21 | 131.29 | 120.28 |
| 5 | E | 288 | ILE | C-N-CA | 8.21 | 131.29 | 120.28 |
| 7 | M | 1356 | LEU | CA-C-N | 8.21 | 132.11 | 120.28 |
| 7 | M | 1356 | LEU | C-N-CA | 8.21 | 132.11 | 120.28 |
| 20 | n | 984 | PHE | N-CA-C | -8.21 | 101.76 | 112.68 |
| 7 | M | 191 | ASP | CA-C-N | 8.21 | 131.71 | 120.46 |
| 7 | M | 191 | ASP | C-N-CA | 8.21 | 131.71 | 120.46 |
| 8 | P | 414 | ASN | CA-CB-CG | 8.21 | 120.81 | 112.60 |
| 20 | n | 86 | LEU | N-CA-C | -8.21 | 95.26 | 108.55 |
| 1 | 0 | 1396 | ASN | CA-C-N | 8.20 | 131.62 | 120.38 |
| 1 | 0 | 1396 | ASN | C-N-CA | 8.20 | 131.62 | 120.38 |
| 2 | 1 | 1122 | ASP | CA-CB-CG | 8.20 | 120.80 | 112.60 |
| 6 | C | 461 | HIS | CG-CD2-NE2 | 8.20 | 115.40 | 107.20 |
| 5 | H | 323 | LEU | CB-CA-C | -8.20 | 94.10 | 110.42 |
| 20 | n | 396 | LYS | CA-C-N | 8.20 | 128.25 | 119.89 |
| 20 | n | 396 | LYS | C-N-CA | 8.20 | 128.25 | 119.89 |
| 20 | n | 948 | GLN | CA-C-N | 8.20 | 132.09 | 120.28 |
| 20 | n | 948 | GLN | C-N-CA | 8.20 | 132.09 | 120.28 |
| 16 | j | 542 | GLN | N-CA-C | 8.20 | 120.94 | 111.11 |
| 2 | 1 | 679 | SER | CB-CA-C | 8.19 | 126.73 | 110.42 |
| 7 | M | 250 | ALA | N-CA-C | -8.20 | 103.79 | 113.21 |
| 14 | h | 436 | HIS | ND1-CE1-NE2 | 8.19 | 116.59 | 108.40 |
| 2 | 1 | 661 | ALA | N-CA-C | -8.19 | 103.29 | 113.28 |
| 7 | M | 1475 | ILE | N-CA-C | -8.19 | 102.83 | 110.53 |
| 15 | b | 422 | MET | O-C-N | -8.19 | 113.44 | 122.12 |
| 14 | a | 437 | ASN | N-CA-CB | 8.19 | 122.74 | 110.53 |
| 9 | Q | 52 | ARG | CA-C-N | 8.19 | 131.68 | 120.46 |
| 9 | Q | 52 | ARG | C-N-CA | 8.19 | 131.68 | 120.46 |
| 8 | P | 597 | LEU | N-CA-C | -8.19 | 102.88 | 113.12 |
| 12 | u | 352 | GLU | CA-C-N | 8.19 | 134.55 | 123.00 |
| 12 | u | 352 | GLU | C-N-CA | 8.19 | 134.55 | 123.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | a | 71 | HIS | CG-CD2-NE2 | 8.19 | 115.39 | 107.20 |
| 2 | 1 | 709 | PHE | CB-CA-C | -8.18 | 94.96 | 110.67 |
| 7 | M | 1138 | PHE | CA-CB-CG | -8.18 | 105.62 | 113.80 |
| 15 | i | 627 | TYR | N-CA-C | -8.18 | 103.39 | 112.72 |
| 9 | R | 637 | ILE | N-CA-C | -8.18 | 105.25 | 112.12 |
| 16 | c | 188 | VAL | CA-C-N | 8.18 | 131.08 | 120.44 |
| 16 | c | 188 | VAL | C-N-CA | 8.18 | 131.08 | 120.44 |
| 1 | 0 | 199 | ASN | CA-CB-CG | 8.18 | 120.78 | 112.60 |
| 7 | M | 1324 | ARG | CA-C-N | 8.18 | 131.24 | 120.28 |
| 7 | M | 1324 | ARG | C-N-CA | 8.18 | 131.24 | 120.28 |
| 2 | 1 | 1205 | LEU | N-CA-C | -8.18 | 101.18 | 112.30 |
| 8 | P | 187 | PHE | CA-C-N | 8.18 | 130.86 | 120.56 |
| 8 | P | 187 | PHE | C-N-CA | 8.18 | 130.86 | 120.56 |
| 8 | P | 1069 | ILE | N-CA-CB | 8.18 | 124.63 | 110.65 |
| 8 | P | 1558 | GLN | OE1-CD-NE2 | -8.17 | 114.43 | 122.60 |
| 14 | h | 149 | TRP | N-CA-C | -8.17 | 101.32 | 112.03 |
| 14 | a | 375 | ASN | CA-CB-CG | 8.17 | 120.77 | 112.60 |
| 7 | M | 1312 | ILE | N-CA-CB | 8.17 | 119.20 | 110.62 |
| 9 | T | 222 | PHE | CA-C-N | 8.17 | 132.05 | 120.28 |
| 9 | T | 222 | PHE | C-N-CA | 8.17 | 132.05 | 120.28 |
| 11 | X | 369 | ALA | N-CA-C | 8.17 | 122.81 | 113.01 |
| 8 | P | 163 | ASP | N-CA-C | -8.17 | 101.42 | 112.94 |
| 1 | Y | 1432 | GLU | CA-C-N | 8.17 | 131.43 | 120.65 |
| 1 | Y | 1432 | GLU | C-N-CA | 8.17 | 131.43 | 120.65 |
| 7 | M | 730 | VAL | CA-C-N | 8.16 | 131.22 | 120.28 |
| 7 | M | 730 | VAL | C-N-CA | 8.16 | 131.22 | 120.28 |
| 9 | Q | 17 | GLY | CA-C-N | 8.16 | 131.54 | 120.44 |
| 9 | Q | 17 | GLY | C-N-CA | 8.16 | 131.54 | 120.44 |
| 9 | S | 255 | GLU | N-CA-C | -8.16 | 102.35 | 112.88 |
| 14 | h | 452 | ASP | CA-CB-CG | 8.16 | 120.76 | 112.60 |
| 4 | G | 745 | TYR | CA-C-N | 8.16 | 131.56 | 120.38 |
| 4 | G | 745 | TYR | C-N-CA | 8.16 | 131.56 | 120.38 |
| 4 | z | 651 | SER | CA-C-N | 8.16 | 131.21 | 120.28 |
| 4 | z | 651 | SER | C-N-CA | 8.16 | 131.21 | 120.28 |
| 2 | 1 | 999 | ASP | CA-CB-CG | 8.16 | 120.76 | 112.60 |
| 6 | L | 318 | SER | CA-C-N | 8.16 | 134.55 | 120.68 |
| 6 | L | 318 | SER | C-N-CA | 8.16 | 134.55 | 120.68 |
| 6 | F | 301 | HIS | CA-C-N | 8.15 | 132.02 | 120.28 |
| 6 | F | 301 | HIS | C-N-CA | 8.15 | 132.02 | 120.28 |
| 16 | c | 405 | SER | CA-C-N | 8.15 | 131.04 | 120.44 |
| 16 | c | 405 | SER | C-N-CA | 8.15 | 131.04 | 120.44 |
| 17 | d | 188 | ASN | CA-CB-CG | -8.15 | 104.45 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1555 | VAL | CA-C-O | 8.15 | 127.39 | 119.97 |
| 9 | T | 776 | ILE | N-CA-C | -8.15 | 102.59 | 110.42 |
| 16 | j | 768 | ASN | CA-CB-CG | -8.15 | 104.45 | 112.60 |
| 14 | a | 160 | VAL | N-CA-C | -8.15 | 104.93 | 112.43 |
| 7 | M | 1189 | MET | CA-CB-CG | 8.15 | 130.40 | 114.10 |
| 7 | M | 129 | GLU | CA-C-N | 8.15 | 132.01 | 120.28 |
| 7 | M | 129 | GLU | C-N-CA | 8.15 | 132.01 | 120.28 |
| 7 | O | 763 | HIS | CB-CG-CD2 | -8.15 | 120.61 | 131.20 |
| 14 | h | 669 | ARG | N-CA-C | -8.15 | 102.37 | 112.88 |
| 21 | r | 68 | TYR | N-CA-C | -8.15 | 100.32 | 113.19 |
| 7 | M | 285 | PHE | CA-C-N | 8.14 | 130.98 | 120.56 |
| 7 | M | 285 | PHE | C-N-CA | 8.14 | 130.98 | 120.56 |
| 2 | Z | 247 | PHE | CA-CB-CG | -8.14 | 105.66 | 113.80 |
| 20 | n | 142 | PHE | CA-C-N | 8.14 | 130.02 | 119.84 |
| 20 | n | 142 | PHE | C-N-CA | 8.14 | 130.02 | 119.84 |
| 7 | M | 288 | TRP | CE2-CD2-CE3 | 8.14 | 126.94 | 118.80 |
| 9 | S | 150 | GLN | O-C-N | -8.14 | 113.69 | 122.07 |
| 1 | 0 | 1166 | VAL | CA-C-N | 8.14 | 137.08 | 121.54 |
| 1 | 0 | 1166 | VAL | C-N-CA | 8.14 | 137.08 | 121.54 |
| 9 | Q | 124 | SER | CA-C-N | 8.14 | 130.81 | 120.56 |
| 9 | Q | 124 | SER | C-N-CA | 8.14 | 130.81 | 120.56 |
| 12 | u | 87 | GLU | CA-C-N | 8.13 | 134.03 | 123.13 |
| 12 | u | 87 | GLU | C-N-CA | 8.13 | 134.03 | 123.13 |
| 13 | w | 1309 | ASP | N-CA-CB | 8.13 | 122.20 | 110.16 |
| 21 | o | 56 | THR | CA-C-O | -8.14 | 108.88 | 120.51 |
| 6 | I | 373 | PHE | CA-CB-CG | -8.13 | 105.67 | 113.80 |
| 7 | M | 420 | THR | N-CA-C | -8.13 | 95.32 | 108.41 |
| 4 | D | 756 | ASN | CA-C-N | 8.13 | 131.50 | 120.44 |
| 4 | D | 756 | ASN | C-N-CA | 8.13 | 131.50 | 120.44 |
| 21 | p | 71 | HIS | CB-CG-ND1 | 8.13 | 134.90 | 122.70 |
| 14 | h | 493 | TRP | CA-C-N | 8.13 | 137.07 | 121.54 |
| 14 | h | 493 | TRP | C-N-CA | 8.13 | 137.07 | 121.54 |
| 9 | Q | 660 | LEU | N-CA-CB | 8.13 | 122.07 | 110.12 |
| 2 | Z | 108 | THR | CA-C-N | 8.13 | 130.00 | 119.84 |
| 2 | Z | 108 | THR | C-N-CA | 8.13 | 130.00 | 119.84 |
| 2 | Z | 921 | SER | CB-CA-C | -8.13 | 94.66 | 110.10 |
| 14 | a | 379 | ILE | N-CA-C | -8.13 | 95.74 | 107.77 |
| 6 | L | 450 | PHE | CA-CB-CG | 8.12 | 121.92 | 113.80 |
| 9 | T | 140 | ILE | N-CA-C | 8.12 | 118.22 | 110.42 |
| 16 | j | 465 | PHE | CA-CB-CG | -8.12 | 105.67 | 113.80 |
| 19 | m | 608 | SER | N-CA-C | -8.12 | 102.93 | 112.92 |
| 16 | c | 507 | ILE | CA-C-N | 8.12 | 131.00 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 16 | c | 507 | ILE | C-N-CA | 8.12 | 131.00 | 120.44 |
| 15 | i | 206 | GLU | N-CA-C | 8.12 | 120.13 | 111.28 |
| 8 | N | 1553 | GLN | CA-C-O | 8.12 | 129.40 | 120.63 |
| 14 | h | 724 | PHE | CA-CB-CG | 8.12 | 121.92 | 113.80 |
| 5 | E | 529 | LYS | CA-C-N | 8.11 | 131.81 | 120.29 |
| 5 | E | 529 | LYS | C-N-CA | 8.11 | 131.81 | 120.29 |
| 7 | M | 996 | LEU | CA-C-N | 8.11 | 137.04 | 121.54 |
| 7 | M | 996 | LEU | C-N-CA | 8.11 | 137.04 | 121.54 |
| 7 | O | 603 | GLU | CA-C-O | -8.11 | 108.91 | 120.51 |
| 16 | j | 340 | LEU | N-CA-C | 8.11 | 119.75 | 111.07 |
| 21 | p | 56 | THR | CA-CB-CG2 | -8.11 | 96.71 | 110.50 |
| 20 | g | 790 | HIS | ND1-CE1-NE2 | 8.11 | 116.51 | 108.40 |
| 1 | 0 | 104 | ALA | CA-C-N | 8.11 | 128.94 | 119.94 |
| 1 | 0 | 104 | ALA | C-N-CA | 8.11 | 128.94 | 119.94 |
| 16 | j | 591 | GLU | CA-C-O | 8.11 | 129.02 | 120.42 |
| 8 | P | 1050 | SER | N-CA-C | -8.11 | 93.53 | 110.80 |
| 4 | D | 811 | SER | CA-C-N | 8.11 | 130.98 | 120.44 |
| 4 | D | 811 | SER | C-N-CA | 8.11 | 130.98 | 120.44 |
| 7 | M | 1398 | SER | N-CA-C | -8.10 | 97.54 | 108.24 |
| 14 | h | 871 | HIS | CA-C-N | 8.10 | 130.97 | 120.44 |
| 14 | h | 871 | HIS | C-N-CA | 8.10 | 130.97 | 120.44 |
| 19 | m | 580 | PHE | CA-CB-CG | -8.10 | 105.70 | 113.80 |
| 8 | P | 24 | ASP | CA-CB-CG | 8.10 | 120.70 | 112.60 |
| 9 | S | 424 | ASN | N-CA-C | -8.10 | 95.70 | 108.90 |
| 19 | f | 232 | ASN | N-CA-C | -8.10 | 102.17 | 114.16 |
| 14 | a | 900 | VAL | N-CA-C | -8.10 | 105.12 | 112.90 |
| 7 | M | 919 | ASN | CA-CB-CG | 8.10 | 120.70 | 112.60 |
| 9 | R | 586 | PHE | CA-CB-CG | -8.10 | 105.70 | 113.80 |
| 2 | Z | 1129 | GLU | N-CA-C | -8.10 | 103.35 | 113.55 |
| 5 | H | 346 | GLN | N-CA-CB | 8.09 | 124.17 | 110.49 |
| 4 | J | 771 | ASN | N-CA-C | 8.09 | 120.10 | 111.28 |
| 20 | n | 860 | LEU | N-CA-C | -8.09 | 103.50 | 112.72 |
| 2 | 1 | 881 | ALA | CA-C-N | 8.09 | 131.93 | 120.28 |
| 2 | 1 | 881 | ALA | C-N-CA | 8.09 | 131.93 | 120.28 |
| 7 | O | 754 | ASP | N-CA-CB | 8.09 | 121.99 | 109.94 |
| 8 | N | 272 | ILE | CB-CA-C | -8.09 | 101.44 | 112.04 |
| 10 | W | 272 | ASN | CA-CB-CG | 8.09 | 120.69 | 112.60 |
| 6 | L | 463 | LYS | O-C-N | -8.09 | 113.74 | 122.07 |
| 20 | n | 923 | HIS | ND1-CE1-NE2 | 8.09 | 116.48 | 108.40 |
| 9 | Q | 699 | ASN | CA-CB-CG | -8.08 | 104.52 | 112.60 |
| 14 | a | 317 | ASN | CA-CB-CG | -8.08 | 104.52 | 112.60 |
| 14 | a | 795 | GLU | N-CA-C | 8.08 | 120.79 | 109.15 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 1059 | ASN | CA-CB-CG | -8.08 | 104.52 | 112.60 |
| 7 | M | 288 | TRP | CB-CG-CD2 | 8.08 | 138.11 | 126.80 |
| 19 | m | 163 | ARG | NE-CZ-NH1 | 8.08 | 129.58 | 121.50 |
| 2 | Z | 850 | HIS | ND1-CE1-NE2 | 8.07 | 116.47 | 108.40 |
| 2 | 1 | 481 | GLY | CA-C-N | 8.07 | 127.75 | 119.19 |
| 2 | 1 | 481 | GLY | C-N-CA | 8.07 | 127.75 | 119.19 |
| 17 | k | 171 | ARG | NE-CZ-NH2 | 8.07 | 126.46 | 119.20 |
| 7 | M | 1106 | PHE | N-CA-C | 8.07 | 120.79 | 111.11 |
| 7 | O | 914 | ASP | CA-C-O | -8.06 | 112.00 | 120.55 |
| 7 | M | 1100 | LEU | CA-C-N | 8.06 | 131.00 | 120.60 |
| 7 | M | 1100 | LEU | C-N-CA | 8.06 | 131.00 | 120.60 |
| 2 | Z | 1232 | LYS | N-CA-C | 8.06 | 120.07 | 111.28 |
| 20 | g | 234 | ARG | NE-CZ-NH2 | 8.06 | 126.46 | 119.20 |
| 1 | 0 | 1471 | ILE | N-CA-CB | 8.06 | 119.76 | 110.65 |
| 2 | 1 | 1367 | LYS | N-CA-C | -8.06 | 101.93 | 112.41 |
| 9 | Q | 62 | ALA | N-CA-CB | 8.06 | 124.11 | 110.49 |
| 2 | Z | 1238 | TRP | N-CA-CB | 8.06 | 121.97 | 110.12 |
| 14 | a | 574 | LEU | N-CA-C | 8.06 | 120.85 | 111.02 |
| 8 | N | 519 | SER | O-C-N | -8.06 | 112.67 | 123.15 |
| 9 | Q | 680 | ASN | CA-C-N | 8.06 | 131.88 | 120.28 |
| 9 | Q | 680 | ASN | C-N-CA | 8.06 | 131.88 | 120.28 |
| 2 | Z | 1282 | VAL | N-CA-C | -8.06 | 104.90 | 112.96 |
| 7 | O | 1352 | GLU | CA-C-N | 8.06 | 131.42 | 120.38 |
| 7 | O | 1352 | GLU | C-N-CA | 8.06 | 131.42 | 120.38 |
| 8 | P | 1531 | SER | N-CA-C | 8.05 | 119.69 | 111.07 |
| 1 | Y | 617 | ALA | N-CA-C | 8.05 | 119.69 | 111.07 |
| 7 | O | 276 | ALA | N-CA-C | 8.05 | 120.97 | 111.71 |
| 9 | Q | 712 | GLU | CA-C-N | 8.05 | 131.49 | 120.46 |
| 9 | Q | 712 | GLU | C-N-CA | 8.05 | 131.49 | 120.46 |
| 12 | u | 628 | MET | CA-C-N | 8.05 | 131.07 | 120.28 |
| 12 | u | 628 | MET | C-N-CA | 8.05 | 131.07 | 120.28 |
| 8 | N | 767 | ILE | N-CA-C | -8.05 | 105.03 | 112.43 |
| 2 | 1 | 542 | ALA | N-CA-C | -8.04 | 100.98 | 108.22 |
| 11 | X | 353 | GLU | N-CA-C | -8.04 | 103.26 | 113.72 |
| 9 | T | 640 | SER | CA-C-N | 8.04 | 130.98 | 120.60 |
| 9 | T | 640 | SER | C-N-CA | 8.04 | 130.98 | 120.60 |
| 2 | Z | 455 | PRO | CA-C-N | 8.04 | 135.00 | 122.94 |
| 2 | Z | 455 | PRO | C-N-CA | 8.04 | 135.00 | 122.94 |
| 4 | y | 640 | LEU | CA-C-N | 8.04 | 130.69 | 120.56 |
| 4 | y | 640 | LEU | C-N-CA | 8.04 | 130.69 | 120.56 |
| 7 | O | 668 | ARG | NH1-CZ-NH2 | -8.04 | 108.85 | 119.30 |
| 8 | N | 1046 | LYS | N-CA-CB | 8.04 | 122.70 | 110.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 761 | LEU | N-CA-CB | 8.04 | 124.07 | 110.49 |
| 9 | S | 462 | PHE | CA-CB-CG | 8.04 | 121.84 | 113.80 |
| 14 | h | 821 | HIS | CE1-NE2-CD2 | -8.04 | 100.96 | 109.00 |
| 2 | 1 | 1282 | VAL | CA-C-O | 8.03 | 126.37 | 119.38 |
| 7 | O | 770 | ILE | CA-C-N | 8.03 | 131.38 | 120.38 |
| 7 | O | 770 | ILE | C-N-CA | 8.03 | 131.38 | 120.38 |
| 20 | n | 804 | ILE | CA-C-O | -8.03 | 110.74 | 120.78 |
| 1 | 0 | 858 | ASP | CA-CB-CG | 8.03 | 120.63 | 112.60 |
| 2 | Z | 1124 | ASP | CA-CB-CG | 8.03 | 120.63 | 112.60 |
| 18 | e | 17 | TYR | CA-C-O | -8.03 | 112.20 | 120.71 |
| 20 | g | 864 | PHE | CA-CB-CG | 8.03 | 121.83 | 113.80 |
| 8 | N | 756 | TRP | N-CA-C | -8.02 | 97.12 | 109.24 |
| 7 | O | 1216 | PHE | CA-CB-CG | -8.02 | 105.78 | 113.80 |
| 20 | g | 614 | TRP | CA-C-N | 8.02 | 133.94 | 121.19 |
| 20 | g | 614 | TRP | C-N-CA | 8.02 | 133.94 | 121.19 |
| 20 | n | 109 | ASN | CA-CB-CG | 8.02 | 120.62 | 112.60 |
| 10 | U | 279 | ASP | N-CA-C | -8.02 | 103.51 | 112.57 |
| 8 | P | 840 | LEU | N-CA-C | -8.01 | 102.77 | 112.54 |
| 8 | P | 1008 | THR | CA-C-O | -8.01 | 109.18 | 120.16 |
| 7 | M | 1173 | THR | CA-C-N | 8.01 | 131.92 | 120.79 |
| 7 | M | 1173 | THR | C-N-CA | 8.01 | 131.92 | 120.79 |
| 7 | O | 1216 | PHE | N-CA-C | -8.01 | 102.55 | 112.88 |
| 8 | P | 365 | LEU | N-CA-C | 8.01 | 120.01 | 111.28 |
| 9 | S | 86 | PHE | CA-C-N | 8.01 | 130.93 | 120.60 |
| 9 | S | 86 | PHE | C-N-CA | 8.01 | 130.93 | 120.60 |
| 9 | R | 630 | ARG | NE-CZ-NH1 | 8.01 | 129.51 | 121.50 |
| 12 | u | 545 | LEU | CA-C-N | 8.01 | 128.87 | 119.98 |
| 1 | 0 | 183 | TRP | CA-CB-CG | 8.01 | 128.81 | 113.60 |
| 2 | 1 | 1356 | ASP | CA-CB-CG | 8.01 | 120.61 | 112.60 |
| 8 | N | 59 | ARG | NE-CZ-NH2 | -8.01 | 112.00 | 119.20 |
| 11 | X | 280 | ILE | N-CA-C | -8.01 | 105.33 | 113.10 |
| 12 | u | 545 | LEU | C-N-CA | 8.01 | 128.87 | 119.98 |
| 16 | j | 459 | PHE | CA-CB-CG | -8.01 | 105.79 | 113.80 |
| 21 | p | 38 | GLU | N-CA-C | 8.01 | 120.00 | 111.28 |
| 8 | P | 816 | ALA | CA-C-N | 8.00 | 127.66 | 119.82 |
| 8 | P | 816 | ALA | C-N-CA | 8.00 | 127.66 | 119.82 |
| 9 | S | 777 | ILE | N-CA-C | -8.00 | 105.22 | 112.90 |
| 7 | O | 1308 | GLN | O-C-N | 8.00 | 130.60 | 122.12 |
| 18 | e | 70 | ARG | N-CA-C | 8.00 | 122.10 | 110.42 |
| 18 | e | 229 | GLN | OE1-CD-NE2 | 8.00 | 130.60 | 122.60 |
| 6 | C | 389 | ARG | O-C-N | 8.00 | 130.60 | 122.12 |
| 15 | b | 618 | ASN | N-CA-C | -8.00 | 101.10 | 113.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 1095 | GLU | N-CA-CB | -8.00 | 96.97 | 110.49 |
| 7 | O | 1312 | ILE | N-CA-CB | 8.00 | 119.02 | 110.62 |
| 15 | i | 422 | MET | N-CA-C | 8.00 | 120.00 | 111.28 |
| 8 | N | 1214 | PHE | N-CA-C | 7.99 | 119.99 | 111.28 |
| 4 | G | 726 | VAL | CA-CB-CG2 | -7.99 | 96.81 | 110.40 |
| 1 | 0 | 669 | PHE | CA-CB-CG | 7.99 | 121.79 | 113.80 |
| 19 | m | 617 | ILE | N-CA-C | -7.99 | 105.70 | 113.53 |
| 14 | a | 183 | LEU | N-CA-C | -7.99 | 97.31 | 110.17 |
| 8 | P | 1557 | LEU | O-C-N | 7.99 | 130.29 | 122.07 |
| 1 | 0 | 100 | PRO | CA-C-N | 7.98 | 130.81 | 120.44 |
| 1 | 0 | 100 | PRO | C-N-CA | 7.98 | 130.81 | 120.44 |
| 16 | j | 541 | ALA | N-CA-C | -7.98 | 104.02 | 114.31 |
| 9 | Q | 136 | PHE | CA-C-N | 7.98 | 130.81 | 120.44 |
| 9 | Q | 136 | PHE | C-N-CA | 7.98 | 130.81 | 120.44 |
| 7 | M | 1148 | LEU | CA-C-N | 7.98 | 130.97 | 120.28 |
| 7 | M | 1148 | LEU | C-N-CA | 7.98 | 130.97 | 120.28 |
| 8 | P | 449 | ASP | CA-C-N | 7.98 | 132.80 | 120.75 |
| 8 | P | 449 | ASP | C-N-CA | 7.98 | 132.80 | 120.75 |
| 14 | h | 89 | HIS | N-CA-C | -7.98 | 101.64 | 113.61 |
| 11 | V | 395 | LEU | CA-C-O | -7.98 | 111.97 | 120.42 |
| 1 | 0 | 509 | PHE | CA-CB-CG | -7.97 | 105.83 | 113.80 |
| 5 | B | 320 | GLU | N-CA-CB | 7.97 | 123.97 | 110.49 |
| 9 | Q | 367 | PHE | CA-CB-CG | -7.97 | 105.83 | 113.80 |
| 20 | g | 858 | ASN | N-CA-C | -7.97 | 103.70 | 113.50 |
| 1 | Y | 613 | GLY | N-CA-C | 7.96 | 122.12 | 112.48 |
| 2 | Z | 1385 | ASP | CA-CB-CG | 7.96 | 120.56 | 112.60 |
| 12 | u | 546 | GLY | CA-C-N | 7.96 | 131.37 | 120.46 |
| 12 | u | 546 | GLY | C-N-CA | 7.96 | 131.37 | 120.46 |
| 20 | n | 1032 | GLU | N-CA-C | -7.96 | 102.53 | 114.64 |
| 9 | T | 533 | ARG | CA-C-N | 7.96 | 131.16 | 120.65 |
| 9 | T | 533 | ARG | C-N-CA | 7.96 | 131.16 | 120.65 |
| 4 | z | 755 | LEU | CA-C-N | 7.96 | 131.29 | 120.54 |
| 4 | z | 755 | LEU | C-N-CA | 7.96 | 131.29 | 120.54 |
| 14 | a | 957 | ASP | N-CA-CB | 7.96 | 123.95 | 110.49 |
| 9 | S | 787 | HIS | CA-CB-CG | 7.96 | 121.76 | 113.80 |
| 2 | Z | 510 | CYS | CA-C-N | 7.95 | 131.02 | 122.11 |
| 2 | Z | 510 | CYS | C-N-CA | 7.95 | 131.02 | 122.11 |
| 21 | q | 72 | GLU | CA-C-O | -7.95 | 111.27 | 120.49 |
| 4 | y | 794 | ILE | N-CA-C | 7.95 | 118.71 | 110.36 |
| 2 | Z | 192 | HIS | CE1-NE2-CD2 | -7.95 | 101.05 | 109.00 |
| 16 | j | 353 | ASN | N-CA-C | -7.95 | 102.36 | 112.93 |
| 2 | Z | 380 | ASP | N-CA-CB | 7.94 | 121.62 | 110.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | i | 708 | ASN | CA-CB-CG | -7.94 | 104.66 | 112.60 |
| 7 | M | 514 | CYS | N-CA-C | -7.94 | 103.57 | 113.18 |
| 7 | M | 1100 | LEU | N-CA-C | 7.94 | 121.91 | 111.75 |
| 14 | a | 71 | HIS | CE1-NE2-CD2 | -7.94 | 101.06 | 109.00 |
| 14 | a | 821 | HIS | CE1-NE2-CD2 | -7.94 | 101.06 | 109.00 |
| 8 | N | 577 | MET | N-CA-CB | 7.94 | 123.99 | 110.50 |
| 9 | S | 678 | ASP | CA-CB-CG | -7.94 | 104.66 | 112.60 |
| 15 | b | 240 | PHE | CA-CB-CG | -7.94 | 105.86 | 113.80 |
| 5 | K | 300 | ASP | O-C-N | -7.93 | 116.25 | 121.88 |
| 19 | m | 303 | LEU | N-CA-C | -7.93 | 103.74 | 113.50 |
| 2 | Z | 456 | THR | CA-CB-OG1 | -7.93 | 97.70 | 109.60 |
| 1 | 0 | 1111 | THR | N-CA-C | -7.93 | 102.68 | 113.30 |
| 9 | R | 507 | ALA | CA-C-N | 7.93 | 130.55 | 120.56 |
| 9 | R | 507 | ALA | C-N-CA | 7.93 | 130.55 | 120.56 |
| 16 | j | 181 | ARG | NE-CZ-NH2 | 7.92 | 126.33 | 119.20 |
| 20 | n | 87 | ASN | CA-CB-CG | -7.92 | 104.67 | 112.60 |
| 19 | f | 160 | PHE | CA-CB-CG | 7.92 | 121.72 | 113.80 |
| 9 | R | 723 | ILE | CA-C-N | 7.92 | 130.90 | 120.28 |
| 9 | R | 723 | ILE | C-N-CA | 7.92 | 130.90 | 120.28 |
| 8 | N | 903 | LEU | O-C-N | 7.92 | 130.23 | 122.07 |
| 4 | D | 693 | ILE | CA-C-N | 7.92 | 131.21 | 120.44 |
| 4 | D | 693 | ILE | C-N-CA | 7.92 | 131.21 | 120.44 |
| 8 | N | 419 | ASP | CA-CB-CG | 7.92 | 120.52 | 112.60 |
| 14 | h | 772 | GLN | CA-C-N | 7.92 | 131.53 | 120.29 |
| 14 | h | 772 | GLN | C-N-CA | 7.92 | 131.53 | 120.29 |
| 20 | n | 337 | HIS | CA-C-N | 7.92 | 129.74 | 119.84 |
| 20 | n | 337 | HIS | C-N-CA | 7.92 | 129.74 | 119.84 |
| 20 | n | 725 | PHE | CA-CB-CG | -7.92 | 105.88 | 113.80 |
| 16 | c | 234 | TRP | CA-C-N | 7.92 | 131.53 | 120.29 |
| 16 | c | 234 | TRP | C-N-CA | 7.92 | 131.53 | 120.29 |
| 19 | f | 720 | ARG | NE-CZ-NH1 | -7.92 | 113.58 | 121.50 |
| 20 | g | 142 | PHE | CA-C-N | 7.92 | 129.74 | 119.84 |
| 20 | g | 142 | PHE | C-N-CA | 7.92 | 129.74 | 119.84 |
| 8 | N | 1419 | LYS | CA-C-O | 7.92 | 127.23 | 118.52 |
| 9 | T | 122 | LEU | CB-CA-C | -7.92 | 98.45 | 110.88 |
| 1 | Y | 910 | LEU | N-CA-C | -7.92 | 103.12 | 114.12 |
| 7 | O | 521 | LEU | N-CA-C | -7.92 | 102.65 | 113.18 |
| 17 | k | 137 | SER | O-C-N | 7.92 | 126.02 | 121.27 |
| 14 | a | 765 | PHE | CA-C-N | 7.92 | 131.68 | 120.28 |
| 14 | a | 765 | PHE | C-N-CA | 7.92 | 131.68 | 120.28 |
| 2 | Z | 820 | ASP | CA-C-N | 7.91 | 131.68 | 120.28 |
| 2 | Z | 820 | ASP | C-N-CA | 7.91 | 131.68 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | u | 277 | ARG | NE-CZ-NH1 | 7.91 | 129.41 | 121.50 |
| 7 | M | 356 | ILE | CA-C-O | -7.91 | 112.50 | 119.62 |
| 20 | g | 860 | LEU | N-CA-C | -7.91 | 103.19 | 112.92 |
| 9 | S | 150 | GLN | CA-C-O | 7.91 | 129.12 | 120.82 |
| 15 | b | 344 | ARG | NE-CZ-NH1 | 7.91 | 129.41 | 121.50 |
| 16 | c | 132 | ILE | O-C-N | 7.91 | 129.66 | 121.91 |
| 8 | N | 714 | LEU | N-CA-CB | 7.91 | 121.92 | 110.06 |
| 8 | P | 14 | THR | CA-C-N | 7.91 | 133.36 | 120.63 |
| 8 | P | 14 | THR | C-N-CA | 7.91 | 133.36 | 120.63 |
| 6 | L | 292 | HIS | N-CA-CB | 7.91 | 121.74 | 110.12 |
| 8 | P | 932 | LEU | N-CA-C | -7.91 | 102.70 | 113.30 |
| 7 | M | 1007 | THR | N-CA-C | 7.91 | 119.90 | 111.28 |
| 14 | h | 106 | TYR | CA-C-N | 7.91 | 134.65 | 122.08 |
| 14 | h | 106 | TYR | C-N-CA | 7.91 | 134.65 | 122.08 |
| 7 | M | 658 | SER | N-CA-CB | 7.90 | 121.83 | 109.82 |
| 1 | 0 | 633 | THR | CA-C-O | 7.90 | 128.16 | 119.15 |
| 7 | M | 1075 | LEU | CA-C-N | 7.90 | 130.87 | 120.28 |
| 7 | M | 1075 | LEU | C-N-CA | 7.90 | 130.87 | 120.28 |
| 9 | S | 39 | LEU | N-CA-C | -7.90 | 96.05 | 109.24 |
| 9 | R | 98 | PRO | N-CA-CB | 7.89 | 112.01 | 103.33 |
| 12 | v | 379 | ASN | CA-CB-CG | 7.89 | 120.49 | 112.60 |
| 19 | m | 518 | ILE | CA-C-N | 7.89 | 132.71 | 121.02 |
| 19 | m | 518 | ILE | C-N-CA | 7.89 | 132.71 | 121.02 |
| 7 | O | 3 | TRP | N-CA-CB | 7.89 | 121.99 | 114.10 |
| 9 | Q | 370 | TYR | N-CA-C | -7.89 | 102.73 | 113.30 |
| 12 | u | 88 | ILE | CB-CA-C | -7.89 | 100.73 | 110.99 |
| 7 | O | 1387 | THR | N-CA-CB | 7.88 | 121.44 | 110.01 |
| 15 | i | 406 | LEU | CA-C-N | 7.88 | 128.30 | 119.32 |
| 15 | i | 406 | LEU | C-N-CA | 7.88 | 128.30 | 119.32 |
| 14 | h | 635 | LEU | N-CA-C | -7.88 | 103.46 | 113.23 |
| 7 | O | 560 | GLN | O-C-N | -7.88 | 113.84 | 122.03 |
| 1 | Y | 262 | SER | N-CA-C | -7.88 | 96.06 | 108.90 |
| 7 | M | 198 | TYR | CA-C-N | 7.87 | 128.72 | 119.98 |
| 7 | M | 198 | TYR | C-N-CA | 7.87 | 128.72 | 119.98 |
| 15 | i | 483 | PRO | CA-C-N | 7.87 | 130.49 | 120.88 |
| 15 | i | 483 | PRO | C-N-CA | 7.87 | 130.49 | 120.88 |
| 2 | 1 | 309 | LEU | CB-CA-C | 7.87 | 125.06 | 110.10 |
| 9 | R | 672 | GLN | CA-C-N | 7.87 | 127.93 | 119.90 |
| 9 | R | 672 | GLN | C-N-CA | 7.87 | 127.93 | 119.90 |
| 9 | R | 783 | SER | N-CA-C | 7.87 | 119.86 | 111.28 |
| 1 | Y | 158 | ASP | CA-C-O | -7.87 | 112.20 | 120.55 |
| 1 | Y | 175 | ILE | N-CA-C | -7.87 | 101.47 | 110.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 217 | VAL | N-CA-C | -7.87 | 96.57 | 107.75 |
| 19 | f | 604 | VAL | N-CA-C | -7.87 | 96.68 | 108.17 |
| 12 | u | 260 | HIS | CA-C-N | 7.87 | 131.16 | 120.54 |
| 12 | u | 260 | HIS | C-N-CA | 7.87 | 131.16 | 120.54 |
| 1 | 0 | 393 | ILE | O-C-N | -7.87 | 115.40 | 123.03 |
| 2 | 1 | 1204 | ASP | N-CA-C | -7.86 | 103.26 | 113.17 |
| 7 | M | 563 | SER | CA-C-N | 7.86 | 131.72 | 120.79 |
| 7 | M | 563 | SER | C-N-CA | 7.86 | 131.72 | 120.79 |
| 9 | Q | 669 | ASP | N-CA-C | -7.86 | 94.05 | 110.80 |
| 20 | n | 842 | GLU | CA-C-N | 7.86 | 130.82 | 120.28 |
| 20 | n | 842 | GLU | C-N-CA | 7.86 | 130.82 | 120.28 |
| 17 | d | 56 | VAL | O-C-N | -7.86 | 114.92 | 123.18 |
| 9 | T | 234 | ILE | CB-CA-C | -7.86 | 102.31 | 110.88 |
| 12 | u | 171 | ASN | CA-CB-CG | 7.86 | 120.46 | 112.60 |
| 16 | j | 294 | ILE | CA-C-N | 7.86 | 130.66 | 120.44 |
| 16 | j | 294 | ILE | C-N-CA | 7.86 | 130.66 | 120.44 |
| 2 | 1 | 1361 | ILE | N-CA-C | -7.86 | 97.11 | 108.11 |
| 14 | h | 1035 | ARG | NE-CZ-NH1 | 7.86 | 129.36 | 121.50 |
| 18 | e | 300 | HIS | CA-CB-CG | 7.86 | 121.66 | 113.80 |
| 9 | Q | 587 | THR | N-CA-C | -7.85 | 103.84 | 113.50 |
| 20 | g | 337 | HIS | CE1-NE2-CD2 | -7.85 | 101.15 | 109.00 |
| 15 | b | 86 | ASP | CA-CB-CG | 7.85 | 120.45 | 112.60 |
| 1 | 0 | 379 | ALA | N-CA-CB | 7.85 | 123.86 | 110.68 |
| 2 | 1 | 430 | VAL | N-CA-CB | 7.85 | 120.41 | 110.99 |
| 7 | M | 271 | LYS | O-C-N | -7.85 | 114.61 | 121.20 |
| 10 | W | 326 | ARG | N-CA-C | -7.85 | 103.73 | 113.38 |
| 20 | n | 177 | ASP | CA-C-O | -7.85 | 113.06 | 121.38 |
| 8 | N | 1539 | ASN | N-CA-C | -7.84 | 102.76 | 112.88 |
| 14 | a | 488 | THR | N-CA-CB | 7.84 | 121.48 | 110.26 |
| 14 | a | 855 | GLU | N-CA-C | -7.84 | 101.75 | 112.03 |
| 8 | N | 762 | LEU | N-CA-C | -7.84 | 100.56 | 113.50 |
| 9 | R | 537 | ILE | CA-C-N | 7.84 | 130.64 | 120.44 |
| 9 | R | 537 | ILE | C-N-CA | 7.84 | 130.64 | 120.44 |
| 19 | m | 590 | LEU | CA-C-N | 7.84 | 131.20 | 120.46 |
| 19 | m | 590 | LEU | C-N-CA | 7.84 | 131.20 | 120.46 |
| 14 | a | 800 | GLU | CA-C-N | 7.84 | 133.68 | 121.99 |
| 14 | a | 800 | GLU | C-N-CA | 7.84 | 133.68 | 121.99 |
| 7 | M | 862 | ALA | CA-C-N | 7.84 | 130.79 | 120.28 |
| 7 | M | 862 | ALA | C-N-CA | 7.84 | 130.79 | 120.28 |
| 19 | f | 705 | PHE | N-CA-C | -7.84 | 96.49 | 108.96 |
| 2 | 1 | 1109 | LEU | N-CA-C | -7.84 | 104.24 | 113.88 |
| 7 | O | 437 | ASP | N-CA-C | -7.84 | 102.82 | 111.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | R | 225 | SER | CA-C-N | 7.84 | 130.78 | 120.28 |
| 9 | R | 225 | SER | C-N-CA | 7.84 | 130.78 | 120.28 |
| 20 | g | 316 | ILE | CA-CB-CG1 | 7.84 | 123.73 | 110.40 |
| 8 | P | 759 | ASN | OD1-CG-ND2 | -7.84 | 114.76 | 122.60 |
| 19 | f | 48 | GLN | CA-C-N | 7.84 | 130.78 | 120.28 |
| 19 | f | 48 | GLN | C-N-CA | 7.84 | 130.78 | 120.28 |
| 5 | H | 440 | PHE | CA-CB-CG | -7.83 | 105.97 | 113.80 |
| 9 | S | 501 | MET | N-CA-CB | 7.83 | 122.36 | 110.14 |
| 1 | Y | 1264 | ASP | CA-CB-CG | -7.83 | 104.77 | 112.60 |
| 15 | i | 328 | LEU | CA-C-N | 7.83 | 130.78 | 120.28 |
| 15 | i | 328 | LEU | C-N-CA | 7.83 | 130.78 | 120.28 |
| 14 | a | 724 | PHE | CA-CB-CG | 7.83 | 121.64 | 113.80 |
| 1 | 0 | 202 | GLN | N-CA-C | -7.83 | 97.38 | 109.52 |
| 7 | M | 1299 | ASN | OD1-CG-ND2 | -7.83 | 114.77 | 122.60 |
| 8 | P | 25 | ALA | CA-C-N | 7.83 | 133.24 | 122.19 |
| 8 | P | 25 | ALA | C-N-CA | 7.83 | 133.24 | 122.19 |
| 8 | P | 1534 | TYR | O-C-N | 7.83 | 131.08 | 122.15 |
| 19 | f | 330 | ARG | N-CA-C | 7.83 | 119.90 | 111.36 |
| 7 | M | 1238 | ASP | CA-CB-CG | -7.83 | 104.77 | 112.60 |
| 12 | v | 70 | HIS | CA-C-O | 7.83 | 129.49 | 120.80 |
| 19 | f | 48 | GLN | OE1-CD-NE2 | -7.83 | 114.77 | 122.60 |
| 2 | 1 | 760 | SER | N-CA-CB | 7.83 | 121.75 | 110.16 |
| 15 | i | 251 | GLN | OE1-CD-NE2 | 7.83 | 130.43 | 122.60 |
| 15 | b | 97 | ARG | NE-CZ-NH2 | 7.83 | 126.25 | 119.20 |
| 19 | f | 634 | PHE | CA-CB-CG | -7.83 | 105.97 | 113.80 |
| 20 | g | 492 | GLY | N-CA-C | -7.83 | 104.39 | 115.43 |
| 7 | M | 791 | PHE | CA-CB-CG | -7.83 | 105.97 | 113.80 |
| 7 | M | 1273 | LYS | CA-C-O | -7.83 | 109.32 | 120.51 |
| 17 | k | 275 | ASP | CA-CB-CG | 7.82 | 120.42 | 112.60 |
| 4 | A | 704 | GLN | N-CA-C | 7.82 | 119.81 | 111.28 |
| 12 | u | 150 | THR | N-CA-C | -7.82 | 96.48 | 109.07 |
| 7 | M | 1157 | TRP | CA-C-N | 7.82 | 130.76 | 120.28 |
| 7 | M | 1157 | TRP | C-N-CA | 7.82 | 130.76 | 120.28 |
| 8 | N | 576 | TYR | CB-CA-C | -7.82 | 98.27 | 110.78 |
| 20 | g | 420 | PHE | CA-C-N | 7.82 | 128.84 | 120.47 |
| 20 | g | 420 | PHE | C-N-CA | 7.82 | 128.84 | 120.47 |
| 14 | h | 666 | ASN | CA-C-N | 7.82 | 133.27 | 122.79 |
| 14 | h | 666 | ASN | C-N-CA | 7.82 | 133.27 | 122.79 |
| 17 | k | 63 | HIS | CA-C-N | 7.82 | 127.81 | 119.76 |
| 17 | k | 63 | HIS | C-N-CA | 7.82 | 127.81 | 119.76 |
| 7 | O | 60 | ASP | N-CA-C | -7.81 | 104.23 | 114.31 |
| 9 | S | 91 | GLN | CA-C-N | 7.81 | 130.60 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | S | 91 | GLN | C-N-CA | 7.81 | 130.60 | 120.44 |
| 1 | Y | 1442 | SER | N-CA-C | 7.81 | 120.70 | 111.71 |
| 8 | P | 134 | ARG | N-CA-C | -7.81 | 103.73 | 113.18 |
| 20 | g | 501 | ALA | N-CA-C | 7.81 | 123.13 | 112.90 |
| 8 | N | 980 | LYS | CA-C-N | 7.81 | 132.20 | 120.17 |
| 8 | N | 980 | LYS | C-N-CA | 7.81 | 132.20 | 120.17 |
| 15 | b | 457 | TYR | CA-C-O | 7.81 | 129.64 | 120.43 |
| 7 | O | 110 | ARG | CA-C-N | 7.81 | 133.53 | 120.88 |
| 7 | O | 110 | ARG | C-N-CA | 7.81 | 133.53 | 120.88 |
| 9 | R | 65 | ASP | N-CA-C | 7.81 | 127.43 | 110.80 |
| 15 | b | 94 | ARG | NH1-CZ-NH2 | -7.81 | 109.15 | 119.30 |
| 2 | 1 | 571 | VAL | O-C-N | -7.81 | 112.20 | 121.10 |
| 7 | O | 1437 | LEU | CA-C-N | 7.81 | 130.40 | 120.56 |
| 7 | O | 1437 | LEU | C-N-CA | 7.81 | 130.40 | 120.56 |
| 20 | g | 246 | LYS | CA-C-O | 7.81 | 129.50 | 121.07 |
| 6 | C | 328 | GLN | CA-C-N | 7.80 | 130.74 | 120.28 |
| 6 | C | 328 | GLN | C-N-CA | 7.80 | 130.74 | 120.28 |
| 19 | m | 341 | HIS | CA-C-O | -7.80 | 113.63 | 120.19 |
| 6 | F | 451 | MET | CA-C-N | 7.80 | 131.05 | 120.44 |
| 6 | F | 451 | MET | C-N-CA | 7.80 | 131.05 | 120.44 |
| 1 | 0 | 1007 | ILE | CA-C-O | 7.80 | 127.02 | 118.98 |
| 20 | n | 239 | LYS | CA-C-N | 7.80 | 127.86 | 119.90 |
| 20 | n | 239 | LYS | C-N-CA | 7.80 | 127.86 | 119.90 |
| 8 | P | 1195 | GLN | CA-C-N | 7.80 | 131.07 | 120.54 |
| 8 | P | 1195 | GLN | C-N-CA | 7.80 | 131.07 | 120.54 |
| 11 | V | 395 | LEU | O-C-N | 7.80 | 131.04 | 122.15 |
| 2 | Z | 1248 | ALA | N-CA-CB | 7.80 | 117.80 | 110.39 |
| 8 | N | 794 | ILE | CB-CA-C | 7.80 | 124.08 | 111.29 |
| 2 | Z | 803 | ASN | CA-CB-CG | 7.80 | 120.40 | 112.60 |
| 7 | O | 938 | ALA | N-CA-C | -7.80 | 101.89 | 111.40 |
| 6 | C | 380 | TYR | N-CA-CB | 7.79 | 121.31 | 110.01 |
| 6 | L | 369 | LEU | CB-CA-C | -7.79 | 95.29 | 110.10 |
| 6 | L | 466 | THR | N-CA-CB | 7.79 | 121.70 | 110.16 |
| 14 | a | 805 | ASP | CA-CB-CG | 7.79 | 120.39 | 112.60 |
| 4 | A | 746 | LYS | N-CA-C | 7.79 | 120.46 | 111.11 |
| 9 | T | 821 | GLN | N-CA-C | -7.79 | 103.67 | 113.02 |
| 17 | k | 237 | ASP | N-CA-C | -7.79 | 103.77 | 113.28 |
| 4 | J | 641 | VAL | CA-C-N | 7.79 | 131.35 | 120.29 |
| 4 | J | 641 | VAL | C-N-CA | 7.79 | 131.35 | 120.29 |
| 1 | 0 | 919 | VAL | N-CA-C | 7.79 | 118.33 | 110.23 |
| 2 | Z | 916 | PHE | N-CA-CB | 7.79 | 123.74 | 110.50 |
| 4 | G | 654 | HIS | CA-CB-CG | 7.79 | 121.59 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | f | 422 | LEU | CA-C-N | 7.79 | 130.72 | 120.28 |
| 19 | f | 422 | LEU | C-N-CA | 7.79 | 130.72 | 120.28 |
| 14 | a | 727 | TYR | O-C-N | 7.79 | 130.09 | 122.07 |
| 9 | R | 476 | ASN | OD1-CG-ND2 | 7.79 | 130.39 | 122.60 |
| 2 | 1 | 640 | ALA | N-CA-C | 7.79 | 119.55 | 111.14 |
| 7 | O | 241 | PHE | CA-CB-CG | -7.79 | 106.02 | 113.80 |
| 9 | S | 425 | ILE | N-CA-C | -7.78 | 102.81 | 109.19 |
| 6 | F | 271 | PRO | N-CA-C | -7.78 | 103.36 | 114.18 |
| 14 | a | 190 | ASP | CA-CB-CG | 7.78 | 120.38 | 112.60 |
| 1 | Y | 453 | GLY | N-CA-C | -7.78 | 99.37 | 110.96 |
| 2 | Z | 564 | THR | N-CA-C | -7.78 | 102.65 | 114.16 |
| 2 | 1 | 813 | ASN | CA-CB-CG | 7.78 | 120.38 | 112.60 |
| 7 | M | 652 | ALA | N-CA-C | -7.78 | 104.01 | 113.97 |
| 12 | v | 392 | THR | CA-C-O | -7.78 | 112.31 | 120.55 |
| 9 | Q | 729 | ASN | OD1-CG-ND2 | -7.78 | 114.83 | 122.60 |
| 14 | h | 981 | LEU | CA-C-N | 7.78 | 131.03 | 120.38 |
| 14 | h | 981 | LEU | C-N-CA | 7.78 | 131.03 | 120.38 |
| 5 | B | 390 | HIS | CE1-NE2-CD2 | -7.77 | 101.23 | 109.00 |
| 20 | g | 391 | THR | N-CA-C | -7.77 | 95.36 | 108.26 |
| 1 | Y | 711 | VAL | N-CA-CB | 7.77 | 124.05 | 111.23 |
| 7 | M | 436 | ASP | N-CA-C | -7.77 | 102.75 | 111.14 |
| 7 | O | 427 | THR | CA-C-N | 7.77 | 130.54 | 120.44 |
| 7 | O | 427 | THR | C-N-CA | 7.77 | 130.54 | 120.44 |
| 9 | R | 612 | HIS | CE1-NE2-CD2 | -7.77 | 101.23 | 109.00 |
| 1 | Y | 1027 | HIS | CE1-NE2-CD2 | -7.77 | 101.23 | 109.00 |
| 20 | g | 829 | VAL | N-CA-C | -7.77 | 105.28 | 112.43 |
| 15 | b | 545 | GLN | OE1-CD-NE2 | -7.77 | 114.83 | 122.60 |
| 8 | N | 151 | ASN | CA-CB-CG | 7.76 | 120.36 | 112.60 |
| 8 | P | 1124 | ASP | N-CA-C | -7.76 | 100.82 | 112.54 |
| 12 | u | 148 | ASP | CA-CB-CG | 7.76 | 120.36 | 112.60 |
| 18 | l | 189 | GLU | N-CA-CB | 7.76 | 123.61 | 110.49 |
| 2 | 1 | 143 | VAL | N-CA-C | -7.76 | 96.84 | 108.17 |
| 1 | Y | 614 | LEU | CA-C-N | 7.76 | 131.73 | 120.71 |
| 1 | Y | 614 | LEU | C-N-CA | 7.76 | 131.73 | 120.71 |
| 8 | N | 271 | LEU | CA-C-N | 7.76 | 131.47 | 120.53 |
| 8 | N | 271 | LEU | C-N-CA | 7.76 | 131.47 | 120.53 |
| 7 | O | 271 | LYS | CA-C-N | 7.76 | 127.94 | 119.87 |
| 7 | O | 271 | LYS | C-N-CA | 7.76 | 127.94 | 119.87 |
| 2 | 1 | 1039 | LEU | N-CA-CB | 7.76 | 123.69 | 110.50 |
| 9 | R | 496 | TYR | CA-C-O | -7.76 | 112.25 | 120.63 |
| 4 | y | 768 | GLU | CA-C-N | 7.76 | 131.09 | 120.46 |
| 4 | y | 768 | GLU | C-N-CA | 7.76 | 131.09 | 120.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 1062 | VAL | CA-C-N | 7.76 | 130.68 | 120.28 |
| 20 | g | 1062 | VAL | C-N-CA | 7.76 | 130.68 | 120.28 |
| 10 | U | 341 | GLY | CA-C-O | 7.75 | 128.04 | 120.75 |
| 20 | n | 224 | ASN | CA-CB-CG | 7.75 | 120.35 | 112.60 |
| 6 | F | 463 | LYS | CA-C-N | 7.75 | 131.44 | 120.28 |
| 6 | F | 463 | LYS | C-N-CA | 7.75 | 131.44 | 120.28 |
| 9 | T | 824 | MET | N-CA-C | 7.75 | 115.20 | 108.22 |
| 15 | i | 634 | TYR | CA-C-O | -7.75 | 112.20 | 120.42 |
| 21 | q | 18 | ASP | N-CA-C | 7.75 | 119.73 | 111.28 |
| 8 | N | 131 | ASP | N-CA-C | 7.75 | 132.70 | 111.00 |
| 16 | j | 523 | ASN | CA-CB-CG | 7.75 | 120.35 | 112.60 |
| 8 | N | 265 | PHE | CA-C-N | 7.75 | 131.00 | 120.54 |
| 8 | N | 265 | PHE | C-N-CA | 7.75 | 131.00 | 120.54 |
| 20 | n | 779 | ASN | CA-C-N | 7.75 | 130.88 | 120.65 |
| 20 | n | 779 | ASN | C-N-CA | 7.75 | 130.88 | 120.65 |
| 2 | 1 | 627 | ASN | OD1-CG-ND2 | 7.75 | 130.35 | 122.60 |
| 1 | Y | 1007 | ILE | N-CA-C | -7.75 | 105.59 | 113.10 |
| 18 | l | 164 | HIS | CA-CB-CG | -7.75 | 106.06 | 113.80 |
| 9 | T | 239 | ILE | CB-CA-C | 7.74 | 122.59 | 112.14 |
| 1 | Y | 616 | ASN | CA-CB-CG | 7.74 | 120.34 | 112.60 |
| 16 | j | 428 | ASN | CA-CB-CG | -7.74 | 104.86 | 112.60 |
| 7 | O | 1562 | ASP | CA-C-N | 7.74 | 131.82 | 120.90 |
| 7 | O | 1562 | ASP | C-N-CA | 7.74 | 131.82 | 120.90 |
| 15 | i | 190 | PHE | CA-C-N | 7.74 | 135.91 | 121.97 |
| 15 | i | 190 | PHE | C-N-CA | 7.74 | 135.91 | 121.97 |
| 20 | n | 309 | ASP | CA-CB-CG | 7.74 | 120.34 | 112.60 |
| 15 | b | 626 | PRO | CA-C-N | 7.74 | 130.97 | 120.44 |
| 15 | b | 626 | PRO | C-N-CA | 7.74 | 130.97 | 120.44 |
| 7 | M | 1532 | ARG | NE-CZ-NH2 | 7.74 | 126.17 | 119.20 |
| 9 | S | 676 | GLY | CA-C-O | -7.74 | 110.45 | 121.52 |
| 19 | m | 253 | GLN | N-CA-C | -7.74 | 97.64 | 109.41 |
| 7 | O | 45 | ASN | CA-CB-CG | 7.74 | 120.34 | 112.60 |
| 12 | v | 412 | SER | CA-C-N | 7.74 | 133.52 | 121.99 |
| 12 | v | 412 | SER | C-N-CA | 7.74 | 133.52 | 121.99 |
| 1 | Y | 1021 | TYR | CB-CA-C | 7.74 | 124.80 | 110.10 |
| 19 | m | 373 | THR | N-CA-C | 7.74 | 127.28 | 110.80 |
| 15 | b | 662 | TYR | N-CA-C | -7.74 | 102.71 | 114.16 |
| 16 | j | 485 | GLN | N-CA-CB | 7.73 | 123.56 | 110.49 |
| 15 | b | 582 | GLU | N-CA-C | -7.73 | 98.21 | 108.34 |
| 2 | Z | 766 | PHE | CA-CB-CG | -7.73 | 106.07 | 113.80 |
| 12 | u | 282 | GLN | O-C-N | 7.73 | 131.66 | 122.85 |
| 13 | x | 1288 | ILE | CB-CA-C | -7.73 | 101.70 | 112.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 963 | LYS | N-CA-C | -7.73 | 100.87 | 112.54 |
| 19 | m | 295 | GLN | OE1-CD-NE2 | 7.73 | 130.33 | 122.60 |
| 12 | u | 695 | LYS | CA-C-N | 7.73 | 130.64 | 120.28 |
| 12 | u | 695 | LYS | C-N-CA | 7.73 | 130.64 | 120.28 |
| 8 | N | 1062 | ARG | NE-CZ-NH2 | -7.73 | 112.25 | 119.20 |
| 1 | Y | 609 | ILE | N-CA-C | -7.73 | 100.28 | 109.01 |
| 9 | Q | 622 | THR | CA-C-N | 7.73 | 131.39 | 120.42 |
| 9 | Q | 622 | THR | C-N-CA | 7.73 | 131.39 | 120.42 |
| 7 | M | 569 | ILE | CB-CA-C | -7.72 | 104.26 | 111.06 |
| 7 | M | 910 | ARG | CA-C-N | 7.72 | 130.63 | 120.28 |
| 7 | M | 910 | ARG | C-N-CA | 7.72 | 130.63 | 120.28 |
| 7 | O | 494 | GLU | N-CA-C | 7.72 | 121.64 | 111.75 |
| 1 | Y | 113 | HIS | CA-CB-CG | -7.72 | 106.08 | 113.80 |
| 15 | b | 117 | ASP | CA-C-O | -7.72 | 112.23 | 120.42 |
| 14 | a | 224 | ILE | N-CA-C | -7.72 | 106.37 | 113.71 |
| 4 | D | 651 | SER | CA-C-N | 7.72 | 130.48 | 120.44 |
| 4 | D | 651 | SER | C-N-CA | 7.72 | 130.48 | 120.44 |
| 16 | c | 217 | PHE | CA-CB-CG | -7.72 | 106.08 | 113.80 |
| 10 | U | 353 | LEU | N-CA-C | -7.72 | 103.92 | 112.72 |
| 14 | h | 821 | HIS | ND1-CE1-NE2 | 7.72 | 116.12 | 108.40 |
| 7 | M | 295 | ARG | N-CA-C | -7.71 | 103.87 | 113.28 |
| 14 | h | 776 | ILE | O-C-N | -7.71 | 113.08 | 122.18 |
| 7 | O | 101 | ASN | N-CA-C | -7.71 | 102.81 | 111.14 |
| 15 | i | 545 | GLN | N-CA-C | -7.71 | 102.93 | 112.88 |
| 1 | 0 | 630 | THR | N-CA-C | -7.71 | 104.36 | 114.31 |
| 14 | h | 546 | THR | N-CA-C | -7.71 | 103.45 | 113.17 |
| 21 | t | 17 | THR | CA-C-N | 7.71 | 130.95 | 120.38 |
| 21 | t | 17 | THR | C-N-CA | 7.71 | 130.95 | 120.38 |
| 20 | g | 267 | VAL | N-CA-C | -7.71 | 103.70 | 111.88 |
| 7 | O | 674 | PHE | CA-CB-CG | 7.71 | 121.50 | 113.80 |
| 15 | b | 517 | ASP | N-CA-C | -7.71 | 103.70 | 113.72 |
| 2 | 1 | 360 | LYS | N-CA-C | -7.70 | 102.52 | 112.23 |
| 14 | h | 941 | ASP | CA-CB-CG | -7.70 | 104.90 | 112.60 |
| 7 | O | 171 | TYR | CA-C-N | 7.70 | 132.38 | 120.75 |
| 7 | O | 171 | TYR | C-N-CA | 7.70 | 132.38 | 120.75 |
| 8 | P | 495 | ASP | CA-C-N | 7.70 | 131.68 | 120.82 |
| 8 | P | 495 | ASP | C-N-CA | 7.70 | 131.68 | 120.82 |
| 8 | P | 1232 | HIS | CE1-NE2-CD2 | -7.70 | 101.30 | 109.00 |
| 20 | g | 100 | ASN | CB-CA-C | 7.70 | 122.39 | 109.84 |
| 9 | Q | 590 | LEU | N-CA-CB | 7.70 | 123.50 | 110.49 |
| 20 | n | 613 | ILE | N-CA-C | -7.70 | 103.18 | 110.42 |
| 1 | 0 | 365 | ARG | CA-C-N | 7.70 | 134.85 | 121.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 365 | ARG | C-N-CA | 7.70 | 134.85 | 121.07 |
| 21 | s | 54 | GLY | CA-C-N | 7.70 | 132.06 | 121.05 |
| 21 | s | 54 | GLY | C-N-CA | 7.70 | 132.06 | 121.05 |
| 2 | 1 | 98 | VAL | N-CA-C | 7.70 | 118.47 | 110.62 |
| 16 | c | 610 | TRP | N-CA-C | -7.70 | 97.37 | 109.07 |
| 14 | a | 267 | PRO | N-CA-C | 7.70 | 123.44 | 114.20 |
| 8 | N | 1211 | ILE | N-CA-CB | 7.69 | 119.55 | 110.55 |
| 15 | b | 317 | PHE | CA-CB-CG | -7.69 | 106.11 | 113.80 |
| 5 | B | 378 | HIS | CB-CG-CD2 | -7.69 | 121.20 | 131.20 |
| 7 | O | 1092 | THR | CA-C-N | 7.69 | 130.59 | 120.28 |
| 7 | O | 1092 | THR | C-N-CA | 7.69 | 130.59 | 120.28 |
| 10 | W | 330 | GLU | CA-C-N | 7.69 | 130.44 | 120.44 |
| 10 | W | 330 | GLU | C-N-CA | 7.69 | 130.44 | 120.44 |
| 1 | Y | 654 | THR | CA-C-N | 7.69 | 128.09 | 119.32 |
| 1 | Y | 654 | THR | C-N-CA | 7.69 | 128.09 | 119.32 |
| 12 | v | 53 | LEU | CA-C-O | -7.69 | 112.73 | 121.19 |
| 20 | n | 134 | VAL | CA-C-N | 7.69 | 129.70 | 120.09 |
| 20 | n | 134 | VAL | C-N-CA | 7.69 | 129.70 | 120.09 |
| 8 | P | 1309 | ARG | NE-CZ-NH2 | -7.69 | 112.28 | 119.20 |
| 14 | h | 817 | VAL | N-CA-CB | 7.69 | 121.97 | 111.21 |
| 18 | l | 131 | ASP | N-CA-C | -7.69 | 103.73 | 113.72 |
| 17 | d | 279 | THR | N-CA-C | -7.69 | 95.88 | 108.41 |
| 8 | N | 370 | SER | N-CA-CB | 7.69 | 123.48 | 110.49 |
| 14 | a | 914 | TYR | N-CA-C | -7.69 | 102.18 | 114.09 |
| 8 | P | 264 | LEU | CA-C-O | -7.68 | 112.75 | 120.82 |
| 11 | V | 268 | LEU | CA-C-O | -7.68 | 110.43 | 118.65 |
| 21 | q | 23 | ASP | O-C-N | -7.68 | 113.39 | 122.15 |
| 14 | a | 139 | PHE | CA-CB-CG | -7.68 | 106.12 | 113.80 |
| 8 | N | 1220 | VAL | N-CA-C | 7.68 | 115.49 | 109.19 |
| 2 | 1 | 722 | GLN | CA-C-N | 7.68 | 133.32 | 123.10 |
| 2 | 1 | 722 | GLN | C-N-CA | 7.68 | 133.32 | 123.10 |
| 9 | Q | 502 | ASP | CA-CB-CG | -7.68 | 104.92 | 112.60 |
| 2 | 1 | 418 | ASN | CA-CB-CG | -7.68 | 104.92 | 112.60 |
| 6 | L | 378 | HIS | CG-CD2-NE2 | 7.68 | 114.88 | 107.20 |
| 8 | N | 941 | SER | N-CA-CB | 7.68 | 124.04 | 110.37 |
| 10 | W | 283 | ILE | N-CA-C | 7.68 | 118.93 | 106.72 |
| 20 | n | 332 | LYS | N-CA-C | -7.68 | 102.91 | 111.82 |
| 9 | S | 85 | ALA | N-CA-C | 7.68 | 120.32 | 111.11 |
| 4 | D | 747 | THR | N-CA-C | -7.68 | 102.92 | 111.82 |
| 9 | R | 656 | LEU | O-C-N | 7.67 | 130.25 | 122.12 |
| 19 | m | 170 | ASP | CA-CB-CG | 7.67 | 120.27 | 112.60 |
| 20 | g | 634 | VAL | CB-CA-C | 7.67 | 122.07 | 112.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 1018 | PRO | CA-C-N | 7.67 | 131.19 | 120.29 |
| 20 | g | 1018 | PRO | C-N-CA | 7.67 | 131.19 | 120.29 |
| 19 | f | 540 | ASN | N-CA-C | -7.67 | 104.05 | 113.41 |
| 8 | N | 574 | HIS | ND1-CE1-NE2 | 7.67 | 116.07 | 108.40 |
| 14 | h | 869 | HIS | CG-CD2-NE2 | 7.67 | 114.87 | 107.20 |
| 18 | l | 120 | HIS | CA-CB-CG | 7.67 | 121.47 | 113.80 |
| 9 | R | 304 | LYS | N-CA-C | -7.67 | 103.03 | 113.30 |
| 2 | 1 | 104 | ARG | NE-CZ-NH2 | 7.67 | 126.10 | 119.20 |
| 1 | Y | 446 | LEU | N-CA-C | -7.66 | 96.73 | 109.07 |
| 4 | y | 656 | GLU | CA-C-N | 7.66 | 130.40 | 120.44 |
| 4 | y | 656 | GLU | C-N-CA | 7.66 | 130.40 | 120.44 |
| 7 | O | 1202 | ASN | N-CA-CB | 7.66 | 121.77 | 110.35 |
| 1 | 0 | 780 | LEU | CA-C-O | -7.66 | 112.70 | 120.90 |
| 9 | Q | 139 | PHE | CA-C-N | 7.66 | 130.36 | 120.56 |
| 9 | Q | 139 | PHE | C-N-CA | 7.66 | 130.36 | 120.56 |
| 16 | j | 525 | HIS | CE1-NE2-CD2 | -7.66 | 101.34 | 109.00 |
| 2 | 1 | 927 | HIS | CE1-NE2-CD2 | -7.66 | 101.34 | 109.00 |
| 9 | S | 789 | LEU | CA-C-N | 7.66 | 131.16 | 120.29 |
| 9 | S | 789 | LEU | C-N-CA | 7.66 | 131.16 | 120.29 |
| 13 | w | 1121 | GLY | CA-C-N | 7.66 | 134.27 | 122.25 |
| 13 | w | 1121 | GLY | C-N-CA | 7.66 | 134.27 | 122.25 |
| 2 | 1 | 487 | LYS | N-CA-C | 7.65 | 119.41 | 111.14 |
| 15 | b | 601 | ALA | CA-C-N | 7.65 | 131.16 | 120.29 |
| 15 | b | 601 | ALA | C-N-CA | 7.65 | 131.16 | 120.29 |
| 15 | b | 653 | ILE | N-CA-C | -7.65 | 103.81 | 111.77 |
| 4 | G | 672 | GLY | CA-C-N | 7.65 | 128.42 | 120.00 |
| 4 | G | 672 | GLY | C-N-CA | 7.65 | 128.42 | 120.00 |
| 9 | S | 764 | ASP | CA-CB-CG | 7.65 | 120.25 | 112.60 |
| 1 | Y | 1480 | ASP | CA-CB-CG | 7.65 | 120.25 | 112.60 |
| 15 | b | 180 | THR | O-C-N | -7.65 | 113.43 | 122.15 |
| 7 | M | 539 | ASN | CA-CB-CG | -7.65 | 104.95 | 112.60 |
| 9 | T | 125 | ILE | CB-CA-C | -7.65 | 102.18 | 111.97 |
| 4 | A | 820 | SER | CA-C-N | 7.64 | 132.84 | 120.30 |
| 4 | A | 820 | SER | C-N-CA | 7.64 | 132.84 | 120.30 |
| 7 | M | 1113 | ASP | CA-C-N | 7.64 | 127.65 | 119.78 |
| 7 | M | 1113 | ASP | C-N-CA | 7.64 | 127.65 | 119.78 |
| 7 | O | 951 | ARG | N-CA-CB | 7.64 | 123.41 | 110.49 |
| 2 | 1 | 442 | SER | CA-C-N | 7.64 | 132.21 | 121.66 |
| 2 | 1 | 442 | SER | C-N-CA | 7.64 | 132.21 | 121.66 |
| 8 | P | 899 | GLN | OE1-CD-NE2 | 7.64 | 130.24 | 122.60 |
| 19 | m | 519 | GLU | N-CA-CB | 7.64 | 121.59 | 109.51 |
| 7 | O | 603 | GLU | N-CA-CB | -7.64 | 97.58 | 110.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | i | 193 | ASP | CA-C-N | 7.64 | 134.75 | 121.07 |
| 15 | i | 193 | ASP | C-N-CA | 7.64 | 134.75 | 121.07 |
| 8 | P | 84 | ASP | CA-CB-CG | 7.64 | 120.24 | 112.60 |
| 10 | U | 350 | LEU | N-CA-C | -7.64 | 102.18 | 112.26 |
| 16 | c | 661 | MET | CA-C-N | 7.64 | 130.85 | 120.54 |
| 16 | c | 661 | MET | C-N-CA | 7.64 | 130.85 | 120.54 |
| 8 | N | 913 | ASN | N-CA-C | -7.64 | 103.53 | 112.92 |
| 5 | H | 537 | TYR | N-CA-C | -7.64 | 102.48 | 112.41 |
| 8 | N | 1201 | ILE | N-CA-C | 7.64 | 117.75 | 110.42 |
| 9 | S | 156 | MET | N-CA-C | 7.64 | 119.24 | 111.07 |
| 21 | s | 86 | PHE | CA-CB-CG | -7.64 | 106.16 | 113.80 |
| 1 | Y | 1278 | LEU | N-CA-C | -7.63 | 104.02 | 112.72 |
| 8 | N | 223 | PHE | CA-CB-CG | 7.63 | 121.43 | 113.80 |
| 2 | Z | 502 | ILE | CA-C-O | 7.63 | 130.32 | 120.78 |
| 17 | d | 23 | ARG | NE-CZ-NH1 | 7.63 | 129.13 | 121.50 |
| 7 | M | 299 | THR | N-CA-C | -7.63 | 104.10 | 113.41 |
| 10 | W | 343 | VAL | N-CA-C | -7.63 | 97.47 | 108.53 |
| 14 | h | 151 | HIS | O-C-N | 7.63 | 132.20 | 123.27 |
| 19 | m | 579 | GLN | CA-C-O | 7.63 | 128.83 | 120.82 |
| 20 | g | 920 | CYS | CA-C-N | 7.63 | 130.50 | 120.28 |
| 20 | g | 920 | CYS | C-N-CA | 7.63 | 130.50 | 120.28 |
| 14 | a | 821 | HIS | ND1-CE1-NE2 | 7.63 | 116.03 | 108.40 |
| 1 | 0 | 711 | VAL | N-CA-CB | 7.62 | 123.81 | 111.23 |
| 17 | k | 275 | ASP | N-CA-C | -7.62 | 104.12 | 113.50 |
| 9 | T | 487 | LEU | CA-C-N | 7.62 | 130.35 | 120.44 |
| 9 | T | 487 | LEU | C-N-CA | 7.62 | 130.35 | 120.44 |
| 8 | N | 204 | VAL | CA-C-O | -7.62 | 114.20 | 119.38 |
| 1 | Y | 290 | GLY | N-CA-C | -7.62 | 103.64 | 112.79 |
| 18 | l | 131 | ASP | CA-CB-CG | 7.62 | 120.22 | 112.60 |
| 7 | O | 832 | PHE | CA-CB-CG | -7.62 | 106.18 | 113.80 |
| 16 | j | 439 | ARG | NE-CZ-NH1 | 7.62 | 129.12 | 121.50 |
| 18 | l | 141 | GLU | CA-C-O | -7.62 | 112.59 | 119.75 |
| 8 | P | 385 | PHE | N-CA-C | -7.62 | 102.19 | 113.61 |
| 20 | g | 748 | ILE | N-CA-C | -7.62 | 102.64 | 113.07 |
| 2 | Z | 120 | GLY | CA-C-N | 7.61 | 131.52 | 120.71 |
| 2 | Z | 120 | GLY | C-N-CA | 7.61 | 131.52 | 120.71 |
| 16 | c | 616 | VAL | N-CA-CB | 7.61 | 120.89 | 110.54 |
| 20 | n | 884 | HIS | CA-CB-CG | 7.61 | 121.41 | 113.80 |
| 4 | G | 640 | LEU | N-CA-C | -7.61 | 103.97 | 113.55 |
| 9 | S | 331 | VAL | CA-C-N | 7.61 | 129.35 | 119.84 |
| 9 | S | 331 | VAL | C-N-CA | 7.61 | 129.35 | 119.84 |
| 19 | f | 180 | PHE | CA-CB-CG | -7.61 | 106.19 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 1242 | PHE | CA-CB-CG | -7.61 | 106.19 | 113.80 |
| 12 | u | 665 | ILE | CA-C-N | 7.61 | 130.33 | 120.44 |
| 12 | u | 665 | ILE | C-N-CA | 7.61 | 130.33 | 120.44 |
| 8 | P | 189 | LEU | CA-C-N | 7.60 | 130.47 | 120.28 |
| 8 | P | 189 | LEU | C-N-CA | 7.60 | 130.47 | 120.28 |
| 11 | V | 285 | ILE | CA-C-N | 7.60 | 131.87 | 120.31 |
| 11 | V | 285 | ILE | C-N-CA | 7.60 | 131.87 | 120.31 |
| 9 | R | 101 | PRO | N-CA-CB | 7.60 | 110.79 | 103.19 |
| 20 | g | 508 | ASN | CA-CB-CG | -7.60 | 105.00 | 112.60 |
| 8 | N | 193 | GLN | N-CA-C | 7.60 | 120.53 | 111.33 |
| 2 | 1 | 1340 | LYS | N-CA-CB | 7.60 | 121.38 | 110.13 |
| 8 | P | 52 | ILE | CA-C-O | 7.60 | 125.67 | 119.29 |
| 9 | S | 306 | LYS | N-CA-CB | 7.60 | 121.09 | 110.07 |
| 2 | 1 | 644 | ALA | CA-C-O | 7.60 | 127.81 | 119.15 |
| 8 | P | 657 | CYS | N-CA-C | -7.60 | 97.68 | 109.76 |
| 2 | Z | 490 | SER | N-CA-C | -7.60 | 101.70 | 113.02 |
| 4 | y | 765 | LEU | CA-C-N | 7.60 | 130.87 | 120.46 |
| 4 | y | 765 | LEU | C-N-CA | 7.60 | 130.87 | 120.46 |
| 7 | M | 323 | LEU | CA-C-N | 7.60 | 130.87 | 120.46 |
| 7 | M | 323 | LEU | C-N-CA | 7.60 | 130.87 | 120.46 |
| 8 | P | 1194 | LEU | CA-C-N | 7.60 | 130.79 | 120.54 |
| 8 | P | 1194 | LEU | C-N-CA | 7.60 | 130.79 | 120.54 |
| 5 | H | 371 | GLN | CA-C-N | 7.59 | 131.22 | 120.28 |
| 5 | H | 371 | GLN | C-N-CA | 7.59 | 131.22 | 120.28 |
| 8 | N | 179 | LEU | CA-C-O | 7.59 | 128.79 | 120.82 |
| 21 | r | 38 | GLU | N-CA-C | 7.59 | 119.56 | 111.28 |
| 19 | f | 509 | HIS | CA-C-N | 7.59 | 130.67 | 120.65 |
| 19 | f | 509 | HIS | C-N-CA | 7.59 | 130.67 | 120.65 |
| 9 | R | 824 | MET | N-CA-C | -7.59 | 99.83 | 110.31 |
| 15 | i | 99 | ASP | N-CA-C | -7.59 | 97.37 | 109.59 |
| 5 | B | 350 | ILE | CA-C-N | 7.59 | 131.90 | 121.05 |
| 5 | B | 350 | ILE | C-N-CA | 7.59 | 131.90 | 121.05 |
| 2 | Z | 1138 | ASN | N-CA-C | -7.59 | 103.99 | 113.55 |
| 7 | M | 524 | SER | CB-CA-C | -7.59 | 98.97 | 110.88 |
| 5 | B | 322 | ILE | CA-CB-CG1 | 7.59 | 123.30 | 110.40 |
| 7 | M | 780 | ILE | CA-C-N | 7.59 | 130.45 | 120.28 |
| 7 | M | 780 | ILE | C-N-CA | 7.59 | 130.45 | 120.28 |
| 1 | 0 | 1102 | ILE | N-CA-C | -7.58 | 105.16 | 112.29 |
| 9 | T | 425 | ILE | O-C-N | -7.58 | 116.91 | 121.69 |
| 5 | H | 362 | ASN | O-C-N | 7.58 | 130.16 | 122.12 |
| 1 | Y | 895 | ALA | CA-C-N | 7.58 | 130.44 | 120.28 |
| 1 | Y | 895 | ALA | C-N-CA | 7.58 | 130.44 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 17 | k | 39 | GLU | N-CA-C | -7.58 | 103.14 | 113.30 |
| 9 | R | 72 | LEU | CA-C-N | 7.58 | 130.44 | 120.28 |
| 9 | R | 72 | LEU | C-N-CA | 7.58 | 130.44 | 120.28 |
| 9 | R | 623 | ILE | CB-CA-C | -7.58 | 102.27 | 111.97 |
| 20 | n | 584 | LYS | N-CA-CB | 7.58 | 121.51 | 110.06 |
| 2 | Z | 456 | THR | N-CA-CB | 7.58 | 124.02 | 110.83 |
| 8 | N | 201 | ASN | CA-CB-CG | -7.58 | 105.02 | 112.60 |
| 9 | R | 556 | TYR | N-CA-C | -7.58 | 104.08 | 112.72 |
| 12 | u | 206 | PHE | CA-CB-CG | 7.58 | 121.38 | 113.80 |
| 7 | M | 422 | VAL | N-CA-C | -7.58 | 97.57 | 108.48 |
| 12 | u | 310 | GLY | N-CA-C | -7.58 | 102.43 | 115.61 |
| 18 | l | 159 | ILE | N-CA-CB | 7.57 | 121.81 | 111.21 |
| 15 | b | 392 | GLN | O-C-N | -7.57 | 112.61 | 121.32 |
| 9 | Q | 430 | LEU | N-CA-C | -7.57 | 100.06 | 111.34 |
| 20 | n | 353 | ASP | CA-CB-CG | 7.57 | 120.17 | 112.60 |
| 1 | Y | 1436 | THR | CA-C-N | 7.57 | 133.67 | 123.00 |
| 1 | Y | 1436 | THR | C-N-CA | 7.57 | 133.67 | 123.00 |
| 2 | Z | 543 | PRO | CA-C-N | 7.57 | 132.22 | 121.02 |
| 2 | Z | 543 | PRO | C-N-CA | 7.57 | 132.22 | 121.02 |
| 6 | L | 378 | HIS | ND1-CE1-NE2 | 7.57 | 115.97 | 108.40 |
| 16 | j | 232 | ASN | CA-CB-CG | -7.57 | 105.03 | 112.60 |
| 15 | b | 281 | SER | CA-C-N | 7.57 | 130.76 | 120.54 |
| 15 | b | 281 | SER | C-N-CA | 7.57 | 130.76 | 120.54 |
| 8 | N | 1421 | ILE | CA-C-N | 7.57 | 130.42 | 120.28 |
| 8 | N | 1421 | ILE | C-N-CA | 7.57 | 130.42 | 120.28 |
| 20 | n | 260 | ILE | N-CA-C | -7.57 | 97.44 | 108.71 |
| 2 | 1 | 185 | ILE | CA-C-O | -7.56 | 113.15 | 121.17 |
| 4 | J | 798 | ASN | N-CA-C | -7.56 | 102.98 | 111.07 |
| 4 | A | 684 | VAL | CA-C-N | 7.56 | 130.41 | 120.28 |
| 4 | A | 684 | VAL | C-N-CA | 7.56 | 130.41 | 120.28 |
| 4 | J | 812 | THR | CA-CB-OG1 | 7.56 | 120.94 | 109.60 |
| 2 | Z | 911 | GLU | O-C-N | -7.56 | 114.10 | 122.12 |
| 2 | Z | 1085 | LYS | N-CA-C | 7.56 | 119.52 | 111.28 |
| 11 | V | 400 | ILE | CA-C-N | 7.56 | 132.67 | 122.84 |
| 11 | V | 400 | ILE | C-N-CA | 7.56 | 132.67 | 122.84 |
| 19 | m | 276 | VAL | N-CA-C | -7.56 | 103.92 | 113.22 |
| 20 | n | 728 | ALA | CA-C-O | -7.56 | 112.41 | 120.42 |
| 9 | T | 717 | LEU | CA-C-N | 7.56 | 130.74 | 120.38 |
| 9 | T | 717 | LEU | C-N-CA | 7.56 | 130.74 | 120.38 |
| 13 | x | 1401 | LEU | O-C-N | -7.56 | 114.28 | 122.07 |
| 14 | h | 777 | PHE | N-CA-C | 7.56 | 119.16 | 111.07 |
| 19 | m | 454 | ASP | CA-CB-CG | 7.56 | 120.16 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | n | 82 | ASN | N-CA-C | -7.56 | 94.61 | 107.23 |
| 1 | Y | 666 | PRO | CA-C-N | 7.56 | 130.39 | 120.26 |
| 1 | Y | 666 | PRO | C-N-CA | 7.56 | 130.39 | 120.26 |
| 15 | i | 686 | ASP | CA-CB-CG | 7.56 | 120.16 | 112.60 |
| 14 | a | 649 | GLN | O-C-N | 7.56 | 129.89 | 122.03 |
| 2 | 1 | 594 | TYR | N-CA-C | -7.55 | 102.63 | 113.21 |
| 2 | 1 | 752 | VAL | CA-C-N | 7.55 | 131.79 | 120.31 |
| 2 | 1 | 752 | VAL | C-N-CA | 7.55 | 131.79 | 120.31 |
| 8 | P | 817 | PRO | N-CA-CB | 7.55 | 110.70 | 103.52 |
| 14 | a | 694 | ASN | CA-CB-CG | 7.55 | 120.15 | 112.60 |
| 7 | M | 185 | PHE | CA-CB-CG | -7.55 | 106.25 | 113.80 |
| 1 | Y | 1455 | TRP | CB-CG-CD1 | -7.55 | 115.58 | 126.90 |
| 18 | l | 94 | SER | CA-C-N | 7.55 | 136.21 | 121.41 |
| 18 | l | 94 | SER | C-N-CA | 7.55 | 136.21 | 121.41 |
| 1 | Y | 113 | HIS | CA-C-N | 7.55 | 130.39 | 120.28 |
| 1 | Y | 113 | HIS | C-N-CA | 7.55 | 130.39 | 120.28 |
| 12 | u | 255 | PHE | N-CA-C | 7.55 | 119.14 | 111.07 |
| 15 | b | 396 | ASP | CA-CB-CG | 7.55 | 120.15 | 112.60 |
| 15 | b | 464 | TYR | CB-CA-C | 7.55 | 119.32 | 109.28 |
| 14 | a | 723 | PHE | CA-CB-CG | -7.55 | 106.25 | 113.80 |
| 20 | g | 517 | PRO | N-CA-C | 7.54 | 119.91 | 110.70 |
| 2 | 1 | 417 | ASN | CA-CB-CG | -7.54 | 105.06 | 112.60 |
| 20 | g | 353 | ASP | CA-CB-CG | 7.54 | 120.14 | 112.60 |
| 5 | K | 293 | LEU | N-CA-C | -7.54 | 103.02 | 112.90 |
| 6 | L | 287 | GLN | OE1-CD-NE2 | 7.54 | 130.14 | 122.60 |
| 7 | M | 742 | GLN | CA-C-O | 7.54 | 127.97 | 120.88 |
| 20 | g | 437 | TYR | N-CA-C | -7.54 | 101.18 | 110.61 |
| 11 | X | 385 | ILE | CA-C-N | 7.54 | 127.99 | 119.92 |
| 11 | X | 385 | ILE | C-N-CA | 7.54 | 127.99 | 119.92 |
| 15 | i | 610 | ASP | CA-CB-CG | 7.54 | 120.14 | 112.60 |
| 1 | 0 | 1054 | MET | CA-C-N | 7.54 | 130.38 | 120.28 |
| 1 | 0 | 1054 | MET | C-N-CA | 7.54 | 130.38 | 120.28 |
| 7 | O | 947 | LYS | CA-C-N | 7.54 | 130.24 | 120.44 |
| 7 | O | 947 | LYS | C-N-CA | 7.54 | 130.24 | 120.44 |
| 16 | j | 302 | ASP | N-CA-C | -7.54 | 101.15 | 110.65 |
| 16 | c | 418 | ILE | CA-C-N | 7.54 | 128.29 | 120.00 |
| 16 | c | 418 | ILE | C-N-CA | 7.54 | 128.29 | 120.00 |
| 5 | B | 319 | THR | CA-CB-OG1 | -7.54 | 98.29 | 109.60 |
| 7 | M | 1316 | ASP | N-CA-C | -7.54 | 102.31 | 113.61 |
| 14 | h | 71 | HIS | N-CA-CB | 7.54 | 121.42 | 109.51 |
| 16 | j | 254 | GLN | N-CA-C | -7.54 | 104.23 | 113.50 |
| 8 | P | 1595 | LYS | CA-C-N | 7.54 | 130.38 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1595 | LYS | C-N-CA | 7.54 | 130.38 | 120.28 |
| 4 | G | 800 | HIS | CB-CG-CD2 | -7.53 | 121.41 | 131.20 |
| 16 | j | 134 | ASN | CA-C-N | 7.53 | 130.99 | 120.29 |
| 16 | j | 134 | ASN | C-N-CA | 7.53 | 130.99 | 120.29 |
| 2 | 1 | 616 | THR | CA-C-N | 7.53 | 127.24 | 119.56 |
| 2 | 1 | 616 | THR | C-N-CA | 7.53 | 127.24 | 119.56 |
| 12 | u | 280 | LYS | CA-C-N | 7.53 | 132.24 | 120.34 |
| 12 | u | 280 | LYS | C-N-CA | 7.53 | 132.24 | 120.34 |
| 8 | N | 690 | LEU | N-CA-C | -7.53 | 103.68 | 113.17 |
| 1 | Y | 657 | GLU | O-C-N | -7.53 | 114.12 | 122.10 |
| 7 | O | 1085 | LYS | CA-C-N | 7.53 | 130.37 | 120.28 |
| 7 | O | 1085 | LYS | C-N-CA | 7.53 | 130.37 | 120.28 |
| 9 | R | 804 | ASP | N-CA-C | -7.53 | 102.67 | 112.68 |
| 19 | m | 302 | LEU | O-C-N | -7.53 | 113.31 | 122.34 |
| 19 | f | 34 | ASP | O-C-N | -7.53 | 114.69 | 121.39 |
| 14 | a | 397 | ILE | N-CA-C | -7.53 | 105.22 | 113.43 |
| 1 | 0 | 467 | PHE | CA-C-N | 7.53 | 128.13 | 120.38 |
| 1 | 0 | 467 | PHE | C-N-CA | 7.53 | 128.13 | 120.38 |
| 9 | Q | 621 | HIS | ND1-CE1-NE2 | 7.53 | 115.92 | 108.40 |
| 20 | g | 137 | ARG | NE-CZ-NH2 | -7.53 | 112.43 | 119.20 |
| 12 | v | 231 | LEU | CA-C-N | 7.52 | 130.31 | 120.60 |
| 12 | v | 231 | LEU | C-N-CA | 7.52 | 130.31 | 120.60 |
| 1 | Y | 687 | CYS | N-CA-C | -7.52 | 105.01 | 114.56 |
| 2 | Z | 988 | CYS | N-CA-CB | 7.52 | 123.20 | 110.49 |
| 2 | Z | 1352 | GLN | OE1-CD-NE2 | -7.52 | 115.08 | 122.60 |
| 20 | n | 455 | ILE | CA-C-N | 7.52 | 130.04 | 120.56 |
| 20 | n | 455 | ILE | C-N-CA | 7.52 | 130.04 | 120.56 |
| 8 | P | 600 | ASN | CA-CB-CG | -7.52 | 105.08 | 112.60 |
| 8 | P | 745 | HIS | CE1-NE2-CD2 | -7.52 | 101.48 | 109.00 |
| 9 | T | 125 | ILE | N-CA-C | 7.52 | 117.64 | 110.42 |
| 20 | n | 553 | LEU | N-CA-C | -7.52 | 103.18 | 112.88 |
| 20 | n | 934 | VAL | CB-CA-C | 7.52 | 122.03 | 110.83 |
| 20 | n | 1011 | ASP | N-CA-CB | 7.52 | 123.20 | 110.49 |
| 7 | M | 328 | ASP | N-CA-C | 7.52 | 119.47 | 111.28 |
| 2 | Z | 921 | SER | CA-CB-OG | 7.52 | 126.13 | 111.10 |
| 18 | e | 129 | GLY | O-C-N | -7.52 | 117.43 | 123.14 |
| 1 | 0 | 1028 | LEU | N-CA-C | -7.51 | 103.73 | 113.12 |
| 5 | B | 400 | LYS | CA-C-N | 7.51 | 130.35 | 120.28 |
| 5 | B | 400 | LYS | C-N-CA | 7.51 | 130.35 | 120.28 |
| 6 | F | 370 | ASP | N-CA-C | -7.51 | 94.79 | 110.80 |
| 9 | Q | 329 | ASN | CA-CB-CG | 7.51 | 120.11 | 112.60 |
| 9 | T | 337 | ILE | N-CA-C | -7.51 | 103.61 | 111.58 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 17 | d | 269 | LEU | CB-CA-C | 7.51 | 121.93 | 109.53 |
| 5 | B | 435 | LYS | CA-C-N | 7.51 | 130.66 | 120.44 |
| 5 | B | 435 | LYS | C-N-CA | 7.51 | 130.66 | 120.44 |
| 4 | D | 797 | LEU | CA-C-N | 7.51 | 130.35 | 120.28 |
| 4 | D | 797 | LEU | C-N-CA | 7.51 | 130.35 | 120.28 |
| 9 | S | 660 | LEU | N-CA-CB | 7.51 | 120.96 | 110.07 |
| 2 | Z | 345 | LEU | N-CA-C | -7.51 | 95.79 | 108.26 |
| 10 | W | 329 | GLN | N-CA-C | -7.51 | 103.68 | 112.92 |
| 18 | l | 13 | HIS | ND1-CE1-NE2 | 7.51 | 115.91 | 108.40 |
| 20 | n | 586 | ASP | CA-CB-CG | 7.51 | 120.11 | 112.60 |
| 8 | N | 1027 | TRP | CB-CG-CD1 | 7.51 | 138.16 | 126.90 |
| 7 | O | 248 | PRO | CA-C-N | 7.51 | 130.67 | 120.38 |
| 7 | O | 248 | PRO | C-N-CA | 7.51 | 130.67 | 120.38 |
| 7 | M | 73 | GLU | N-CA-C | -7.51 | 103.74 | 113.12 |
| 7 | M | 1580 | VAL | CB-CA-C | -7.51 | 102.36 | 111.97 |
| 9 | R | 654 | ILE | CA-CB-CG1 | 7.50 | 123.16 | 110.40 |
| 16 | j | 515 | ILE | N-CA-C | -7.50 | 105.70 | 112.90 |
| 20 | n | 441 | ARG | N-CA-CB | 7.50 | 121.17 | 110.44 |
| 15 | b | 420 | THR | N-CA-C | -7.50 | 103.07 | 112.90 |
| 5 | E | 335 | TRP | CB-CG-CD2 | -7.50 | 116.30 | 126.80 |
| 9 | Q | 141 | ASN | N-CA-C | 7.50 | 119.46 | 111.28 |
| 1 | Y | 890 | SER | CA-C-O | -7.50 | 113.12 | 121.00 |
| 7 | O | 997 | ALA | N-CA-C | -7.50 | 102.71 | 113.21 |
| 8 | P | 610 | LYS | CA-C-O | 7.50 | 127.02 | 119.97 |
| 14 | a | 462 | SER | CA-C-O | -7.50 | 113.43 | 121.45 |
| 5 | B | 530 | ASP | N-CA-CB | 7.50 | 121.14 | 110.12 |
| 9 | Q | 92 | THR | N-CA-C | 7.50 | 119.09 | 111.07 |
| 9 | R | 459 | LEU | CA-C-O | -7.50 | 112.88 | 121.72 |
| 21 | r | 63 | LYS | CB-CA-C | -7.50 | 96.96 | 109.55 |
| 7 | O | 608 | PHE | CA-CB-CG | -7.49 | 106.31 | 113.80 |
| 17 | k | 207 | VAL | N-CA-C | -7.49 | 99.83 | 109.80 |
| 16 | c | 378 | GLU | N-CA-C | -7.49 | 106.08 | 114.62 |
| 8 | P | 1308 | TYR | N-CA-C | -7.49 | 104.14 | 113.20 |
| 16 | j | 338 | LEU | N-CA-C | 7.49 | 119.44 | 111.28 |
| 21 | t | 54 | GLY | CA-C-O | 7.49 | 128.36 | 122.29 |
| 14 | a | 882 | PHE | CA-CB-CG | -7.49 | 106.31 | 113.80 |
| 19 | m | 656 | ARG | CA-C-N | 7.49 | 131.06 | 120.28 |
| 19 | m | 656 | ARG | C-N-CA | 7.49 | 131.06 | 120.28 |
| 5 | E | 382 | LYS | CA-C-N | 7.49 | 130.31 | 120.28 |
| 5 | E | 382 | LYS | C-N-CA | 7.49 | 130.31 | 120.28 |
| 19 | f | 468 | LEU | N-CA-C | -7.48 | 103.72 | 112.92 |
| 2 | Z | 1387 | HIS | N-CA-CB | 7.48 | 123.13 | 110.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 924 | SER | N-CA-CB | 7.48 | 123.13 | 110.49 |
| 2 | 1 | 927 | HIS | ND1-CE1-NE2 | 7.48 | 115.88 | 108.40 |
| 9 | R | 591 | GLY | CA-C-O | 7.48 | 127.73 | 120.92 |
| 7 | M | 1496 | ASP | N-CA-C | -7.48 | 96.12 | 108.76 |
| 20 | n | 748 | ILE | N-CA-C | -7.48 | 105.43 | 112.83 |
| 19 | f | 696 | ASN | CA-CB-CG | 7.47 | 120.08 | 112.60 |
| 14 | a | 89 | HIS | CE1-NE2-CD2 | -7.47 | 101.53 | 109.00 |
| 14 | h | 83 | PRO | CA-C-O | -7.47 | 113.17 | 121.32 |
| 7 | O | 569 | ILE | N-CA-C | -7.47 | 105.85 | 111.90 |
| 9 | Q | 651 | ASP | N-CA-C | 7.47 | 119.42 | 111.28 |
| 9 | R | 349 | ALA | N-CA-CB | 7.47 | 121.10 | 110.12 |
| 1 | Y | 901 | GLN | CA-C-N | 7.47 | 133.19 | 120.72 |
| 1 | Y | 901 | GLN | C-N-CA | 7.47 | 133.19 | 120.72 |
| 9 | T | 629 | ARG | NE-CZ-NH2 | -7.46 | 112.48 | 119.20 |
| 18 | e | 5 | ASP | N-CA-CB | 7.46 | 121.01 | 110.04 |
| 19 | f | 344 | ARG | CA-C-N | 7.46 | 130.69 | 120.46 |
| 19 | f | 344 | ARG | C-N-CA | 7.46 | 130.69 | 120.46 |
| 14 | a | 960 | CYS | N-CA-C | -7.46 | 104.20 | 113.38 |
| 2 | Z | 1370 | GLU | N-CA-C | -7.46 | 104.42 | 113.97 |
| 20 | n | 948 | GLN | OE1-CD-NE2 | 7.46 | 130.06 | 122.60 |
| 7 | M | 903 | ASN | CA-CB-CG | 7.46 | 120.06 | 112.60 |
| 16 | j | 439 | ARG | N-CA-C | 7.46 | 120.47 | 111.82 |
| 8 | P | 857 | LEU | N-CA-CB | 7.46 | 121.25 | 110.06 |
| 1 | Y | 1185 | TYR | N-CA-C | -7.46 | 103.31 | 113.30 |
| 20 | g | 719 | ASN | CA-CB-CG | -7.46 | 105.14 | 112.60 |
| 7 | O | 694 | ASN | CA-C-N | 7.45 | 130.27 | 120.28 |
| 7 | O | 694 | ASN | C-N-CA | 7.45 | 130.27 | 120.28 |
| 14 | a | 403 | ASP | CA-CB-CG | 7.45 | 120.05 | 112.60 |
| 14 | a | 865 | LYS | N-CA-C | -7.45 | 101.91 | 113.02 |
| 2 | Z | 398 | LEU | N-CA-C | -7.45 | 103.99 | 113.23 |
| 16 | j | 477 | PHE | CA-CB-CG | -7.45 | 106.35 | 113.80 |
| 19 | f | 623 | PHE | O-C-N | -7.45 | 114.04 | 122.09 |
| 4 | J | 755 | LEU | CA-C-N | 7.45 | 130.12 | 120.44 |
| 4 | J | 755 | LEU | C-N-CA | 7.45 | 130.12 | 120.44 |
| 9 | T | 626 | GLN | CA-C-N | 7.45 | 130.12 | 120.44 |
| 9 | T | 626 | GLN | C-N-CA | 7.45 | 130.12 | 120.44 |
| 11 | V | 378 | ARG | NE-CZ-NH1 | 7.45 | 128.95 | 121.50 |
| 15 | i | 196 | ASP | CA-C-N | 7.45 | 135.38 | 121.97 |
| 15 | i | 196 | ASP | C-N-CA | 7.45 | 135.38 | 121.97 |
| 7 | M | 1394 | SER | O-C-N | -7.45 | 114.46 | 122.06 |
| 1 | Y | 132 | ASP | CA-CB-CG | -7.45 | 105.15 | 112.60 |
| 19 | f | 317 | LEU | CA-C-O | -7.45 | 113.94 | 120.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 13 | x | 1456 | LEU | N-CA-CB | 7.44 | 123.16 | 110.50 |
| 7 | M | 866 | GLN | N-CA-CB | 7.44 | 121.06 | 110.12 |
| 2 | Z | 1078 | GLN | N-CA-C | -7.44 | 103.33 | 114.64 |
| 13 | w | 1354 | ALA | N-CA-C | 7.44 | 119.03 | 111.07 |
| 18 | e | 13 | HIS | CB-CG-CD2 | -7.44 | 121.53 | 131.20 |
| 8 | N | 68 | HIS | CE1-NE2-CD2 | -7.44 | 101.56 | 109.00 |
| 8 | N | 653 | SER | CA-C-N | 7.44 | 130.65 | 120.46 |
| 8 | N | 653 | SER | C-N-CA | 7.44 | 130.65 | 120.46 |
| 15 | i | 120 | ASP | CA-CB-CG | 7.44 | 120.04 | 112.60 |
| 8 | N | 1594 | ASP | CA-C-N | 7.44 | 132.60 | 120.63 |
| 8 | N | 1594 | ASP | C-N-CA | 7.44 | 132.60 | 120.63 |
| 15 | b | 49 | VAL | CA-C-N | 7.44 | 127.86 | 119.83 |
| 15 | b | 49 | VAL | C-N-CA | 7.44 | 127.86 | 119.83 |
| 15 | b | 120 | ASP | O-C-N | -7.44 | 114.51 | 123.29 |
| 14 | a | 781 | ASP | CA-C-O | -7.44 | 112.94 | 121.72 |
| 12 | v | 202 | GLY | O-C-N | -7.44 | 116.49 | 122.51 |
| 11 | X | 402 | ASN | N-CA-C | -7.43 | 90.18 | 111.00 |
| 7 | O | 324 | ILE | N-CA-CB | 7.43 | 120.65 | 110.54 |
| 2 | Z | 355 | HIS | ND1-CE1-NE2 | 7.43 | 115.83 | 108.40 |
| 12 | v | 288 | ASN | CB-CA-C | 7.43 | 124.81 | 110.17 |
| 19 | f | 392 | LEU | N-CA-CB | 7.43 | 121.16 | 110.16 |
| 7 | O | 331 | ILE | N-CA-CB | 7.43 | 120.09 | 110.13 |
| 19 | m | 652 | LEU | CA-C-N | 7.43 | 131.12 | 120.79 |
| 19 | m | 652 | LEU | C-N-CA | 7.43 | 131.12 | 120.79 |
| 21 | o | 80 | TYR | CA-C-O | -7.43 | 112.71 | 121.11 |
| 2 | Z | 1176 | LEU | N-CA-C | -7.43 | 102.15 | 113.89 |
| 1 | 0 | 626 | ASN | OD1-CG-ND2 | -7.43 | 115.17 | 122.60 |
| 18 | e | 113 | SER | O-C-N | -7.43 | 115.01 | 123.40 |
| 8 | N | 913 | ASN | CA-CB-CG | 7.42 | 120.03 | 112.60 |
| 9 | S | 612 | HIS | CE1-NE2-CD2 | -7.42 | 101.58 | 109.00 |
| 12 | u | 595 | GLN | CA-C-N | 7.42 | 130.23 | 120.28 |
| 12 | u | 595 | GLN | C-N-CA | 7.42 | 130.23 | 120.28 |
| 20 | n | 105 | VAL | N-CA-CB | 7.42 | 121.13 | 112.15 |
| 16 | c | 551 | ASN | OD1-CG-ND2 | 7.42 | 130.02 | 122.60 |
| 6 | C | 306 | ASP | CA-CB-CG | 7.42 | 120.02 | 112.60 |
| 7 | M | 841 | PHE | CA-CB-CG | 7.42 | 121.22 | 113.80 |
| 7 | O | 166 | GLN | N-CA-CB | 7.42 | 121.27 | 110.06 |
| 14 | h | 211 | PHE | CA-CB-CG | 7.42 | 121.22 | 113.80 |
| 20 | n | 1063 | LYS | CA-C-O | -7.42 | 112.68 | 120.55 |
| 12 | v | 356 | LEU | CA-C-N | 7.42 | 132.68 | 122.07 |
| 12 | v | 356 | LEU | C-N-CA | 7.42 | 132.68 | 122.07 |
| 9 | Q | 634 | ASP | N-CA-C | -7.42 | 104.23 | 113.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | S | 697 | PHE | N-CA-CB | 7.42 | 123.02 | 110.49 |
| 20 | n | 78 | SER | N-CA-C | -7.42 | 104.74 | 114.31 |
| 5 | K | 470 | ALA | N-CA-C | 7.42 | 119.36 | 111.28 |
| 8 | P | 802 | LEU | CA-C-N | 7.42 | 130.54 | 120.38 |
| 8 | P | 802 | LEU | C-N-CA | 7.42 | 130.54 | 120.38 |
| 9 | R | 705 | GLN | CB-CG-CD | -7.42 | 99.99 | 112.60 |
| 8 | N | 698 | VAL | N-CA-C | -7.41 | 105.61 | 112.43 |
| 9 | S | 707 | HIS | CG-CD2-NE2 | 7.41 | 114.61 | 107.20 |
| 16 | c | 647 | GLN | N-CA-CB | 7.41 | 120.87 | 109.97 |
| 2 | 1 | 508 | PHE | N-CA-C | -7.41 | 98.03 | 109.52 |
| 1 | Y | 1071 | ALA | N-CA-C | 7.41 | 119.00 | 111.07 |
| 12 | u | 701 | LEU | CA-C-N | 7.41 | 130.21 | 120.28 |
| 12 | u | 701 | LEU | C-N-CA | 7.41 | 130.21 | 120.28 |
| 16 | c | 609 | LYS | O-C-N | 7.41 | 132.45 | 122.59 |
| 16 | c | 762 | LYS | CA-C-N | 7.41 | 131.84 | 120.13 |
| 16 | c | 762 | LYS | C-N-CA | 7.41 | 131.84 | 120.13 |
| 18 | e | 313 | ASN | OD1-CG-ND2 | 7.41 | 130.01 | 122.60 |
| 20 | g | 809 | LYS | CA-C-O | 7.41 | 127.20 | 119.05 |
| 7 | M | 696 | PHE | N-CA-C | 7.41 | 120.06 | 111.02 |
| 7 | M | 796 | ILE | CA-CB-CG2 | -7.41 | 97.91 | 110.50 |
| 1 | Y | 1155 | ARG | N-CA-C | -7.41 | 103.38 | 113.30 |
| 2 | Z | 371 | ASN | N-CA-CB | 7.41 | 123.01 | 110.49 |
| 13 | w | 1446 | LYS | CA-C-O | -7.41 | 112.70 | 120.55 |
| 20 | g | 538 | ILE | CA-CB-CG1 | 7.41 | 122.99 | 110.40 |
| 1 | 0 | 1211 | PHE | CA-CB-CG | 7.40 | 121.20 | 113.80 |
| 8 | N | 1334 | ASP | CA-C-N | 7.40 | 130.94 | 120.28 |
| 8 | N | 1334 | ASP | C-N-CA | 7.40 | 130.94 | 120.28 |
| 9 | S | 554 | VAL | N-CA-C | -7.40 | 104.76 | 113.42 |
| 18 | l | 214 | LEU | N-CA-CB | 7.40 | 120.59 | 109.19 |
| 20 | g | 977 | ASN | N-CA-C | -7.40 | 98.06 | 109.24 |
| 4 | G | 659 | THR | CA-C-O | 7.40 | 128.26 | 120.42 |
| 9 | S | 612 | HIS | CG-CD2-NE2 | 7.40 | 114.60 | 107.20 |
| 10 | U | 351 | LYS | N-CA-C | -7.40 | 102.20 | 113.89 |
| 9 | T | 466 | ILE | N-CA-C | 7.40 | 117.48 | 110.53 |
| 6 | C | 343 | ASP | N-CA-C | -7.40 | 102.51 | 112.94 |
| 6 | C | 347 | THR | CA-CB-OG1 | 7.40 | 120.70 | 109.60 |
| 8 | P | 1343 | VAL | N-CA-C | -7.40 | 99.15 | 109.21 |
| 9 | S | 508 | ILE | O-C-N | -7.40 | 114.66 | 121.91 |
| 1 | 0 | 770 | PHE | CA-C-N | 7.40 | 130.19 | 120.28 |
| 1 | 0 | 770 | PHE | C-N-CA | 7.40 | 130.19 | 120.28 |
| 4 | D | 654 | HIS | CE1-NE2-CD2 | -7.40 | 101.60 | 109.00 |
| 4 | G | 715 | GLU | CA-C-N | 7.40 | 130.06 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | G | 715 | GLU | C-N-CA | 7.40 | 130.06 | 120.44 |
| 7 | O | 1542 | ASN | CA-CB-CG | 7.40 | 120.00 | 112.60 |
| 7 | O | 941 | SER | N-CA-C | -7.39 | 103.15 | 111.14 |
| 8 | P | 738 | ILE | CA-C-O | -7.39 | 112.66 | 120.57 |
| 1 | Y | 835 | SER | CA-C-N | 7.39 | 130.19 | 120.28 |
| 1 | Y | 835 | SER | C-N-CA | 7.39 | 130.19 | 120.28 |
| 14 | a | 206 | LYS | N-CA-C | -7.39 | 98.50 | 109.81 |
| 14 | a | 458 | ASN | CA-CB-CG | -7.39 | 105.20 | 112.60 |
| 1 | Y | 1460 | ARG | CA-C-O | 7.39 | 128.37 | 119.43 |
| 9 | T | 129 | LEU | CA-C-N | 7.39 | 130.18 | 120.28 |
| 9 | T | 129 | LEU | C-N-CA | 7.39 | 130.18 | 120.28 |
| 8 | N | 1622 | GLU | CA-C-N | 7.39 | 130.78 | 120.29 |
| 8 | N | 1622 | GLU | C-N-CA | 7.39 | 130.78 | 120.29 |
| 17 | k | 34 | LYS | N-CA-CB | 7.39 | 120.95 | 110.24 |
| 5 | K | 319 | THR | CA-C-O | 7.39 | 131.07 | 120.51 |
| 9 | S | 826 | ARG | NE-CZ-NH1 | -7.39 | 114.11 | 121.50 |
| 2 | Z | 1281 | VAL | CA-C-O | -7.39 | 111.55 | 120.78 |
| 12 | v | 282 | GLN | N-CA-CB | 7.39 | 122.17 | 110.65 |
| 16 | j | 318 | LEU | N-CA-C | -7.39 | 104.29 | 113.38 |
| 21 | q | 36 | GLN | N-CA-C | -7.39 | 103.85 | 114.12 |
| 19 | f | 210 | MET | CA-C-N | 7.39 | 130.94 | 120.53 |
| 19 | f | 210 | MET | C-N-CA | 7.39 | 130.94 | 120.53 |
| 20 | g | 515 | ASN | OD1-CG-ND2 | 7.39 | 129.99 | 122.60 |
| 14 | a | 598 | LYS | CA-C-N | 7.39 | 133.39 | 123.20 |
| 14 | a | 598 | LYS | C-N-CA | 7.39 | 133.39 | 123.20 |
| 11 | V | 301 | LEU | CB-CA-C | -7.38 | 98.90 | 111.31 |
| 13 | x | 1304 | ALA | CA-C-N | 7.38 | 130.17 | 120.28 |
| 13 | x | 1304 | ALA | C-N-CA | 7.38 | 130.17 | 120.28 |
| 15 | i | 338 | VAL | CA-C-N | 7.38 | 130.91 | 120.42 |
| 15 | i | 338 | VAL | C-N-CA | 7.38 | 130.91 | 120.42 |
| 17 | k | 149 | ASN | CA-CB-CG | -7.38 | 105.22 | 112.60 |
| 2 | Z | 1318 | HIS | CA-CB-CG | 7.38 | 121.18 | 113.80 |
| 1 | 0 | 1209 | LYS | CA-C-O | 7.38 | 129.04 | 121.07 |
| 6 | C | 285 | GLN | CA-C-O | 7.38 | 128.25 | 120.42 |
| 5 | E | 369 | VAL | CA-CB-CG1 | -7.38 | 97.85 | 110.40 |
| 8 | N | 1018 | GLU | CA-C-N | 7.38 | 130.91 | 120.28 |
| 8 | N | 1018 | GLU | C-N-CA | 7.38 | 130.91 | 120.28 |
| 20 | n | 810 | ASP | O-C-N | 7.38 | 128.72 | 121.85 |
| 19 | f | 678 | LEU | CA-C-N | 7.38 | 133.28 | 121.18 |
| 19 | f | 678 | LEU | C-N-CA | 7.38 | 133.28 | 121.18 |
| 8 | N | 647 | GLN | OE1-CD-NE2 | -7.38 | 115.22 | 122.60 |
| 8 | N | 1288 | PHE | CA-CB-CG | 7.38 | 121.18 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 147 | GLY | O-C-N | 7.38 | 129.25 | 122.90 |
| 8 | N | 1497 | ASN | CA-CB-CG | 7.38 | 119.98 | 112.60 |
| 7 | O | 39 | THR | N-CA-C | -7.38 | 104.17 | 113.02 |
| 15 | i | 461 | MET | N-CA-C | 7.38 | 119.32 | 111.28 |
| 17 | k | 224 | SER | CA-C-N | 7.38 | 130.44 | 120.63 |
| 17 | k | 224 | SER | C-N-CA | 7.38 | 130.44 | 120.63 |
| 14 | a | 686 | PHE | CA-CB-CG | -7.38 | 106.42 | 113.80 |
| 7 | O | 267 | SER | N-CA-C | -7.38 | 103.87 | 114.12 |
| 7 | O | 962 | ARG | N-CA-C | -7.38 | 99.51 | 110.06 |
| 4 | A | 676 | ILE | N-CA-C | 7.37 | 120.31 | 111.09 |
| 16 | j | 356 | LYS | CA-C-N | 7.37 | 129.85 | 120.56 |
| 16 | j | 356 | LYS | C-N-CA | 7.37 | 129.85 | 120.56 |
| 19 | f | 386 | LEU | N-CA-C | 7.37 | 119.32 | 111.28 |
| 7 | M | 48 | ARG | NE-CZ-NH2 | 7.37 | 125.83 | 119.20 |
| 8 | P | 105 | GLU | CA-C-N | 7.37 | 130.02 | 120.44 |
| 8 | P | 105 | GLU | C-N-CA | 7.37 | 130.02 | 120.44 |
| 16 | c | 768 | ASN | OD1-CG-ND2 | -7.37 | 115.23 | 122.60 |
| 8 | P | 372 | ASP | N-CA-CB | 7.37 | 123.49 | 110.37 |
| 8 | P | 1125 | GLU | CA-C-N | 7.37 | 130.02 | 120.44 |
| 8 | P | 1125 | GLU | C-N-CA | 7.37 | 130.02 | 120.44 |
| 12 | v | 217 | LEU | N-CA-C | -7.37 | 101.40 | 110.61 |
| 13 | w | 1401 | LEU | CA-C-N | 7.37 | 130.02 | 120.44 |
| 13 | w | 1401 | LEU | C-N-CA | 7.37 | 130.02 | 120.44 |
| 19 | m | 517 | LEU | CA-C-N | 7.37 | 130.62 | 121.85 |
| 19 | m | 517 | LEU | C-N-CA | 7.37 | 130.62 | 121.85 |
| 4 | J | 802 | ASP | CA-CB-CG | 7.37 | 119.97 | 112.60 |
| 8 | P | 844 | TYR | N-CA-C | 7.37 | 118.95 | 111.07 |
| 9 | R | 69 | ALA | CA-C-N | 7.37 | 130.01 | 120.44 |
| 9 | R | 69 | ALA | C-N-CA | 7.37 | 130.01 | 120.44 |
| 9 | R | 542 | THR | N-CA-C | 7.37 | 120.18 | 111.71 |
| 2 | Z | 767 | ASN | N-CA-C | -7.37 | 95.11 | 110.80 |
| 15 | i | 682 | LEU | N-CA-C | -7.37 | 97.12 | 108.76 |
| 9 | R | 773 | ASN | CA-CB-CG | -7.36 | 105.24 | 112.60 |
| 9 | T | 658 | ASN | OD1-CG-ND2 | 7.36 | 129.96 | 122.60 |
| 1 | Y | 1369 | ASN | N-CA-C | -7.36 | 104.29 | 113.20 |
| 12 | u | 402 | LEU | N-CA-C | -7.36 | 103.71 | 114.39 |
| 14 | h | 328 | ILE | CA-C-N | 7.36 | 131.17 | 120.71 |
| 14 | h | 328 | ILE | C-N-CA | 7.36 | 131.17 | 120.71 |
| 19 | f | 438 | GLU | CB-CG-CD | -7.36 | 100.08 | 112.60 |
| 8 | P | 704 | ASP | N-CA-C | -7.36 | 102.04 | 112.13 |
| 9 | Q | 51 | ARG | CA-C-N | 7.36 | 130.01 | 120.44 |
| 9 | Q | 51 | ARG | C-N-CA | 7.36 | 130.01 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | U | 277 | LEU | N-CA-C | -7.36 | 102.57 | 113.61 |
| 14 | a | 876 | LEU | N-CA-C | -7.36 | 103.44 | 113.30 |
| 8 | N | 1504 | LEU | CA-C-N | 7.36 | 130.14 | 120.28 |
| 8 | N | 1504 | LEU | C-N-CA | 7.36 | 130.14 | 120.28 |
| 2 | Z | 240 | ARG | NE-CZ-NH1 | 7.36 | 128.86 | 121.50 |
| 20 | g | 502 | VAL | N-CA-C | -7.36 | 102.27 | 112.50 |
| 20 | g | 891 | ILE | N-CA-C | -7.36 | 104.56 | 111.48 |
| 9 | S | 829 | TYR | CA-C-N | 7.36 | 130.14 | 120.28 |
| 9 | S | 829 | TYR | C-N-CA | 7.36 | 130.14 | 120.28 |
| 7 | M | 1584 | ASN | CA-C-N | 7.36 | 126.62 | 118.97 |
| 7 | M | 1584 | ASN | C-N-CA | 7.36 | 126.62 | 118.97 |
| 7 | O | 654 | PHE | N-CA-C | 7.36 | 118.94 | 111.07 |
| 1 | Y | 1417 | ILE | CA-C-O | 7.36 | 127.52 | 120.31 |
| 1 | 0 | 431 | ASN | OD1-CG-ND2 | -7.36 | 115.25 | 122.60 |
| 1 | Y | 1469 | ASN | N-CA-C | 7.36 | 119.99 | 111.02 |
| 20 | g | 84 | ASP | CA-C-N | 7.36 | 134.42 | 122.65 |
| 20 | g | 84 | ASP | C-N-CA | 7.36 | 134.42 | 122.65 |
| 8 | N | 1595 | LYS | CA-C-N | 7.35 | 130.13 | 120.28 |
| 8 | N | 1595 | LYS | C-N-CA | 7.35 | 130.13 | 120.28 |
| 9 | Q | 70 | HIS | CA-C-N | 7.35 | 130.00 | 120.44 |
| 9 | Q | 70 | HIS | C-N-CA | 7.35 | 130.00 | 120.44 |
| 20 | g | 632 | LYS | N-CA-C | -7.35 | 96.33 | 108.76 |
| 2 | 1 | 747 | ILE | CA-CB-CG1 | 7.35 | 122.90 | 110.40 |
| 8 | N | 610 | LYS | N-CA-CB | 7.35 | 122.53 | 110.69 |
| 9 | R | 487 | LEU | CA-C-N | 7.35 | 130.35 | 120.65 |
| 9 | R | 487 | LEU | C-N-CA | 7.35 | 130.35 | 120.65 |
| 15 | i | 215 | SER | CB-CA-C | -7.35 | 99.28 | 110.90 |
| 21 | t | 71 | HIS | ND1-CE1-NE2 | 7.35 | 115.75 | 108.40 |
| 16 | c | 561 | LEU | N-CA-C | 7.35 | 121.83 | 113.01 |
| 1 | Y | 765 | ILE | CA-C-N | 7.35 | 135.58 | 121.54 |
| 1 | Y | 765 | ILE | C-N-CA | 7.35 | 135.58 | 121.54 |
| 20 | g | 108 | TRP | N-CA-C | -7.35 | 98.23 | 109.85 |
| 14 | a | 727 | TYR | CA-C-O | -7.35 | 113.10 | 120.82 |
| 2 | 1 | 595 | SER | N-CA-C | -7.35 | 103.91 | 114.12 |
| 7 | M | 1537 | ALA | CA-C-N | 7.35 | 129.99 | 120.44 |
| 7 | M | 1537 | ALA | C-N-CA | 7.35 | 129.99 | 120.44 |
| 7 | O | 1205 | ASN | OD1-CG-ND2 | 7.35 | 129.95 | 122.60 |
| 7 | O | 1645 | LEU | CA-C-N | 7.35 | 129.99 | 120.44 |
| 7 | O | 1645 | LEU | C-N-CA | 7.35 | 129.99 | 120.44 |
| 18 | l | 42 | THR | N-CA-C | -7.35 | 98.15 | 109.24 |
| 1 | Y | 156 | ILE | CA-C-N | 7.34 | 127.39 | 119.90 |
| 1 | Y | 156 | ILE | C-N-CA | 7.34 | 127.39 | 119.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | A | 717 | LYS | CA-C-O | 7.34 | 128.41 | 119.97 |
| 9 | R | 698 | ASP | CA-CB-CG | 7.34 | 119.94 | 112.60 |
| 2 | 1 | 353 | VAL | CA-C-N | 7.34 | 134.55 | 122.07 |
| 2 | 1 | 353 | VAL | C-N-CA | 7.34 | 134.55 | 122.07 |
| 7 | M | 782 | LYS | CA-C-N | 7.34 | 130.52 | 120.46 |
| 7 | M | 782 | LYS | C-N-CA | 7.34 | 130.52 | 120.46 |
| 7 | O | 1614 | SER | CA-C-N | 7.34 | 132.35 | 120.60 |
| 7 | O | 1614 | SER | C-N-CA | 7.34 | 132.35 | 120.60 |
| 8 | P | 318 | HIS | CE1-NE2-CD2 | -7.34 | 101.66 | 109.00 |
| 20 | n | 232 | THR | CA-CB-OG1 | 7.34 | 120.61 | 109.60 |
| 1 | Y | 1406 | HIS | CE1-NE2-CD2 | -7.34 | 101.66 | 109.00 |
| 19 | m | 43 | ARG | CA-C-O | -7.34 | 112.64 | 120.42 |
| 15 | b | 579 | SER | CA-C-N | 7.34 | 135.56 | 121.54 |
| 15 | b | 579 | SER | C-N-CA | 7.34 | 135.56 | 121.54 |
| 8 | N | 1490 | ARG | CA-C-N | 7.34 | 130.85 | 120.28 |
| 8 | N | 1490 | ARG | C-N-CA | 7.34 | 130.85 | 120.28 |
| 12 | v | 285 | PHE | CA-CB-CG | -7.34 | 106.46 | 113.80 |
| 8 | N | 683 | ASP | N-CA-CB | 7.34 | 122.89 | 110.49 |
| 8 | P | 575 | SER | CA-C-N | 7.34 | 135.56 | 121.54 |
| 8 | P | 575 | SER | C-N-CA | 7.34 | 135.56 | 121.54 |
| 8 | P | 595 | ILE | CB-CA-C | -7.34 | 102.24 | 112.14 |
| 9 | T | 505 | HIS | CA-CB-CG | -7.34 | 106.46 | 113.80 |
| 12 | u | 167 | ASN | CA-CB-CG | -7.33 | 105.27 | 112.60 |
| 14 | a | 415 | TYR | N-CA-C | -7.33 | 104.86 | 113.88 |
| 7 | O | 418 | TYR | N-CA-CB | 7.33 | 120.73 | 110.17 |
| 1 | Y | 847 | ASN | CA-CB-CG | 7.33 | 119.93 | 112.60 |
| 1 | Y | 1027 | HIS | ND1-CE1-NE2 | 7.33 | 115.73 | 108.40 |
| 12 | u | 447 | PHE | CA-CB-CG | 7.33 | 121.13 | 113.80 |
| 14 | h | 121 | VAL | N-CA-C | -7.33 | 97.47 | 108.17 |
| 14 | a | 208 | LEU | N-CA-C | -7.33 | 101.44 | 111.56 |
| 8 | N | 650 | ASP | CA-C-N | 7.33 | 131.08 | 120.38 |
| 8 | N | 650 | ASP | C-N-CA | 7.33 | 131.08 | 120.38 |
| 8 | P | 363 | ASN | OD1-CG-ND2 | 7.33 | 129.93 | 122.60 |
| 8 | P | 774 | ILE | N-CA-C | -7.33 | 105.40 | 112.29 |
| 9 | R | 54 | PHE | CA-C-N | 7.33 | 129.97 | 120.44 |
| 9 | R | 54 | PHE | C-N-CA | 7.33 | 129.97 | 120.44 |
| 20 | n | 366 | ILE | N-CA-CB | 7.33 | 120.57 | 111.41 |
| 7 | O | 535 | PHE | CA-CB-CG | -7.33 | 106.47 | 113.80 |
| 7 | O | 1138 | PHE | N-CA-C | -7.33 | 95.19 | 110.80 |
| 9 | S | 316 | ALA | N-CA-C | -7.33 | 102.43 | 112.03 |
| 7 | M | 1403 | SER | CA-C-N | 7.33 | 130.09 | 120.28 |
| 7 | M | 1403 | SER | C-N-CA | 7.33 | 130.09 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 527 | SER | CA-C-O | -7.32 | 110.13 | 120.16 |
| 2 | 1 | 915 | LYS | CB-CA-C | -7.32 | 95.85 | 110.42 |
| 2 | 1 | 1102 | LEU | CA-C-N | 7.32 | 130.69 | 120.29 |
| 2 | 1 | 1102 | LEU | C-N-CA | 7.32 | 130.69 | 120.29 |
| 20 | n | 434 | ASP | N-CA-C | -7.32 | 104.37 | 113.38 |
| 1 | Y | 241 | PHE | CA-C-N | 7.32 | 133.56 | 122.65 |
| 1 | Y | 241 | PHE | C-N-CA | 7.32 | 133.56 | 122.65 |
| 1 | Y | 1162 | TYR | N-CA-C | 7.32 | 121.12 | 111.75 |
| 2 | Z | 248 | ASN | CA-CB-CG | -7.32 | 105.28 | 112.60 |
| 19 | m | 250 | LEU | N-CA-CB | 7.32 | 121.11 | 110.20 |
| 21 | p | 71 | HIS | CB-CG-CD2 | -7.32 | 121.68 | 131.20 |
| 19 | f | 429 | ILE | O-C-N | -7.32 | 112.75 | 121.10 |
| 9 | R | 269 | ASN | CA-CB-CG | -7.32 | 105.28 | 112.60 |
| 8 | N | 644 | ILE | N-CA-CB | 7.32 | 119.11 | 110.55 |
| 8 | P | 675 | TYR | CA-C-N | 7.32 | 130.42 | 120.54 |
| 8 | P | 675 | TYR | C-N-CA | 7.32 | 130.42 | 120.54 |
| 20 | g | 223 | THR | N-CA-C | -7.32 | 97.81 | 109.59 |
| 7 | O | 1492 | LEU | N-CA-CB | 7.32 | 120.84 | 109.94 |
| 2 | Z | 927 | HIS | CA-C-N | 7.32 | 130.81 | 120.28 |
| 2 | Z | 927 | HIS | C-N-CA | 7.32 | 130.81 | 120.28 |
| 12 | v | 75 | THR | N-CA-CB | 7.31 | 122.85 | 110.49 |
| 14 | a | 139 | PHE | N-CA-C | -7.31 | 103.95 | 113.17 |
| 5 | B | 436 | MET | O-C-N | 7.31 | 129.99 | 122.09 |
| 19 | m | 385 | LEU | CA-C-N | 7.31 | 130.40 | 120.38 |
| 19 | m | 385 | LEU | C-N-CA | 7.31 | 130.40 | 120.38 |
| 20 | n | 437 | TYR | N-CA-CB | 7.31 | 122.85 | 110.49 |
| 8 | N | 986 | SER | N-CA-C | -7.31 | 95.23 | 110.80 |
| 1 | 0 | 980 | SER | N-CA-C | -7.31 | 104.22 | 113.43 |
| 2 | 1 | 1053 | ARG | N-CA-C | 7.31 | 119.25 | 111.28 |
| 7 | O | 1430 | LEU | N-CA-CB | 7.31 | 121.30 | 110.33 |
| 8 | P | 162 | HIS | CA-CB-CG | -7.31 | 106.49 | 113.80 |
| 2 | Z | 933 | ASP | CA-CB-CG | 7.31 | 119.91 | 112.60 |
| 12 | u | 111 | ILE | CA-CB-CG1 | 7.31 | 122.83 | 110.40 |
| 6 | F | 373 | PHE | O-C-N | 7.31 | 129.87 | 122.12 |
| 14 | a | 389 | LEU | N-CA-C | -7.31 | 102.65 | 113.61 |
| 14 | h | 317 | ASN | CA-CB-CG | -7.31 | 105.29 | 112.60 |
| 1 | Y | 1155 | ARG | NE-CZ-NH1 | 7.30 | 128.81 | 121.50 |
| 6 | I | 440 | VAL | N-CA-C | -7.30 | 106.02 | 113.10 |
| 9 | R | 810 | ALA | N-CA-C | 7.30 | 118.88 | 111.07 |
| 1 | Y | 1396 | ASN | CA-C-N | 7.30 | 130.38 | 120.38 |
| 1 | Y | 1396 | ASN | C-N-CA | 7.30 | 130.38 | 120.38 |
| 12 | v | 201 | GLU | CA-C-N | 7.30 | 131.13 | 120.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | v | 201 | GLU | C-N-CA | 7.30 | 131.13 | 120.11 |
| 14 | a | 841 | ALA | N-CA-C | 7.30 | 118.88 | 111.07 |
| 8 | N | 423 | LYS | N-CA-C | -7.30 | 98.72 | 110.32 |
| 8 | N | 904 | LEU | CA-C-N | 7.30 | 130.39 | 120.54 |
| 8 | N | 904 | LEU | C-N-CA | 7.30 | 130.39 | 120.54 |
| 8 | P | 340 | SER | N-CA-C | -7.30 | 95.25 | 110.80 |
| 1 | 0 | 120 | VAL | CA-C-N | 7.30 | 131.86 | 121.42 |
| 1 | 0 | 120 | VAL | C-N-CA | 7.30 | 131.86 | 121.42 |
| 1 | 0 | 272 | ASP | CA-CB-CG | 7.30 | 119.90 | 112.60 |
| 7 | M | 738 | THR | N-CA-C | -7.30 | 96.27 | 108.75 |
| 18 | e | 324 | ASP | CA-CB-CG | 7.30 | 119.90 | 112.60 |
| 20 | g | 727 | PHE | CA-CB-CG | -7.30 | 106.50 | 113.80 |
| 7 | M | 1372 | THR | CA-CB-OG1 | 7.30 | 120.55 | 109.60 |
| 2 | Z | 1110 | GLU | CA-C-N | 7.30 | 131.40 | 120.31 |
| 2 | Z | 1110 | GLU | C-N-CA | 7.30 | 131.40 | 120.31 |
| 12 | u | 178 | ARG | NE-CZ-NH2 | 7.30 | 125.77 | 119.20 |
| 7 | O | 1195 | PHE | N-CA-C | -7.29 | 101.46 | 110.65 |
| 19 | m | 288 | ILE | CA-C-N | 7.29 | 130.65 | 120.29 |
| 19 | m | 288 | ILE | C-N-CA | 7.29 | 130.65 | 120.29 |
| 6 | F | 318 | SER | N-CA-C | 7.29 | 119.23 | 111.28 |
| 9 | T | 352 | VAL | O-C-N | -7.29 | 115.07 | 122.14 |
| 15 | i | 461 | MET | CA-C-N | 7.29 | 130.93 | 120.79 |
| 15 | i | 461 | MET | C-N-CA | 7.29 | 130.93 | 120.79 |
| 19 | m | 148 | ILE | N-CA-C | -7.29 | 102.67 | 113.39 |
| 4 | J | 684 | VAL | N-CA-C | 7.29 | 118.06 | 110.62 |
| 9 | Q | 462 | PHE | CA-CB-CG | 7.29 | 121.09 | 113.80 |
| 16 | j | 445 | LEU | CA-C-N | 7.29 | 131.76 | 120.75 |
| 16 | j | 445 | LEU | C-N-CA | 7.29 | 131.76 | 120.75 |
| 16 | c | 535 | SER | CA-C-N | 7.29 | 129.92 | 120.44 |
| 16 | c | 535 | SER | C-N-CA | 7.29 | 129.92 | 120.44 |
| 6 | F | 291 | SER | CA-C-N | 7.29 | 130.27 | 120.65 |
| 6 | F | 291 | SER | C-N-CA | 7.29 | 130.27 | 120.65 |
| 17 | k | 54 | GLY | CA-C-N | 7.29 | 128.95 | 119.84 |
| 17 | k | 54 | GLY | C-N-CA | 7.29 | 128.95 | 119.84 |
| 6 | C | 278 | GLU | CA-C-N | 7.29 | 129.91 | 120.44 |
| 6 | C | 278 | GLU | C-N-CA | 7.29 | 129.91 | 120.44 |
| 7 | O | 207 | MET | N-CA-C | -7.29 | 101.59 | 111.87 |
| 6 | F | 370 | ASP | CB-CA-C | 7.29 | 124.92 | 110.42 |
| 4 | z | 807 | LEU | CA-C-O | -7.29 | 112.70 | 120.42 |
| 18 | e | 78 | ASP | CA-CB-CG | 7.29 | 119.89 | 112.60 |
| 6 | L | 280 | LEU | CA-C-N | 7.28 | 129.91 | 120.44 |
| 6 | L | 280 | LEU | C-N-CA | 7.28 | 129.91 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | S | 691 | ARG | N-CA-C | -7.28 | 104.42 | 113.38 |
| 14 | h | 161 | ARG | NE-CZ-NH2 | 7.28 | 125.75 | 119.20 |
| 14 | h | 429 | GLU | CA-C-O | 7.28 | 128.19 | 119.59 |
| 18 | l | 54 | HIS | O-C-N | 7.28 | 131.55 | 123.25 |
| 8 | P | 776 | TYR | N-CA-C | -7.28 | 103.54 | 113.30 |
| 8 | P | 1433 | ILE | CA-C-N | 7.28 | 131.17 | 120.90 |
| 8 | P | 1433 | ILE | C-N-CA | 7.28 | 131.17 | 120.90 |
| 14 | h | 661 | GLN | OE1-CD-NE2 | -7.28 | 115.32 | 122.60 |
| 15 | i | 260 | GLN | N-CA-C | -7.28 | 105.58 | 114.75 |
| 1 | 0 | 134 | ASN | N-CA-C | -7.28 | 98.77 | 109.11 |
| 9 | R | 806 | LEU | N-CA-CB | 7.28 | 120.93 | 110.16 |
| 14 | h | 722 | THR | N-CA-C | -7.28 | 103.25 | 112.93 |
| 8 | P | 1617 | ILE | O-C-N | -7.28 | 113.46 | 120.59 |
| 15 | i | 346 | ILE | CA-C-N | 7.28 | 130.03 | 120.28 |
| 15 | i | 346 | ILE | C-N-CA | 7.28 | 130.03 | 120.28 |
| 17 | k | 36 | PHE | CA-CB-CG | -7.28 | 106.52 | 113.80 |
| 13 | x | 1387 | LYS | CB-CA-C | -7.28 | 98.48 | 110.85 |
| 21 | o | 71 | HIS | ND1-CE1-NE2 | 7.28 | 115.67 | 108.40 |
| 8 | N | 262 | SER | O-C-N | 7.27 | 130.97 | 122.17 |
| 8 | N | 407 | ALA | O-C-N | -7.27 | 112.95 | 121.32 |
| 7 | O | 1537 | ALA | CA-C-N | 7.27 | 129.90 | 120.44 |
| 7 | O | 1537 | ALA | C-N-CA | 7.27 | 129.90 | 120.44 |
| 8 | P | 1431 | ILE | N-CA-C | -7.27 | 105.50 | 113.43 |
| 12 | u | 653 | GLN | CA-C-N | 7.27 | 130.62 | 120.29 |
| 12 | u | 653 | GLN | C-N-CA | 7.27 | 130.62 | 120.29 |
| 7 | M | 233 | TYR | CA-C-N | 7.27 | 129.18 | 120.09 |
| 7 | M | 233 | TYR | C-N-CA | 7.27 | 129.18 | 120.09 |
| 8 | N | 637 | VAL | N-CA-C | 7.27 | 117.26 | 110.42 |
| 8 | P | 267 | ILE | CA-C-N | 7.27 | 130.36 | 120.54 |
| 8 | P | 267 | ILE | C-N-CA | 7.27 | 130.36 | 120.54 |
| 4 | y | 692 | LYS | O-C-N | -7.27 | 114.41 | 122.12 |
| 16 | c | 230 | ASP | CA-C-N | 7.27 | 130.03 | 120.28 |
| 16 | c | 230 | ASP | C-N-CA | 7.27 | 130.03 | 120.28 |
| 7 | O | 477 | ASP | CA-C-N | 7.27 | 129.89 | 120.44 |
| 7 | O | 477 | ASP | C-N-CA | 7.27 | 129.89 | 120.44 |
| 9 | Q | 815 | ILE | CA-C-N | 7.27 | 129.89 | 120.44 |
| 9 | Q | 815 | ILE | C-N-CA | 7.27 | 129.89 | 120.44 |
| 4 | A | 805 | ARG | N-CA-C | 7.27 | 118.99 | 111.14 |
| 1 | Y | 187 | ASP | CA-CB-CG | 7.27 | 119.87 | 112.60 |
| 2 | Z | 105 | ASP | N-CA-C | -7.27 | 104.41 | 113.28 |
| 14 | a | 537 | THR | CA-CB-OG1 | 7.27 | 120.50 | 109.60 |
| 7 | M | 286 | ILE | CA-C-N | 7.27 | 128.17 | 120.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 286 | ILE | C-N-CA | 7.27 | 128.17 | 120.03 |
| 18 | e | 61 | ILE | N-CA-C | -7.27 | 98.03 | 108.42 |
| 14 | a | 637 | PHE | CA-C-N | 7.27 | 129.78 | 120.70 |
| 14 | a | 637 | PHE | C-N-CA | 7.27 | 129.78 | 120.70 |
| 1 | 0 | 609 | ILE | N-CA-C | -7.27 | 100.80 | 109.01 |
| 5 | B | 329 | HIS | CA-CB-CG | 7.26 | 121.06 | 113.80 |
| 1 | Y | 379 | ALA | N-CA-C | -7.26 | 97.06 | 108.90 |
| 15 | i | 489 | ILE | N-CA-C | -7.26 | 106.05 | 113.10 |
| 14 | a | 662 | PHE | CA-CB-CG | 7.26 | 121.06 | 113.80 |
| 1 | 0 | 1046 | LYS | CA-C-N | 7.26 | 130.01 | 120.28 |
| 1 | 0 | 1046 | LYS | C-N-CA | 7.26 | 130.01 | 120.28 |
| 5 | E | 401 | ALA | CB-CA-C | -7.26 | 98.74 | 110.79 |
| 4 | J | 711 | LEU | N-CA-C | 7.26 | 119.19 | 111.28 |
| 1 | Y | 292 | ASN | CA-CB-CG | -7.26 | 105.34 | 112.60 |
| 7 | M | 1474 | PHE | CA-C-N | 7.26 | 129.85 | 120.56 |
| 7 | M | 1474 | PHE | C-N-CA | 7.26 | 129.85 | 120.56 |
| 14 | h | 578 | ASP | CA-C-N | 7.26 | 124.81 | 120.24 |
| 14 | h | 578 | ASP | C-N-CA | 7.26 | 124.81 | 120.24 |
| 19 | f | 232 | ASN | CA-CB-CG | -7.26 | 105.34 | 112.60 |
| 1 | 0 | 279 | SER | N-CA-C | -7.25 | 105.61 | 114.75 |
| 1 | 0 | 1374 | ILE | CA-C-N | 7.25 | 129.48 | 120.34 |
| 1 | 0 | 1374 | ILE | C-N-CA | 7.25 | 129.48 | 120.34 |
| 7 | O | 501 | SER | N-CA-C | -7.25 | 101.73 | 113.19 |
| 13 | w | 1274 | ASN | O-C-N | -7.25 | 114.60 | 122.07 |
| 18 | e | 314 | LEU | O-C-N | 7.25 | 129.63 | 122.09 |
| 12 | v | 330 | ASP | CA-CB-CG | 7.25 | 119.85 | 112.60 |
| 13 | w | 1361 | GLU | O-C-N | 7.25 | 129.80 | 122.12 |
| 10 | W | 305 | TYR | CA-C-N | 7.25 | 128.90 | 119.84 |
| 10 | W | 305 | TYR | C-N-CA | 7.25 | 128.90 | 119.84 |
| 2 | Z | 997 | PHE | O-C-N | 7.25 | 129.54 | 122.07 |
| 18 | l | 318 | ILE | CB-CA-C | -7.25 | 102.53 | 111.88 |
| 20 | n | 935 | GLU | N-CA-C | -7.25 | 102.74 | 113.61 |
| 14 | a | 532 | PHE | N-CA-CB | 7.25 | 121.20 | 110.33 |
| 9 | Q | 77 | GLY | N-CA-C | -7.25 | 101.35 | 114.46 |
| 2 | Z | 541 | SER | N-CA-CB | 7.25 | 122.98 | 110.81 |
| 2 | Z | 145 | ASN | N-CA-C | -7.24 | 97.62 | 108.99 |
| 12 | u | 275 | GLU | N-CA-C | -7.24 | 95.37 | 110.80 |
| 20 | n | 605 | ARG | N-CA-C | -7.24 | 97.09 | 108.90 |
| 8 | N | 205 | PRO | CA-C-O | -7.24 | 113.16 | 121.56 |
| 9 | R | 700 | ALA | CA-C-N | 7.24 | 128.14 | 120.03 |
| 9 | R | 700 | ALA | C-N-CA | 7.24 | 128.14 | 120.03 |
| 9 | S | 137 | ASP | CA-C-N | 7.24 | 129.85 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | S | 137 | ASP | C-N-CA | 7.24 | 129.85 | 120.44 |
| 9 | R | 85 | ALA | CA-C-N | 7.24 | 129.98 | 120.28 |
| 9 | R | 85 | ALA | C-N-CA | 7.24 | 129.98 | 120.28 |
| 1 | Y | 1455 | TRP | CB-CG-CD2 | 7.24 | 136.94 | 126.80 |
| 2 | Z | 242 | HIS | CG-CD2-NE2 | 7.24 | 114.44 | 107.20 |
| 19 | m | 162 | LEU | CA-C-N | 7.24 | 129.85 | 120.44 |
| 19 | m | 162 | LEU | C-N-CA | 7.24 | 129.85 | 120.44 |
| 8 | N | 642 | PHE | N-CA-C | -7.24 | 104.70 | 113.97 |
| 8 | N | 1124 | ASP | N-CA-C | -7.24 | 103.60 | 113.30 |
| 7 | O | 296 | ARG | N-CA-C | -7.24 | 98.66 | 108.86 |
| 10 | W | 258 | TYR | CA-C-N | 7.24 | 127.27 | 119.89 |
| 10 | W | 258 | TYR | C-N-CA | 7.24 | 127.27 | 119.89 |
| 21 | t | 36 | GLN | N-CA-C | -7.24 | 102.45 | 113.89 |
| 1 | 0 | 176 | PHE | CB-CA-C | -7.24 | 102.14 | 110.17 |
| 2 | Z | 913 | ALA | N-CA-C | 7.24 | 120.88 | 110.24 |
| 2 | 1 | 997 | PHE | N-CA-C | 7.24 | 119.17 | 111.28 |
| 8 | N | 295 | PHE | CA-CB-CG | -7.24 | 106.56 | 113.80 |
| 20 | n | 890 | GLN | CA-C-N | 7.24 | 129.71 | 120.88 |
| 20 | n | 890 | GLN | C-N-CA | 7.24 | 129.71 | 120.88 |
| 19 | f | 467 | PHE | CA-CB-CG | -7.24 | 106.56 | 113.80 |
| 7 | M | 1484 | ARG | N-CA-C | 7.23 | 119.84 | 111.02 |
| 16 | j | 497 | LEU | CA-C-O | -7.23 | 113.06 | 121.16 |
| 1 | 0 | 582 | ASP | CA-C-N | 7.23 | 131.30 | 120.31 |
| 1 | 0 | 582 | ASP | C-N-CA | 7.23 | 131.30 | 120.31 |
| 1 | 0 | 1335 | VAL | N-CA-C | -7.23 | 105.96 | 112.90 |
| 6 | L | 354 | LEU | N-CA-CB | 7.23 | 121.03 | 110.47 |
| 8 | N | 494 | PRO | CA-C-O | -7.23 | 112.63 | 121.31 |
| 8 | N | 1497 | ASN | CA-C-N | 7.23 | 129.43 | 122.27 |
| 8 | N | 1497 | ASN | C-N-CA | 7.23 | 129.43 | 122.27 |
| 9 | Q | 808 | ASN | N-CA-CB | 7.23 | 120.47 | 109.91 |
| 2 | 1 | 544 | ASP | CA-C-N | 7.23 | 129.97 | 120.28 |
| 2 | 1 | 544 | ASP | C-N-CA | 7.23 | 129.97 | 120.28 |
| 8 | N | 1549 | LYS | CA-C-N | 7.23 | 129.97 | 120.28 |
| 8 | N | 1549 | LYS | C-N-CA | 7.23 | 129.97 | 120.28 |
| 8 | P | 1545 | SER | CA-C-N | 7.23 | 129.97 | 120.28 |
| 8 | P | 1545 | SER | C-N-CA | 7.23 | 129.97 | 120.28 |
| 2 | Z | 235 | ILE | N-CA-CB | 7.23 | 118.81 | 110.49 |
| 2 | Z | 457 | SER | N-CA-C | -7.23 | 90.75 | 111.00 |
| 4 | z | 685 | MET | CA-C-O | -7.23 | 112.89 | 120.55 |
| 18 | l | 139 | ALA | CA-C-N | 7.23 | 129.97 | 120.28 |
| 18 | l | 139 | ALA | C-N-CA | 7.23 | 129.97 | 120.28 |
| 19 | m | 510 | LEU | CA-C-N | 7.23 | 130.69 | 120.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | m | 510 | LEU | C-N-CA | 7.23 | 130.69 | 120.42 |
| 19 | m | 689 | ALA | N-CA-C | -7.23 | 103.77 | 112.59 |
| 20 | g | 576 | ASN | CA-CB-CG | 7.23 | 119.83 | 112.60 |
| 7 | O | 107 | PHE | CA-CB-CG | 7.23 | 121.03 | 113.80 |
| 9 | S | 680 | ASN | CA-C-N | 7.23 | 129.97 | 120.28 |
| 9 | S | 680 | ASN | C-N-CA | 7.23 | 129.97 | 120.28 |
| 1 | Y | 1460 | ARG | NE-CZ-NH2 | -7.23 | 112.70 | 119.20 |
| 15 | i | 401 | LYS | CA-C-O | 7.23 | 128.09 | 120.36 |
| 8 | N | 1478 | ILE | CA-C-N | 7.23 | 130.28 | 120.38 |
| 8 | N | 1478 | ILE | C-N-CA | 7.23 | 130.28 | 120.38 |
| 7 | O | 757 | PHE | O-C-N | 7.23 | 129.89 | 122.09 |
| 9 | T | 754 | ARG | N-CA-C | -7.23 | 95.41 | 110.80 |
| 7 | M | 100 | ASN | N-CA-C | -7.22 | 105.08 | 114.04 |
| 8 | N | 1635 | GLU | CA-C-N | 7.22 | 130.83 | 120.79 |
| 8 | N | 1635 | GLU | C-N-CA | 7.22 | 130.83 | 120.79 |
| 8 | P | 421 | PHE | CA-CB-CG | -7.22 | 106.58 | 113.80 |
| 7 | O | 358 | LYS | CA-C-O | 7.22 | 127.19 | 119.03 |
| 12 | u | 356 | LEU | N-CA-C | -7.22 | 104.33 | 113.43 |
| 5 | H | 329 | HIS | ND1-CE1-NE2 | 7.22 | 115.62 | 108.40 |
| 9 | Q | 146 | LEU | N-CA-CB | 7.22 | 122.69 | 110.49 |
| 9 | S | 122 | LEU | CA-C-N | 7.22 | 129.82 | 120.44 |
| 9 | S | 122 | LEU | C-N-CA | 7.22 | 129.82 | 120.44 |
| 19 | m | 619 | LYS | CA-C-O | -7.22 | 110.36 | 119.31 |
| 16 | c | 305 | ARG | CA-C-N | 7.22 | 129.95 | 120.28 |
| 16 | c | 305 | ARG | C-N-CA | 7.22 | 129.95 | 120.28 |
| 20 | g | 317 | LEU | CA-C-O | 7.22 | 128.20 | 120.55 |
| 8 | P | 882 | SER | N-CA-C | 7.22 | 119.23 | 111.36 |
| 2 | 1 | 128 | GLU | N-CA-C | -7.21 | 97.97 | 109.59 |
| 18 | e | 59 | VAL | CB-CA-C | 7.21 | 117.47 | 111.05 |
| 7 | O | 912 | PHE | CA-C-N | 7.21 | 131.27 | 120.31 |
| 7 | O | 912 | PHE | C-N-CA | 7.21 | 131.27 | 120.31 |
| 8 | P | 1027 | TRP | CA-CB-CG | 7.21 | 127.31 | 113.60 |
| 16 | j | 265 | HIS | CA-CB-CG | -7.21 | 106.59 | 113.80 |
| 7 | M | 31 | ASP | CA-C-N | 7.21 | 129.81 | 120.44 |
| 7 | M | 31 | ASP | C-N-CA | 7.21 | 129.81 | 120.44 |
| 8 | N | 141 | LEU | CA-C-N | 7.21 | 130.66 | 120.42 |
| 8 | N | 141 | LEU | C-N-CA | 7.21 | 130.66 | 120.42 |
| 7 | O | 663 | LYS | N-CA-C | -7.21 | 104.05 | 112.92 |
| 14 | h | 692 | PHE | CA-CB-CG | 7.21 | 121.01 | 113.80 |
| 9 | T | 162 | LEU | CB-CA-C | -7.21 | 99.56 | 110.88 |
| 7 | M | 654 | PHE | N-CA-C | 7.21 | 118.78 | 111.07 |
| 7 | O | 715 | ASN | CA-CB-CG | -7.21 | 105.39 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 17 | k | 246 | THR | N-CA-C | -7.21 | 96.52 | 108.34 |
| 20 | n | 884 | HIS | ND1-CE1-NE2 | 7.21 | 115.61 | 108.40 |
| 21 | o | 71 | HIS | CE1-NE2-CD2 | -7.21 | 101.79 | 109.00 |
| 2 | 1 | 131 | GLY | CA-C-O | -7.21 | 111.52 | 121.46 |
| 9 | S | 766 | ASN | OD1-CG-ND2 | 7.21 | 129.81 | 122.60 |
| 16 | c | 149 | THR | N-CA-C | -7.21 | 96.43 | 108.75 |
| 14 | a | 1024 | VAL | N-CA-C | -7.21 | 106.11 | 113.10 |
| 14 | h | 170 | SER | CA-C-O | -7.21 | 113.66 | 120.94 |
| 15 | b | 717 | ASP | N-CA-C | -7.21 | 102.80 | 113.61 |
| 8 | N | 1614 | SER | N-CA-C | 7.20 | 118.78 | 111.07 |
| 8 | P | 1224 | ASP | CA-CB-CG | -7.20 | 105.40 | 112.60 |
| 9 | R | 69 | ALA | N-CA-C | 7.20 | 118.78 | 111.07 |
| 14 | a | 89 | HIS | ND1-CE1-NE2 | 7.20 | 115.60 | 108.40 |
| 8 | P | 1646 | ALA | CA-C-N | 7.20 | 129.80 | 120.44 |
| 8 | P | 1646 | ALA | C-N-CA | 7.20 | 129.80 | 120.44 |
| 7 | O | 860 | ASN | N-CA-C | -7.20 | 102.51 | 113.89 |
| 1 | Y | 915 | GLU | CA-C-N | 7.20 | 134.11 | 122.81 |
| 1 | Y | 915 | GLU | C-N-CA | 7.20 | 134.11 | 122.81 |
| 21 | o | 30 | ASP | CA-CB-CG | 7.20 | 119.80 | 112.60 |
| 20 | g | 565 | GLN | CA-C-N | 7.20 | 129.93 | 120.28 |
| 20 | g | 565 | GLN | C-N-CA | 7.20 | 129.93 | 120.28 |
| 14 | a | 523 | ASP | N-CA-CB | 7.20 | 121.44 | 110.28 |
| 1 | 0 | 1237 | SER | CA-C-O | 7.20 | 128.06 | 119.06 |
| 7 | O | 750 | TRP | CA-C-N | 7.20 | 126.90 | 119.56 |
| 7 | O | 750 | TRP | C-N-CA | 7.20 | 126.90 | 119.56 |
| 9 | R | 596 | ASP | CA-C-O | 7.20 | 125.08 | 119.18 |
| 2 | Z | 486 | GLN | OE1-CD-NE2 | 7.20 | 129.80 | 122.60 |
| 14 | a | 894 | GLU | CA-C-N | 7.20 | 130.51 | 120.29 |
| 14 | a | 894 | GLU | C-N-CA | 7.20 | 130.51 | 120.29 |
| 9 | Q | 711 | LYS | O-C-N | 7.20 | 130.15 | 122.38 |
| 9 | S | 293 | ASN | CA-C-N | 7.20 | 130.64 | 120.28 |
| 9 | S | 293 | ASN | C-N-CA | 7.20 | 130.64 | 120.28 |
| 19 | f | 726 | ASN | CA-CB-CG | -7.20 | 105.40 | 112.60 |
| 15 | b | 678 | ASP | CA-C-N | 7.20 | 130.81 | 123.04 |
| 15 | b | 678 | ASP | C-N-CA | 7.20 | 130.81 | 123.04 |
| 19 | f | 652 | LEU | CA-C-N | 7.20 | 130.79 | 120.79 |
| 19 | f | 652 | LEU | C-N-CA | 7.20 | 130.79 | 120.79 |
| 7 | O | 331 | ILE | O-C-N | 7.19 | 130.01 | 122.67 |
| 8 | P | 1384 | ASP | N-CA-C | -7.19 | 101.01 | 111.30 |
| 1 | 0 | 1162 | TYR | CA-C-O | -7.19 | 112.86 | 120.63 |
| 7 | O | 101 | ASN | CA-C-N | 7.19 | 128.12 | 119.99 |
| 7 | O | 101 | ASN | C-N-CA | 7.19 | 128.12 | 119.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 123 | LEU | N-CA-CB | 7.19 | 122.14 | 110.41 |
| 21 | p | 16 | ILE | CA-C-N | 7.19 | 130.96 | 120.82 |
| 21 | p | 16 | ILE | C-N-CA | 7.19 | 130.96 | 120.82 |
| 7 | O | 847 | GLY | N-CA-C | -7.19 | 104.22 | 116.01 |
| 8 | P | 908 | VAL | N-CA-C | -7.19 | 97.37 | 107.80 |
| 21 | t | 58 | HIS | CG-CD2-NE2 | 7.19 | 114.39 | 107.20 |
| 9 | R | 546 | ARG | NE-CZ-NH2 | -7.19 | 112.73 | 119.20 |
| 16 | c | 403 | VAL | CA-C-N | 7.19 | 130.63 | 120.28 |
| 16 | c | 403 | VAL | C-N-CA | 7.19 | 130.63 | 120.28 |
| 17 | d | 110 | HIS | CB-CG-CD2 | -7.19 | 121.86 | 131.20 |
| 2 | 1 | 500 | THR | O-C-N | -7.19 | 114.60 | 123.44 |
| 2 | 1 | 564 | THR | N-CA-C | -7.19 | 101.73 | 111.87 |
| 8 | N | 1517 | GLU | N-CA-C | 7.19 | 119.11 | 111.28 |
| 19 | m | 724 | LEU | O-C-N | -7.19 | 113.72 | 122.20 |
| 8 | N | 1307 | PHE | CA-CB-CG | -7.19 | 106.61 | 113.80 |
| 7 | O | 1525 | LEU | CA-C-N | 7.19 | 129.62 | 120.56 |
| 7 | O | 1525 | LEU | C-N-CA | 7.19 | 129.62 | 120.56 |
| 9 | T | 257 | TRP | N-CA-CB | 7.19 | 120.65 | 109.94 |
| 2 | 1 | 1178 | ARG | N-CA-C | -7.18 | 98.43 | 109.14 |
| 7 | M | 268 | ILE | N-CA-C | -7.18 | 105.82 | 112.43 |
| 7 | O | 1606 | GLN | CA-C-N | 7.18 | 129.91 | 120.28 |
| 7 | O | 1606 | GLN | C-N-CA | 7.18 | 129.91 | 120.28 |
| 8 | P | 1284 | ILE | N-CA-C | -7.18 | 105.54 | 112.29 |
| 15 | i | 276 | ASP | N-CA-CB | 7.18 | 121.42 | 110.28 |
| 16 | c | 629 | GLU | N-CA-C | -7.18 | 97.19 | 108.90 |
| 12 | v | 341 | ASN | N-CA-CB | 7.18 | 123.09 | 111.74 |
| 14 | a | 444 | ALA | O-C-N | 7.18 | 129.56 | 122.09 |
| 9 | Q | 662 | SER | N-CA-C | 7.18 | 121.30 | 112.54 |
| 1 | Y | 1166 | VAL | N-CA-C | -7.18 | 106.14 | 113.10 |
| 12 | u | 223 | LEU | N-CA-C | 7.18 | 119.73 | 111.11 |
| 1 | Y | 583 | TYR | CA-C-N | 7.18 | 128.10 | 119.99 |
| 1 | Y | 583 | TYR | C-N-CA | 7.18 | 128.10 | 119.99 |
| 2 | Z | 675 | ILE | N-CA-C | -7.18 | 100.33 | 109.30 |
| 7 | M | 18 | GLY | CA-C-O | 7.18 | 126.65 | 119.04 |
| 5 | E | 334 | GLU | N-CA-C | 7.17 | 119.96 | 111.71 |
| 9 | R | 52 | ARG | CA-C-N | 7.17 | 130.65 | 120.53 |
| 9 | R | 52 | ARG | C-N-CA | 7.17 | 130.65 | 120.53 |
| 16 | j | 639 | SER | CA-C-N | 7.17 | 127.94 | 119.98 |
| 16 | j | 639 | SER | C-N-CA | 7.17 | 127.94 | 119.98 |
| 19 | m | 528 | HIS | N-CA-CB | 7.17 | 120.63 | 109.94 |
| 14 | a | 657 | LEU | N-CA-C | 7.17 | 119.10 | 111.28 |
| 6 | I | 352 | VAL | O-C-N | -7.17 | 113.69 | 121.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1240 | HIS | CA-C-O | 7.17 | 126.94 | 118.69 |
| 7 | O | 1336 | ILE | O-C-N | -7.17 | 114.98 | 120.07 |
| 20 | g | 411 | ASN | CA-CB-CG | 7.17 | 119.77 | 112.60 |
| 7 | O | 944 | ILE | CA-C-N | 7.17 | 130.61 | 120.28 |
| 7 | O | 944 | ILE | C-N-CA | 7.17 | 130.61 | 120.28 |
| 20 | g | 450 | ARG | NE-CZ-NH2 | -7.17 | 112.75 | 119.20 |
| 7 | O | 60 | ASP | CA-CB-CG | 7.17 | 119.77 | 112.60 |
| 7 | M | 1075 | LEU | CA-C-O | -7.17 | 111.73 | 119.97 |
| 9 | S | 64 | LYS | CA-C-O | -7.17 | 113.23 | 119.97 |
| 13 | w | 1402 | LEU | N-CA-C | -7.17 | 103.40 | 111.07 |
| 14 | h | 471 | ILE | CB-CA-C | 7.17 | 119.40 | 111.80 |
| 20 | g | 948 | GLN | N-CA-C | 7.17 | 119.17 | 111.36 |
| 1 | 0 | 1398 | PHE | CA-CB-CG | -7.17 | 106.63 | 113.80 |
| 8 | N | 915 | ASP | N-CA-C | -7.17 | 95.53 | 110.80 |
| 7 | O | 671 | PHE | CA-CB-CG | -7.17 | 106.63 | 113.80 |
| 7 | O | 818 | TYR | CA-C-O | 7.17 | 127.85 | 119.32 |
| 9 | S | 267 | ASP | CA-C-N | 7.17 | 130.63 | 120.53 |
| 9 | S | 267 | ASP | C-N-CA | 7.17 | 130.63 | 120.53 |
| 1 | Y | 861 | SER | N-CA-C | -7.17 | 104.11 | 112.92 |
| 1 | Y | 1050 | ALA | CA-C-N | 7.17 | 129.59 | 120.56 |
| 1 | Y | 1050 | ALA | C-N-CA | 7.17 | 129.59 | 120.56 |
| 4 | G | 703 | GLN | CA-C-N | 7.16 | 130.46 | 120.29 |
| 4 | G | 703 | GLN | C-N-CA | 7.16 | 130.46 | 120.29 |
| 9 | Q | 795 | GLN | N-CA-CB | 7.16 | 122.60 | 110.71 |
| 16 | j | 431 | THR | CA-C-O | 7.16 | 128.01 | 120.42 |
| 20 | n | 621 | TYR | CA-CB-CG | -7.16 | 101.00 | 113.90 |
| 16 | c | 392 | GLY | N-CA-C | -7.16 | 102.92 | 112.81 |
| 20 | g | 385 | THR | CA-C-N | 7.16 | 131.04 | 120.87 |
| 20 | g | 385 | THR | C-N-CA | 7.16 | 131.04 | 120.87 |
| 14 | a | 650 | HIS | CE1-NE2-CD2 | -7.16 | 101.84 | 109.00 |
| 6 | F | 447 | PHE | N-CA-C | -7.16 | 103.21 | 112.23 |
| 2 | Z | 434 | PHE | CA-CB-CG | -7.16 | 106.64 | 113.80 |
| 2 | Z | 547 | ILE | CA-C-O | 7.16 | 126.36 | 118.98 |
| 12 | v | 39 | GLN | N-CA-C | -7.16 | 99.14 | 109.31 |
| 7 | M | 257 | SER | N-CA-C | 7.16 | 118.73 | 111.07 |
| 7 | M | 918 | PHE | CA-CB-CG | 7.16 | 120.96 | 113.80 |
| 9 | T | 699 | ASN | N-CA-C | -7.16 | 97.84 | 108.79 |
| 4 | y | 695 | GLN | CA-C-N | 7.16 | 129.87 | 120.28 |
| 4 | y | 695 | GLN | C-N-CA | 7.16 | 129.87 | 120.28 |
| 21 | q | 68 | TYR | CB-CA-C | 7.16 | 120.10 | 110.94 |
| 21 | q | 72 | GLU | O-C-N | 7.16 | 131.82 | 123.02 |
| 1 | 0 | 1258 | LEU | N-CA-C | -7.16 | 95.56 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | i | 91 | TYR | CA-C-O | -7.16 | 110.53 | 119.54 |
| 15 | b | 180 | THR | CA-C-O | 7.16 | 128.00 | 120.42 |
| 15 | b | 576 | PHE | N-CA-C | -7.16 | 104.42 | 113.72 |
| 9 | Q | 672 | GLN | CA-C-O | -7.15 | 113.98 | 120.13 |
| 19 | f | 293 | ILE | N-CA-CB | 7.15 | 120.27 | 110.54 |
| 7 | M | 706 | VAL | CA-C-O | 7.15 | 127.29 | 120.14 |
| 19 | f | 105 | PHE | CA-CB-CG | -7.15 | 106.65 | 113.80 |
| 14 | a | 991 | LEU | O-C-N | -7.15 | 114.42 | 122.86 |
| 9 | T | 106 | SER | N-CA-C | -7.15 | 97.85 | 108.79 |
| 1 | Y | 607 | GLN | CA-C-O | -7.15 | 112.98 | 120.99 |
| 15 | b | 466 | LEU | N-CA-C | -7.15 | 103.42 | 111.07 |
| 20 | g | 750 | TYR | N-CA-C | -7.15 | 104.70 | 113.50 |
| 8 | N | 658 | CYS | N-CA-CB | 7.15 | 121.79 | 110.57 |
| 1 | 0 | 1341 | ASP | CA-CB-CG | 7.15 | 119.75 | 112.60 |
| 9 | Q | 742 | LEU | CA-C-O | 7.15 | 127.83 | 119.32 |
| 16 | j | 587 | VAL | N-CA-C | -7.15 | 105.67 | 111.81 |
| 15 | b | 65 | MET | O-C-N | -7.15 | 117.14 | 121.71 |
| 8 | P | 822 | ASN | N-CA-C | -7.14 | 104.55 | 113.55 |
| 14 | a | 274 | GLU | N-CA-C | -7.14 | 103.12 | 112.41 |
| 8 | N | 1080 | GLU | O-C-N | 7.14 | 129.69 | 122.12 |
| 8 | N | 1487 | PHE | CA-C-O | 7.14 | 127.81 | 120.24 |
| 9 | S | 236 | ASN | CA-CB-CG | -7.14 | 105.46 | 112.60 |
| 1 | Y | 164 | PHE | N-CA-C | 7.14 | 122.01 | 113.16 |
| 1 | 0 | 384 | GLU | N-CA-C | -7.14 | 95.59 | 110.80 |
| 7 | O | 276 | ALA | CB-CA-C | -7.14 | 97.42 | 110.63 |
| 14 | h | 137 | PHE | CA-CB-CG | 7.14 | 120.94 | 113.80 |
| 9 | S | 207 | ILE | N-CA-C | -7.14 | 102.90 | 113.39 |
| 18 | e | 94 | SER | N-CA-C | -7.14 | 96.64 | 108.34 |
| 8 | P | 1609 | PRO | N-CA-C | -7.13 | 104.94 | 113.86 |
| 19 | m | 528 | HIS | CA-CB-CG | 7.13 | 120.93 | 113.80 |
| 1 | Y | 136 | SER | N-CA-C | -7.13 | 98.80 | 108.86 |
| 9 | Q | 443 | ILE | CA-C-O | 7.13 | 129.69 | 120.78 |
| 9 | S | 703 | SER | CA-C-O | -7.13 | 111.77 | 119.97 |
| 15 | i | 469 | PHE | N-CA-C | -7.13 | 102.70 | 111.40 |
| 21 | q | 55 | ASN | CA-CB-CG | 7.13 | 119.73 | 112.60 |
| 14 | a | 135 | LEU | N-CA-C | -7.13 | 101.78 | 111.55 |
| 9 | T | 740 | GLU | N-CA-C | 7.13 | 118.84 | 111.14 |
| 20 | g | 492 | GLY | CA-C-N | 7.13 | 132.14 | 120.23 |
| 20 | g | 492 | GLY | C-N-CA | 7.13 | 132.14 | 120.23 |
| 7 | M | 539 | ASN | N-CA-C | 7.13 | 121.56 | 113.01 |
| 8 | P | 262 | SER | CA-C-N | 7.13 | 130.79 | 120.38 |
| 8 | P | 262 | SER | C-N-CA | 7.13 | 130.79 | 120.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 649 | ILE | CA-C-O | -7.13 | 112.82 | 120.59 |
| 8 | P | 1634 | LEU | N-CA-C | -7.13 | 104.21 | 114.12 |
| 12 | v | 251 | LYS | O-C-N | 7.13 | 129.67 | 122.12 |
| 20 | n | 997 | VAL | N-CA-CB | 7.13 | 122.99 | 111.23 |
| 21 | q | 75 | HIS | O-C-N | -7.13 | 113.02 | 122.28 |
| 7 | O | 1382 | TYR | CA-C-N | 7.12 | 130.16 | 120.54 |
| 7 | O | 1382 | TYR | C-N-CA | 7.12 | 130.16 | 120.54 |
| 15 | i | 157 | VAL | CA-C-O | -7.12 | 113.54 | 120.95 |
| 15 | b | 709 | LEU | N-CA-C | -7.12 | 103.75 | 113.30 |
| 5 | E | 351 | GLN | N-CA-C | 7.12 | 120.04 | 110.35 |
| 9 | S | 300 | THR | N-CA-C | -7.12 | 97.29 | 108.90 |
| 1 | Y | 785 | TRP | CB-CG-CD2 | -7.12 | 116.83 | 126.80 |
| 13 | x | 1446 | LYS | CA-C-N | 7.12 | 129.70 | 120.44 |
| 13 | x | 1446 | LYS | C-N-CA | 7.12 | 129.70 | 120.44 |
| 16 | c | 193 | GLU | CA-C-N | 7.12 | 130.22 | 120.46 |
| 16 | c | 193 | GLU | C-N-CA | 7.12 | 130.22 | 120.46 |
| 14 | a | 947 | SER | CA-C-N | 7.12 | 130.54 | 120.42 |
| 14 | a | 947 | SER | C-N-CA | 7.12 | 130.54 | 120.42 |
| 7 | O | 889 | ILE | CA-C-O | 7.12 | 128.19 | 120.57 |
| 8 | P | 671 | LEU | N-CA-C | -7.12 | 101.71 | 110.61 |
| 14 | a | 549 | LYS | N-CA-C | 7.12 | 119.04 | 111.28 |
| 2 | 1 | 823 | LYS | N-CA-C | 7.12 | 119.90 | 111.71 |
| 4 | D | 668 | VAL | CA-C-N | 7.12 | 129.69 | 120.44 |
| 4 | D | 668 | VAL | C-N-CA | 7.12 | 129.69 | 120.44 |
| 7 | M | 548 | GLY | O-C-N | -7.12 | 115.91 | 122.96 |
| 9 | R | 789 | LEU | N-CA-C | -7.12 | 104.48 | 113.02 |
| 17 | k | 53 | GLU | N-CA-C | -7.12 | 98.13 | 109.59 |
| 21 | t | 39 | ARG | CA-C-N | 7.12 | 129.69 | 120.44 |
| 21 | t | 39 | ARG | C-N-CA | 7.12 | 129.69 | 120.44 |
| 7 | M | 1406 | TYR | CB-CG-CD2 | -7.12 | 110.12 | 120.80 |
| 16 | j | 569 | GLU | CA-C-N | 7.12 | 131.13 | 120.17 |
| 16 | j | 569 | GLU | C-N-CA | 7.12 | 131.13 | 120.17 |
| 16 | c | 631 | GLN | OE1-CD-NE2 | 7.12 | 129.72 | 122.60 |
| 1 | 0 | 176 | PHE | O-C-N | -7.12 | 113.01 | 121.12 |
| 1 | 0 | 1470 | ASP | N-CA-C | 7.12 | 119.03 | 111.28 |
| 9 | T | 116 | LYS | N-CA-C | -7.12 | 103.61 | 112.72 |
| 15 | i | 85 | LYS | CA-C-O | -7.12 | 113.30 | 120.98 |
| 1 | Y | 176 | PHE | N-CA-C | -7.11 | 93.14 | 108.93 |
| 4 | D | 800 | HIS | N-CA-C | -7.11 | 104.75 | 113.50 |
| 8 | P | 400 | PHE | CA-CB-CG | 7.11 | 120.91 | 113.80 |
| 14 | h | 258 | ASP | CA-CB-CG | 7.11 | 119.71 | 112.60 |
| 16 | c | 374 | GLU | CB-CG-CD | -7.11 | 100.51 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 208 | ILE | CA-C-N | 7.11 | 130.20 | 120.46 |
| 8 | P | 208 | ILE | C-N-CA | 7.11 | 130.20 | 120.46 |
| 8 | P | 1265 | PHE | CA-CB-CG | -7.11 | 106.69 | 113.80 |
| 10 | U | 355 | SER | N-CA-CB | 7.11 | 122.41 | 111.46 |
| 2 | Z | 1303 | ALA | N-CA-C | -7.11 | 98.55 | 109.14 |
| 14 | h | 717 | ASN | CA-CB-CG | -7.11 | 105.49 | 112.60 |
| 1 | 0 | 1106 | ASP | N-CA-C | -7.11 | 99.02 | 109.11 |
| 2 | 1 | 502 | ILE | O-C-N | -7.11 | 115.42 | 122.67 |
| 8 | N | 56 | ASN | CA-CB-CG | -7.11 | 105.49 | 112.60 |
| 8 | N | 1339 | PHE | CA-CB-CG | -7.11 | 106.69 | 113.80 |
| 8 | P | 1503 | VAL | CA-C-N | 7.11 | 129.68 | 120.44 |
| 8 | P | 1503 | VAL | C-N-CA | 7.11 | 129.68 | 120.44 |
| 5 | H | 457 | ASN | N-CA-C | -7.11 | 104.58 | 113.18 |
| 7 | M | 1645 | LEU | N-CA-C | 7.11 | 119.03 | 111.28 |
| 1 | Y | 1448 | MET | CA-C-O | -7.11 | 113.02 | 120.55 |
| 19 | m | 139 | VAL | CA-C-N | 7.11 | 128.72 | 119.84 |
| 19 | m | 139 | VAL | C-N-CA | 7.11 | 128.72 | 119.84 |
| 19 | f | 34 | ASP | N-CA-C | -7.11 | 98.03 | 109.40 |
| 4 | G | 655 | PHE | CA-C-N | 7.11 | 130.38 | 120.29 |
| 4 | G | 655 | PHE | C-N-CA | 7.11 | 130.38 | 120.29 |
| 6 | L | 444 | ILE | CA-C-O | -7.11 | 112.58 | 120.25 |
| 9 | S | 571 | LEU | CA-C-N | 7.11 | 130.38 | 120.29 |
| 9 | S | 571 | LEU | C-N-CA | 7.11 | 130.38 | 120.29 |
| 20 | n | 947 | ILE | CA-C-N | 7.11 | 129.80 | 120.28 |
| 20 | n | 947 | ILE | C-N-CA | 7.11 | 129.80 | 120.28 |
| 7 | M | 298 | ASP | CA-CB-CG | 7.10 | 119.70 | 112.60 |
| 18 | l | 68 | TYR | N-CA-C | -7.10 | 103.78 | 113.30 |
| 7 | M | 1137 | ASN | N-CA-C | 7.10 | 130.89 | 111.00 |
| 7 | M | 1452 | SER | CA-C-N | 7.10 | 129.67 | 120.44 |
| 7 | M | 1452 | SER | C-N-CA | 7.10 | 129.67 | 120.44 |
| 9 | R | 249 | ARG | NE-CZ-NH2 | 7.10 | 125.59 | 119.20 |
| 9 | S | 408 | ARG | N-CA-CB | 7.10 | 120.97 | 110.53 |
| 7 | O | 1619 | ASN | CA-C-O | -7.10 | 113.02 | 120.55 |
| 14 | a | 422 | ARG | CA-C-O | -7.10 | 113.83 | 121.78 |
| 9 | T | 627 | ALA | CA-C-N | 7.10 | 129.79 | 120.28 |
| 9 | T | 627 | ALA | C-N-CA | 7.10 | 129.79 | 120.28 |
| 1 | Y | 437 | VAL | N-CA-C | -7.10 | 98.17 | 108.11 |
| 2 | Z | 355 | HIS | CE1-NE2-CD2 | -7.10 | 101.90 | 109.00 |
| 2 | Z | 921 | SER | N-CA-C | 7.10 | 130.88 | 111.00 |
| 8 | N | 1435 | ASP | CA-C-O | -7.10 | 113.40 | 121.07 |
| 1 | Y | 365 | ARG | N-CA-C | -7.10 | 105.55 | 114.56 |
| 12 | v | 356 | LEU | N-CA-C | -7.10 | 104.49 | 113.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | q | 43 | GLY | N-CA-C | 7.10 | 121.25 | 112.73 |
| 8 | N | 1015 | LYS | N-CA-C | -7.10 | 104.75 | 113.41 |
| 8 | N | 1027 | TRP | CB-CG-CD2 | -7.10 | 116.87 | 126.80 |
| 12 | v | 173 | PHE | CA-CB-CG | -7.10 | 106.70 | 113.80 |
| 5 | B | 395 | ALA | O-C-N | 7.09 | 130.24 | 122.15 |
| 8 | N | 220 | PHE | CA-CB-CG | -7.09 | 106.71 | 113.80 |
| 12 | u | 380 | ILE | CA-C-O | 7.09 | 126.53 | 120.22 |
| 16 | j | 445 | LEU | N-CA-C | -7.09 | 101.71 | 110.65 |
| 20 | g | 823 | GLN | OE1-CD-NE2 | -7.09 | 115.51 | 122.60 |
| 14 | a | 373 | PHE | CA-CB-CG | -7.09 | 106.71 | 113.80 |
| 1 | 0 | 922 | PHE | CA-CB-CG | -7.09 | 106.71 | 113.80 |
| 5 | K | 507 | ASN | CA-CB-CG | 7.09 | 119.69 | 112.60 |
| 4 | z | 660 | LYS | N-CA-C | -7.09 | 103.63 | 111.36 |
| 20 | n | 441 | ARG | N-CA-C | -7.09 | 101.38 | 110.53 |
| 7 | M | 1554 | LYS | CA-C-N | 7.09 | 132.84 | 122.99 |
| 7 | M | 1554 | LYS | C-N-CA | 7.09 | 132.84 | 122.99 |
| 1 | 0 | 1271 | ILE | CA-C-O | -7.09 | 113.58 | 120.95 |
| 9 | T | 574 | GLU | CB-CA-C | 7.09 | 122.01 | 110.88 |
| 15 | i | 693 | GLU | CA-C-N | 7.09 | 132.65 | 122.09 |
| 15 | i | 693 | GLU | C-N-CA | 7.09 | 132.65 | 122.09 |
| 17 | k | 225 | VAL | CA-C-O | -7.09 | 112.91 | 121.13 |
| 16 | c | 289 | ASN | N-CA-C | -7.09 | 98.14 | 109.76 |
| 17 | d | 240 | GLN | N-CA-C | -7.09 | 104.52 | 113.02 |
| 1 | 0 | 176 | PHE | CA-C-O | 7.08 | 126.11 | 119.59 |
| 4 | D | 802 | ASP | CA-CB-CG | 7.08 | 119.68 | 112.60 |
| 4 | J | 804 | LEU | N-CA-C | 7.08 | 119.00 | 111.28 |
| 7 | M | 1190 | TYR | N-CA-CB | 7.08 | 120.46 | 109.48 |
| 1 | Y | 1011 | ARG | CA-C-O | 7.08 | 128.57 | 121.20 |
| 1 | Y | 1103 | LEU | CA-C-N | 7.08 | 132.24 | 123.17 |
| 1 | Y | 1103 | LEU | C-N-CA | 7.08 | 132.24 | 123.17 |
| 14 | h | 233 | TYR | CA-CB-CG | -7.08 | 101.15 | 113.90 |
| 17 | k | 79 | VAL | N-CA-CB | 7.08 | 120.83 | 111.90 |
| 15 | b | 741 | GLN | N-CA-CB | 7.08 | 122.46 | 110.49 |
| 20 | g | 836 | PHE | CB-CA-C | -7.08 | 99.46 | 110.37 |
| 9 | T | 80 | PHE | N-CA-CB | 7.08 | 122.46 | 110.49 |
| 1 | Y | 212 | GLN | N-CA-C | -7.08 | 103.88 | 114.64 |
| 1 | Y | 1075 | ASP | N-CA-C | -7.08 | 97.57 | 108.76 |
| 12 | u | 332 | GLU | O-C-N | 7.08 | 131.27 | 123.13 |
| 4 | y | 685 | MET | N-CA-CB | 7.08 | 120.53 | 110.12 |
| 8 | P | 1425 | TYR | N-CA-C | -7.08 | 104.38 | 113.16 |
| 16 | j | 434 | LEU | CA-C-N | 7.08 | 130.10 | 120.54 |
| 16 | j | 434 | LEU | C-N-CA | 7.08 | 130.10 | 120.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 1547 | ILE | CA-C-N | 7.08 | 129.76 | 120.28 |
| 7 | M | 1547 | ILE | C-N-CA | 7.08 | 129.76 | 120.28 |
| 8 | P | 1553 | GLN | CA-C-N | 7.08 | 130.07 | 120.44 |
| 8 | P | 1553 | GLN | C-N-CA | 7.08 | 130.07 | 120.44 |
| 2 | 1 | 1340 | LYS | N-CA-C | -7.08 | 102.77 | 111.40 |
| 9 | Q | 254 | LEU | CA-C-O | 7.08 | 127.92 | 120.42 |
| 9 | R | 257 | TRP | N-CA-CB | 7.08 | 120.48 | 109.94 |
| 9 | R | 341 | LEU | N-CA-C | -7.08 | 104.62 | 113.18 |
| 8 | P | 78 | LEU | N-CA-C | -7.08 | 104.22 | 112.92 |
| 8 | P | 1199 | TYR | N-CA-CB | 7.08 | 120.80 | 110.26 |
| 9 | Q | 540 | ASN | N-CA-C | -7.08 | 104.62 | 113.18 |
| 11 | X | 351 | THR | N-CA-C | -7.08 | 97.87 | 109.40 |
| 2 | Z | 220 | ASN | N-CA-C | -7.08 | 95.73 | 110.80 |
| 1 | 0 | 650 | TYR | N-CA-C | -7.07 | 97.37 | 108.90 |
| 8 | N | 338 | SER | N-CA-C | -7.07 | 104.92 | 113.97 |
| 7 | O | 1586 | LEU | N-CA-C | 7.07 | 118.64 | 111.07 |
| 9 | T | 327 | VAL | CA-C-O | -7.07 | 112.12 | 120.75 |
| 2 | Z | 912 | ALA | CA-C-N | 7.07 | 131.16 | 121.05 |
| 2 | Z | 912 | ALA | C-N-CA | 7.07 | 131.16 | 121.05 |
| 13 | x | 1436 | VAL | CA-C-N | 7.07 | 130.15 | 120.46 |
| 13 | x | 1436 | VAL | C-N-CA | 7.07 | 130.15 | 120.46 |
| 15 | i | 320 | SER | CA-C-O | -7.07 | 113.61 | 121.89 |
| 8 | N | 905 | SER | N-CA-C | 7.07 | 119.60 | 111.11 |
| 1 | 0 | 714 | LYS | N-CA-CB | 7.07 | 122.95 | 110.37 |
| 7 | M | 486 | TYR | O-C-N | -7.07 | 114.62 | 122.12 |
| 4 | y | 769 | ILE | O-C-N | 7.07 | 128.73 | 121.87 |
| 20 | n | 666 | LYS | CA-C-N | 7.07 | 129.63 | 120.44 |
| 20 | n | 666 | LYS | C-N-CA | 7.07 | 129.63 | 120.44 |
| 6 | F | 339 | LEU | N-CA-C | 7.07 | 121.65 | 112.89 |
| 4 | z | 666 | ASP | N-CA-C | 7.07 | 118.98 | 111.28 |
| 20 | g | 1034 | LYS | N-CA-CB | 7.07 | 120.51 | 110.12 |
| 4 | A | 707 | LEU | CA-C-N | 7.07 | 130.61 | 120.79 |
| 4 | A | 707 | LEU | C-N-CA | 7.07 | 130.61 | 120.79 |
| 4 | G | 663 | ASN | CA-C-N | 7.07 | 130.32 | 120.29 |
| 4 | G | 663 | ASN | C-N-CA | 7.07 | 130.32 | 120.29 |
| 7 | O | 22 | PHE | N-CA-CB | 7.07 | 122.43 | 110.49 |
| 9 | R | 798 | THR | N-CA-C | -7.07 | 104.27 | 113.17 |
| 20 | n | 250 | LYS | O-C-N | -7.07 | 113.19 | 121.32 |
| 20 | n | 965 | LYS | CA-C-N | 7.07 | 132.33 | 120.88 |
| 20 | n | 965 | LYS | C-N-CA | 7.07 | 132.33 | 120.88 |
| 20 | g | 323 | LEU | N-CA-C | -7.07 | 102.94 | 112.26 |
| 20 | g | 1124 | ASN | N-CA-C | -7.07 | 104.47 | 113.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 253 | GLU | CA-C-O | -7.06 | 113.13 | 121.11 |
| 6 | C | 285 | GLN | CB-CG-CD | -7.06 | 100.59 | 112.60 |
| 7 | O | 10 | THR | CA-C-N | 7.06 | 129.74 | 120.28 |
| 7 | O | 10 | THR | C-N-CA | 7.06 | 129.74 | 120.28 |
| 7 | O | 301 | ASP | CA-CB-CG | -7.06 | 105.54 | 112.60 |
| 7 | O | 1361 | PHE | CA-CB-CG | -7.06 | 106.74 | 113.80 |
| 4 | G | 713 | ASN | OD1-CG-ND2 | -7.06 | 115.54 | 122.60 |
| 7 | M | 648 | PRO | N-CA-C | -7.06 | 107.34 | 114.68 |
| 7 | O | 198 | TYR | CB-CG-CD1 | 7.06 | 131.39 | 120.80 |
| 7 | O | 1280 | ILE | N-CA-CB | 7.06 | 118.81 | 110.55 |
| 20 | g | 413 | VAL | N-CA-C | -7.06 | 98.19 | 108.71 |
| 7 | M | 1546 | ILE | CA-C-N | 7.06 | 130.44 | 120.42 |
| 7 | M | 1546 | ILE | C-N-CA | 7.06 | 130.44 | 120.42 |
| 18 | e | 167 | SER | N-CA-C | -7.06 | 98.30 | 108.60 |
| 6 | I | 406 | PHE | CA-CB-CG | 7.06 | 120.86 | 113.80 |
| 7 | M | 1313 | ILE | N-CA-C | 7.06 | 117.57 | 110.23 |
| 14 | h | 978 | ALA | CA-C-N | 7.06 | 129.74 | 120.28 |
| 14 | h | 978 | ALA | C-N-CA | 7.06 | 129.74 | 120.28 |
| 9 | S | 150 | GLN | CA-C-N | 7.05 | 129.61 | 120.44 |
| 9 | S | 150 | GLN | C-N-CA | 7.05 | 129.61 | 120.44 |
| 2 | Z | 848 | LYS | CA-C-N | 7.05 | 129.73 | 120.28 |
| 2 | Z | 848 | LYS | C-N-CA | 7.05 | 129.73 | 120.28 |
| 20 | n | 787 | ASP | CA-CB-CG | 7.05 | 119.65 | 112.60 |
| 6 | L | 326 | LEU | CA-C-N | 7.05 | 129.73 | 120.28 |
| 6 | L | 326 | LEU | C-N-CA | 7.05 | 129.73 | 120.28 |
| 7 | M | 757 | PHE | CA-CB-CG | -7.05 | 106.75 | 113.80 |
| 9 | T | 206 | ASN | OD1-CG-ND2 | -7.05 | 115.55 | 122.60 |
| 20 | n | 974 | ARG | NE-CZ-NH1 | 7.05 | 128.55 | 121.50 |
| 16 | c | 540 | ASN | N-CA-CB | 7.05 | 122.83 | 110.42 |
| 9 | R | 551 | ARG | NE-CZ-NH1 | 7.05 | 128.55 | 121.50 |
| 12 | v | 187 | PHE | CA-CB-CG | -7.05 | 106.75 | 113.80 |
| 4 | y | 644 | TRP | CA-C-N | 7.05 | 129.60 | 120.44 |
| 4 | y | 644 | TRP | C-N-CA | 7.05 | 129.60 | 120.44 |
| 2 | 1 | 278 | THR | N-CA-C | -7.04 | 104.71 | 113.38 |
| 9 | S | 419 | ASP | CA-C-O | 7.04 | 128.62 | 120.80 |
| 6 | I | 402 | ASP | CB-CA-C | -7.04 | 99.82 | 110.88 |
| 1 | Y | 1157 | PHE | CA-CB-CG | 7.04 | 120.84 | 113.80 |
| 17 | k | 43 | HIS | CE1-NE2-CD2 | -7.04 | 101.96 | 109.00 |
| 19 | m | 448 | ILE | N-CA-CB | 7.04 | 121.15 | 110.58 |
| 20 | n | 870 | VAL | N-CA-CB | 7.04 | 118.33 | 110.51 |
| 8 | N | 1403 | ASN | CA-CB-CG | 7.04 | 119.64 | 112.60 |
| 9 | S | 662 | SER | CA-C-N | 7.04 | 129.72 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | S | 662 | SER | C-N-CA | 7.04 | 129.72 | 120.28 |
| 1 | Y | 274 | VAL | N-CA-C | -7.04 | 98.03 | 108.45 |
| 1 | Y | 1339 | LYS | O-C-N | 7.04 | 130.56 | 122.25 |
| 18 | e | 19 | PHE | CA-CB-CG | 7.04 | 120.84 | 113.80 |
| 18 | e | 117 | ALA | CB-CA-C | -7.04 | 102.36 | 110.17 |
| 19 | f | 586 | GLN | OE1-CD-NE2 | -7.04 | 115.56 | 122.60 |
| 20 | g | 81 | SER | N-CA-CB | 7.04 | 122.39 | 110.49 |
| 14 | a | 57 | SER | CB-CA-C | -7.04 | 101.93 | 110.94 |
| 14 | a | 199 | PHE | CA-CB-CG | 7.04 | 120.84 | 113.80 |
| 9 | T | 100 | PRO | CB-CA-C | -7.04 | 102.33 | 110.92 |
| 7 | M | 1080 | LEU | CA-C-N | 7.04 | 129.71 | 120.28 |
| 7 | M | 1080 | LEU | C-N-CA | 7.04 | 129.71 | 120.28 |
| 9 | Q | 27 | GLU | CA-C-N | 7.04 | 129.71 | 120.28 |
| 9 | Q | 27 | GLU | C-N-CA | 7.04 | 129.71 | 120.28 |
| 20 | n | 659 | PRO | N-CA-CB | 7.04 | 109.57 | 103.31 |
| 7 | M | 1309 | LEU | N-CA-C | 7.04 | 122.98 | 111.37 |
| 8 | P | 25 | ALA | N-CA-C | -7.04 | 97.49 | 109.24 |
| 2 | Z | 1088 | ALA | N-CA-C | -7.04 | 103.87 | 113.30 |
| 15 | i | 552 | ILE | CA-CB-CG2 | -7.04 | 98.54 | 110.50 |
| 7 | M | 1436 | LYS | CB-CA-C | -7.03 | 99.84 | 110.88 |
| 7 | O | 162 | ILE | N-CA-C | 7.03 | 117.17 | 110.42 |
| 20 | g | 790 | HIS | CE1-NE2-CD2 | -7.03 | 101.97 | 109.00 |
| 2 | 1 | 983 | TYR | CB-CG-CD2 | -7.03 | 110.26 | 120.80 |
| 8 | N | 1012 | VAL | N-CA-C | -7.03 | 105.65 | 111.91 |
| 7 | O | 605 | ALA | CA-C-N | 7.03 | 129.41 | 120.56 |
| 7 | O | 605 | ALA | C-N-CA | 7.03 | 129.41 | 120.56 |
| 8 | P | 742 | LEU | CA-C-N | 7.03 | 131.57 | 120.47 |
| 8 | P | 742 | LEU | C-N-CA | 7.03 | 131.57 | 120.47 |
| 9 | R | 125 | ILE | CA-C-N | 7.03 | 130.03 | 120.54 |
| 9 | R | 125 | ILE | C-N-CA | 7.03 | 130.03 | 120.54 |
| 6 | C | 389 | ARG | CA-C-O | -7.03 | 113.10 | 120.55 |
| 7 | M | 964 | LYS | N-CA-C | 7.03 | 121.30 | 112.87 |
| 8 | N | 819 | THR | CA-C-O | 7.03 | 127.93 | 119.43 |
| 15 | i | 714 | ILE | N-CA-C | -7.03 | 105.88 | 112.83 |
| 20 | g | 655 | PHE | N-CA-C | -7.03 | 105.90 | 114.75 |
| 7 | O | 37 | LEU | N-CA-C | -7.02 | 98.04 | 108.79 |
| 1 | Y | 436 | LEU | O-C-N | -7.02 | 115.39 | 123.33 |
| 2 | Z | 408 | LYS | N-CA-C | -7.02 | 97.17 | 108.55 |
| 1 | 0 | 1430 | LEU | CA-C-O | 7.02 | 128.08 | 119.79 |
| 8 | P | 690 | LEU | CB-CA-C | -7.02 | 98.30 | 110.17 |
| 12 | v | 549 | ILE | CA-C-N | 7.02 | 129.57 | 120.44 |
| 12 | v | 549 | ILE | C-N-CA | 7.02 | 129.57 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 983 | ASN | OD1-CG-ND2 | -7.02 | 115.58 | 122.60 |
| 11 | V | 269 | SER | N-CA-CB | 7.02 | 120.36 | 110.04 |
| 15 | b | 357 | PHE | CA-C-N | 7.02 | 130.00 | 120.38 |
| 15 | b | 357 | PHE | C-N-CA | 7.02 | 130.00 | 120.38 |
| 9 | R | 582 | GLU | N-CA-C | 7.02 | 119.78 | 111.71 |
| 9 | R | 629 | ARG | NE-CZ-NH2 | 7.02 | 125.52 | 119.20 |
| 9 | T | 770 | ASN | CA-CB-CG | 7.02 | 119.62 | 112.60 |
| 16 | c | 489 | HIS | CG-CD2-NE2 | 7.02 | 114.22 | 107.20 |
| 2 | 1 | 1073 | LEU | O-C-N | -7.02 | 114.68 | 122.12 |
| 5 | K | 520 | ILE | N-CA-C | -7.02 | 103.63 | 110.72 |
| 8 | P | 1435 | ASP | CA-CB-CG | 7.02 | 119.62 | 112.60 |
| 19 | m | 274 | GLN | CA-C-N | 7.02 | 133.55 | 122.60 |
| 19 | m | 274 | GLN | C-N-CA | 7.02 | 133.55 | 122.60 |
| 19 | f | 64 | SER | N-CA-CB | 7.02 | 120.44 | 110.12 |
| 10 | W | 331 | ASN | CA-CB-CG | 7.02 | 119.62 | 112.60 |
| 1 | Y | 230 | HIS | N-CA-C | -7.02 | 97.86 | 108.52 |
| 12 | u | 538 | ARG | N-CA-C | 7.02 | 118.93 | 111.28 |
| 14 | h | 573 | GLU | N-CA-C | -7.02 | 103.06 | 111.69 |
| 20 | g | 408 | ASN | CA-CB-CG | -7.01 | 105.59 | 112.60 |
| 2 | Z | 287 | GLN | N-CA-C | -7.01 | 97.78 | 109.07 |
| 8 | N | 57 | THR | CA-C-N | 7.01 | 129.53 | 120.56 |
| 8 | N | 57 | THR | C-N-CA | 7.01 | 129.53 | 120.56 |
| 8 | P | 1288 | PHE | CB-CG-CD1 | 7.01 | 132.62 | 120.70 |
| 9 | S | 546 | ARG | NE-CZ-NH2 | -7.01 | 112.89 | 119.20 |
| 19 | m | 600 | TRP | N-CA-C | 7.01 | 118.92 | 111.28 |
| 16 | c | 372 | LEU | N-CA-C | -7.01 | 101.98 | 111.87 |
| 14 | a | 221 | ASP | CA-C-O | 7.01 | 127.91 | 119.43 |
| 2 | 1 | 1001 | ARG | N-CA-CB | 7.01 | 120.17 | 110.01 |
| 14 | h | 567 | LEU | O-C-N | 7.01 | 129.58 | 122.08 |
| 16 | j | 252 | ASN | OD1-CG-ND2 | 7.01 | 129.61 | 122.60 |
| 16 | c | 547 | ARG | N-CA-CB | 7.01 | 120.41 | 109.69 |
| 14 | a | 217 | LYS | CA-C-N | 7.01 | 130.66 | 120.71 |
| 14 | a | 217 | LYS | C-N-CA | 7.01 | 130.66 | 120.71 |
| 8 | N | 371 | PHE | N-CA-C | -7.01 | 95.87 | 110.80 |
| 8 | N | 956 | PHE | CA-C-N | 7.01 | 129.98 | 120.38 |
| 8 | N | 956 | PHE | C-N-CA | 7.01 | 129.98 | 120.38 |
| 9 | S | 16 | LYS | CA-C-N | 7.01 | 128.90 | 120.14 |
| 9 | S | 16 | LYS | C-N-CA | 7.01 | 128.90 | 120.14 |
| 15 | i | 201 | ARG | CA-C-O | 7.01 | 127.85 | 120.42 |
| 2 | 1 | 795 | MET | CA-C-N | 7.01 | 130.37 | 120.28 |
| 2 | 1 | 795 | MET | C-N-CA | 7.01 | 130.37 | 120.28 |
| 7 | O | 1365 | ASN | N-CA-CB | 7.01 | 122.33 | 110.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 751 | ARG | CA-C-N | 7.01 | 131.33 | 120.82 |
| 14 | h | 751 | ARG | C-N-CA | 7.01 | 131.33 | 120.82 |
| 17 | d | 112 | TYR | N-CA-C | -7.01 | 97.98 | 109.40 |
| 20 | g | 406 | ASN | O-C-N | 7.00 | 131.79 | 122.96 |
| 8 | N | 876 | LEU | N-CA-CB | 7.00 | 122.33 | 110.49 |
| 20 | n | 852 | ILE | CA-C-O | 7.00 | 127.94 | 119.54 |
| 1 | 0 | 648 | GLU | O-C-N | -7.00 | 115.24 | 123.22 |
| 8 | P | 516 | CYS | N-CA-C | -7.00 | 104.35 | 113.17 |
| 2 | 1 | 1123 | PHE | N-CA-C | -7.00 | 95.89 | 110.80 |
| 15 | i | 215 | SER | N-CA-C | 7.00 | 118.70 | 111.14 |
| 9 | S | 582 | GLU | CA-C-N | 7.00 | 132.75 | 122.39 |
| 9 | S | 582 | GLU | C-N-CA | 7.00 | 132.75 | 122.39 |
| 2 | Z | 130 | GLY | CA-C-N | 7.00 | 130.53 | 121.85 |
| 2 | Z | 130 | GLY | C-N-CA | 7.00 | 130.53 | 121.85 |
| 2 | Z | 1318 | HIS | ND1-CE1-NE2 | 7.00 | 115.40 | 108.40 |
| 1 | 0 | 1445 | ASN | CA-C-N | 7.00 | 130.51 | 120.79 |
| 1 | 0 | 1445 | ASN | C-N-CA | 7.00 | 130.51 | 120.79 |
| 5 | B | 394 | THR | CA-C-N | 7.00 | 130.22 | 120.29 |
| 5 | B | 394 | THR | C-N-CA | 7.00 | 130.22 | 120.29 |
| 19 | f | 168 | VAL | CA-C-N | 7.00 | 133.28 | 123.07 |
| 19 | f | 168 | VAL | C-N-CA | 7.00 | 133.28 | 123.07 |
| 7 | M | 1474 | PHE | N-CA-C | -6.99 | 104.25 | 114.39 |
| 12 | v | 47 | ASN | CA-C-N | 6.99 | 129.37 | 120.56 |
| 12 | v | 47 | ASN | C-N-CA | 6.99 | 129.37 | 120.56 |
| 14 | a | 405 | GLU | N-CA-C | -6.99 | 105.29 | 114.31 |
| 8 | P | 188 | ILE | CA-C-N | 6.99 | 129.53 | 120.44 |
| 8 | P | 188 | ILE | C-N-CA | 6.99 | 129.53 | 120.44 |
| 2 | Z | 1177 | VAL | N-CA-C | -6.99 | 104.62 | 113.22 |
| 15 | b | 49 | VAL | CA-C-O | -6.99 | 113.21 | 119.71 |
| 7 | M | 815 | PHE | CA-CB-CG | -6.99 | 106.81 | 113.80 |
| 8 | P | 1080 | GLU | CA-C-N | 6.99 | 131.52 | 120.47 |
| 8 | P | 1080 | GLU | C-N-CA | 6.99 | 131.52 | 120.47 |
| 2 | Z | 1193 | LEU | CA-C-N | 6.99 | 130.22 | 120.29 |
| 2 | Z | 1193 | LEU | C-N-CA | 6.99 | 130.22 | 120.29 |
| 1 | 0 | 1321 | ALA | CA-C-N | 6.99 | 129.53 | 120.44 |
| 1 | 0 | 1321 | ALA | C-N-CA | 6.99 | 129.53 | 120.44 |
| 12 | u | 72 | ILE | CA-C-N | 6.99 | 133.06 | 122.65 |
| 12 | u | 72 | ILE | C-N-CA | 6.99 | 133.06 | 122.65 |
| 14 | h | 359 | THR | N-CA-C | -6.99 | 101.92 | 111.56 |
| 20 | n | 547 | PRO | N-CA-C | 6.99 | 119.23 | 110.70 |
| 5 | H | 322 | ILE | CA-C-N | 6.99 | 134.88 | 121.54 |
| 5 | H | 322 | ILE | C-N-CA | 6.99 | 134.88 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1090 | THR | CA-CB-OG1 | 6.99 | 120.08 | 109.60 |
| 14 | h | 134 | PRO | CA-C-O | -6.99 | 113.22 | 121.95 |
| 2 | 1 | 1084 | LEU | CA-C-O | -6.99 | 113.48 | 120.82 |
| 7 | M | 1449 | GLU | CA-C-N | 6.99 | 127.55 | 119.94 |
| 7 | M | 1449 | GLU | C-N-CA | 6.99 | 127.55 | 119.94 |
| 8 | N | 1016 | LEU | N-CA-C | 6.99 | 118.89 | 111.28 |
| 7 | O | 1279 | CYS | N-CA-C | 6.99 | 118.54 | 111.07 |
| 2 | Z | 975 | ASP | CA-CB-CG | 6.99 | 119.58 | 112.60 |
| 19 | m | 329 | ASN | CA-C-N | 6.99 | 130.21 | 120.29 |
| 19 | m | 329 | ASN | C-N-CA | 6.99 | 130.21 | 120.29 |
| 20 | n | 570 | PHE | N-CA-CB | 6.99 | 120.14 | 110.01 |
| 2 | Z | 1165 | ASP | CA-CB-CG | -6.98 | 105.62 | 112.60 |
| 7 | M | 1120 | THR | CA-C-O | 6.98 | 128.87 | 121.33 |
| 7 | M | 1415 | ARG | NE-CZ-NH2 | -6.98 | 112.92 | 119.20 |
| 20 | n | 138 | CYS | N-CA-C | -6.98 | 95.80 | 108.02 |
| 19 | f | 666 | GLU | CA-C-N | 6.98 | 129.64 | 120.28 |
| 19 | f | 666 | GLU | C-N-CA | 6.98 | 129.64 | 120.28 |
| 7 | O | 985 | GLN | OE1-CD-NE2 | -6.98 | 115.62 | 122.60 |
| 9 | R | 373 | ALA | N-CA-CB | 6.98 | 122.15 | 110.77 |
| 17 | k | 43 | HIS | CG-CD2-NE2 | 6.98 | 114.18 | 107.20 |
| 20 | n | 263 | THR | CB-CA-C | 6.98 | 122.05 | 109.83 |
| 12 | v | 575 | ASP | CA-C-N | 6.98 | 129.51 | 120.44 |
| 12 | v | 575 | ASP | C-N-CA | 6.98 | 129.51 | 120.44 |
| 20 | n | 862 | PHE | CA-CB-CG | 6.98 | 120.78 | 113.80 |
| 7 | M | 845 | ASP | CA-CB-CG | 6.98 | 119.58 | 112.60 |
| 7 | O | 362 | ASP | CB-CA-C | -6.98 | 96.84 | 110.10 |
| 9 | R | 427 | ALA | N-CA-C | -6.98 | 102.00 | 112.54 |
| 2 | Z | 508 | PHE | CA-CB-CG | -6.98 | 106.82 | 113.80 |
| 14 | a | 82 | TYR | CA-C-N | 6.98 | 127.40 | 119.93 |
| 14 | a | 82 | TYR | C-N-CA | 6.98 | 127.40 | 119.93 |
| 8 | P | 896 | PHE | CA-CB-CG | -6.98 | 106.82 | 113.80 |
| 14 | h | 618 | SER | CA-C-N | 6.98 | 129.51 | 120.44 |
| 14 | h | 618 | SER | C-N-CA | 6.98 | 129.51 | 120.44 |
| 1 | 0 | 1298 | ASP | N-CA-C | -6.97 | 104.65 | 113.72 |
| 4 | G | 776 | PHE | CA-CB-CG | 6.97 | 120.78 | 113.80 |
| 8 | N | 192 | LEU | CA-C-N | 6.97 | 129.94 | 120.38 |
| 8 | N | 192 | LEU | C-N-CA | 6.97 | 129.94 | 120.38 |
| 7 | O | 1607 | LEU | CA-C-N | 6.97 | 129.35 | 120.56 |
| 7 | O | 1607 | LEU | C-N-CA | 6.97 | 129.35 | 120.56 |
| 16 | j | 571 | ALA | N-CA-C | -6.97 | 103.76 | 112.90 |
| 9 | R | 308 | PHE | N-CA-C | -6.97 | 104.65 | 113.02 |
| 19 | m | 329 | ASN | CA-CB-CG | 6.97 | 119.57 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | Q | 506 | LEU | N-CA-C | -6.97 | 104.41 | 113.12 |
| 15 | i | 586 | LEU | N-CA-C | -6.97 | 98.37 | 109.59 |
| 15 | b | 577 | GLU | N-CA-C | -6.97 | 103.96 | 113.30 |
| 5 | E | 449 | ASP | CA-C-N | 6.97 | 128.55 | 119.84 |
| 5 | E | 449 | ASP | C-N-CA | 6.97 | 128.55 | 119.84 |
| 8 | N | 997 | VAL | CB-CA-C | 6.97 | 117.18 | 110.63 |
| 8 | P | 1513 | LYS | N-CA-C | -6.97 | 105.40 | 114.04 |
| 8 | P | 1522 | VAL | CA-C-N | 6.97 | 129.62 | 120.28 |
| 8 | P | 1522 | VAL | C-N-CA | 6.97 | 129.62 | 120.28 |
| 20 | g | 245 | GLY | CA-C-N | 6.97 | 131.70 | 121.31 |
| 20 | g | 245 | GLY | C-N-CA | 6.97 | 131.70 | 121.31 |
| 12 | u | 629 | LYS | CA-C-O | 6.97 | 127.94 | 120.55 |
| 6 | F | 286 | LYS | CA-C-N | 6.97 | 129.62 | 120.28 |
| 6 | F | 286 | LYS | C-N-CA | 6.97 | 129.62 | 120.28 |
| 7 | M | 1665 | GLU | N-CA-CB | 6.97 | 122.26 | 110.49 |
| 8 | N | 14 | THR | CA-C-N | 6.97 | 131.75 | 120.60 |
| 8 | N | 14 | THR | C-N-CA | 6.97 | 131.75 | 120.60 |
| 7 | O | 356 | ILE | N-CA-CB | 6.97 | 120.96 | 111.21 |
| 4 | z | 669 | LEU | CA-C-O | -6.96 | 113.41 | 121.07 |
| 20 | n | 875 | PHE | N-CA-C | 6.96 | 118.95 | 111.36 |
| 7 | M | 103 | LYS | CA-C-N | 6.96 | 129.58 | 120.60 |
| 7 | M | 103 | LYS | C-N-CA | 6.96 | 129.58 | 120.60 |
| 7 | M | 1184 | LEU | N-CA-C | -6.96 | 104.78 | 112.72 |
| 8 | N | 106 | ARG | N-CA-C | 6.96 | 118.52 | 111.07 |
| 8 | N | 1130 | PHE | N-CA-C | -6.96 | 102.03 | 112.54 |
| 9 | T | 80 | PHE | N-CA-C | -6.96 | 95.97 | 110.80 |
| 2 | Z | 822 | PHE | CA-CB-CG | -6.96 | 106.84 | 113.80 |
| 12 | v | 261 | GLU | N-CA-CB | 6.96 | 120.40 | 109.82 |
| 14 | a | 859 | GLU | N-CA-C | -6.96 | 104.09 | 112.59 |
| 7 | O | 1111 | ILE | N-CA-CB | 6.96 | 118.24 | 110.51 |
| 7 | O | 1353 | LEU | CA-C-N | 6.96 | 130.00 | 120.46 |
| 7 | O | 1353 | LEU | C-N-CA | 6.96 | 130.00 | 120.46 |
| 20 | g | 337 | HIS | CG-CD2-NE2 | 6.96 | 114.16 | 107.20 |
| 7 | O | 1484 | ARG | CA-C-N | 6.96 | 129.94 | 120.54 |
| 7 | O | 1484 | ARG | C-N-CA | 6.96 | 129.94 | 120.54 |
| 2 | Z | 1285 | VAL | CA-C-N | 6.96 | 131.74 | 120.60 |
| 2 | Z | 1285 | VAL | C-N-CA | 6.96 | 131.74 | 120.60 |
| 15 | b | 229 | SER | N-CA-CB | 6.96 | 122.25 | 110.49 |
| 7 | M | 1241 | LYS | CB-CA-C | 6.96 | 120.81 | 111.14 |
| 2 | 1 | 745 | ILE | N-CA-CB | -6.96 | 99.75 | 111.23 |
| 1 | Y | 1105 | TYR | CA-C-N | 6.96 | 132.02 | 122.77 |
| 1 | Y | 1105 | TYR | C-N-CA | 6.96 | 132.02 | 122.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | m | 231 | PHE | CA-CB-CG | -6.96 | 106.84 | 113.80 |
| 9 | R | 612 | HIS | CG-CD2-NE2 | 6.96 | 114.16 | 107.20 |
| 6 | F | 346 | ASP | CA-CB-CG | 6.95 | 119.55 | 112.60 |
| 9 | S | 411 | VAL | N-CA-CB | 6.95 | 119.86 | 112.21 |
| 14 | h | 186 | LEU | CA-C-O | 6.95 | 127.84 | 120.33 |
| 16 | c | 385 | LEU | CA-C-N | 6.95 | 129.60 | 120.28 |
| 16 | c | 385 | LEU | C-N-CA | 6.95 | 129.60 | 120.28 |
| 6 | C | 317 | LYS | CA-C-O | 6.95 | 127.92 | 120.55 |
| 9 | T | 246 | ASN | N-CA-C | -6.95 | 98.87 | 109.85 |
| 13 | w | 1284 | THR | CA-C-N | 6.95 | 129.59 | 120.28 |
| 13 | w | 1284 | THR | C-N-CA | 6.95 | 129.59 | 120.28 |
| 14 | h | 22 | ASN | CA-CB-CG | 6.95 | 119.55 | 112.60 |
| 19 | m | 279 | TYR | N-CA-C | -6.95 | 105.07 | 113.97 |
| 5 | B | 475 | SER | N-CA-C | -6.95 | 105.35 | 114.31 |
| 9 | R | 352 | VAL | N-CA-CB | 6.95 | 121.52 | 112.28 |
| 9 | S | 269 | ASN | CA-CB-CG | -6.95 | 105.65 | 112.60 |
| 20 | n | 147 | ASP | N-CA-CB | 6.95 | 121.96 | 110.63 |
| 4 | G | 810 | ASN | OD1-CG-ND2 | -6.95 | 115.65 | 122.60 |
| 8 | N | 1215 | VAL | CA-C-O | -6.95 | 113.49 | 120.85 |
| 13 | x | 1389 | SER | N-CA-CB | 6.95 | 122.55 | 110.39 |
| 8 | P | 914 | ASP | CA-CB-CG | 6.95 | 119.55 | 112.60 |
| 9 | T | 508 | ILE | CA-C-N | 6.95 | 127.69 | 119.98 |
| 9 | T | 508 | ILE | C-N-CA | 6.95 | 127.69 | 119.98 |
| 19 | m | 623 | PHE | N-CA-C | -6.95 | 103.64 | 111.14 |
| 7 | O | 1412 | TYR | CA-C-N | 6.94 | 130.28 | 120.28 |
| 7 | O | 1412 | TYR | C-N-CA | 6.94 | 130.28 | 120.28 |
| 7 | M | 698 | ASN | CA-C-O | -6.94 | 113.55 | 120.70 |
| 7 | M | 881 | THR | CA-C-N | 6.94 | 130.52 | 120.38 |
| 7 | M | 881 | THR | C-N-CA | 6.94 | 130.52 | 120.38 |
| 7 | O | 624 | ASP | CA-C-N | 6.94 | 130.28 | 120.28 |
| 7 | O | 624 | ASP | C-N-CA | 6.94 | 130.28 | 120.28 |
| 7 | O | 1412 | TYR | CA-C-O | -6.94 | 113.53 | 120.82 |
| 7 | O | 1611 | VAL | N-CA-C | -6.94 | 104.55 | 111.77 |
| 12 | v | 353 | ARG | N-CA-C | -6.94 | 97.09 | 108.41 |
| 20 | n | 594 | LEU | CB-CA-C | -6.94 | 101.49 | 111.14 |
| 17 | d | 52 | HIS | CA-CB-CG | -6.94 | 106.86 | 113.80 |
| 14 | h | 92 | THR | CA-C-N | 6.94 | 132.64 | 122.99 |
| 14 | h | 92 | THR | C-N-CA | 6.94 | 132.64 | 122.99 |
| 18 | e | 197 | GLY | CA-C-N | 6.94 | 129.58 | 120.28 |
| 18 | e | 197 | GLY | C-N-CA | 6.94 | 129.58 | 120.28 |
| 19 | f | 320 | HIS | CE1-NE2-CD2 | -6.94 | 102.06 | 109.00 |
| 12 | u | 304 | THR | CA-CB-OG1 | -6.94 | 99.19 | 109.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 18 | l | 328 | VAL | N-CA-CB | 6.94 | 118.47 | 110.49 |
| 6 | C | 299 | ILE | N-CA-C | -6.94 | 106.37 | 113.10 |
| 8 | N | 637 | VAL | CA-C-O | -6.94 | 113.13 | 121.18 |
| 12 | u | 393 | LEU | N-CA-CB | 6.94 | 120.32 | 110.12 |
| 2 | Z | 821 | ALA | N-CA-CB | 6.94 | 120.90 | 110.22 |
| 2 | 1 | 196 | GLU | N-CA-C | -6.93 | 105.44 | 114.04 |
| 7 | M | 1006 | LEU | CB-CA-C | -6.93 | 99.28 | 110.79 |
| 8 | N | 289 | TYR | N-CA-CB | 6.93 | 122.21 | 110.49 |
| 8 | N | 1125 | GLU | N-CA-C | -6.93 | 103.29 | 112.72 |
| 15 | i | 80 | ALA | CB-CA-C | -6.93 | 98.65 | 110.16 |
| 2 | 1 | 710 | TYR | CA-C-O | -6.93 | 113.54 | 120.82 |
| 11 | V | 298 | PHE | N-CA-C | -6.93 | 100.52 | 108.49 |
| 5 | H | 348 | ILE | O-C-N | -6.93 | 114.54 | 120.92 |
| 8 | P | 680 | ASP | N-CA-C | -6.93 | 104.86 | 113.38 |
| 9 | R | 783 | SER | O-C-N | 6.93 | 129.47 | 122.12 |
| 16 | j | 589 | ASN | N-CA-CB | 6.93 | 120.31 | 110.12 |
| 1 | 0 | 605 | VAL | N-CA-CB | 6.93 | 118.08 | 110.53 |
| 7 | O | 245 | ARG | NE-CZ-NH2 | -6.93 | 112.96 | 119.20 |
| 8 | P | 295 | PHE | N-CA-C | -6.93 | 105.37 | 114.31 |
| 1 | Y | 1096 | GLN | N-CA-C | 6.93 | 120.62 | 111.75 |
| 2 | Z | 767 | ASN | CA-CB-CG | -6.93 | 105.67 | 112.60 |
| 20 | g | 239 | LYS | CA-C-N | 6.93 | 126.92 | 119.78 |
| 20 | g | 239 | LYS | C-N-CA | 6.93 | 126.92 | 119.78 |
| 9 | S | 503 | ALA | CA-C-N | 6.93 | 130.26 | 120.42 |
| 9 | S | 503 | ALA | C-N-CA | 6.93 | 130.26 | 120.42 |
| 9 | T | 434 | ASP | CB-CA-C | -6.93 | 97.37 | 110.67 |
| 12 | u | 565 | GLN | CA-C-N | 6.93 | 129.56 | 120.28 |
| 12 | u | 565 | GLN | C-N-CA | 6.93 | 129.56 | 120.28 |
| 6 | F | 326 | LEU | CA-C-N | 6.93 | 129.44 | 120.44 |
| 6 | F | 326 | LEU | C-N-CA | 6.93 | 129.44 | 120.44 |
| 19 | m | 471 | PRO | N-CA-C | -6.93 | 105.69 | 114.35 |
| 20 | n | 704 | SER | N-CA-C | -6.93 | 103.51 | 113.21 |
| 7 | O | 1211 | GLU | N-CA-C | -6.92 | 98.50 | 109.23 |
| 18 | l | 302 | ASP | N-CA-C | -6.92 | 104.40 | 112.92 |
| 7 | O | 996 | LEU | N-CA-C | -6.92 | 103.72 | 112.93 |
| 8 | P | 964 | GLN | N-CA-CB | 6.92 | 122.19 | 110.49 |
| 10 | W | 307 | ILE | O-C-N | 6.92 | 130.50 | 122.81 |
| 9 | Q | 676 | GLY | CA-C-N | 6.92 | 128.49 | 119.84 |
| 9 | Q | 676 | GLY | C-N-CA | 6.92 | 128.49 | 119.84 |
| 2 | Z | 615 | ARG | CA-C-N | 6.92 | 130.32 | 120.49 |
| 2 | Z | 615 | ARG | C-N-CA | 6.92 | 130.32 | 120.49 |
| 15 | b | 544 | ASN | CA-C-N | 6.92 | 130.25 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | b | 544 | ASN | C-N-CA | 6.92 | 130.25 | 120.28 |
| 14 | a | 976 | ALA | N-CA-C | -6.92 | 96.06 | 110.80 |
| 2 | Z | 1338 | LEU | N-CA-C | -6.92 | 104.83 | 112.72 |
| 12 | v | 528 | PHE | N-CA-C | 6.92 | 118.47 | 111.07 |
| 18 | l | 37 | LYS | N-CA-C | -6.92 | 96.44 | 108.69 |
| 9 | T | 164 | GLN | N-CA-C | -6.92 | 104.72 | 113.02 |
| 12 | u | 149 | ASP | CB-CA-C | 6.92 | 124.19 | 110.42 |
| 19 | m | 553 | ASN | OD1-CG-ND2 | 6.92 | 129.52 | 122.60 |
| 20 | g | 227 | ARG | N-CA-C | -6.92 | 98.65 | 109.72 |
| 7 | M | 909 | LEU | O-C-N | 6.92 | 131.79 | 122.59 |
| 8 | N | 1566 | TYR | CA-C-O | 6.92 | 130.40 | 120.51 |
| 2 | 1 | 359 | THR | N-CA-C | -6.91 | 104.85 | 113.28 |
| 6 | I | 328 | GLN | CA-C-N | 6.91 | 129.42 | 120.44 |
| 6 | I | 328 | GLN | C-N-CA | 6.91 | 129.42 | 120.44 |
| 9 | R | 125 | ILE | N-CA-C | 6.91 | 117.62 | 110.36 |
| 7 | O | 1665 | GLU | N-CA-CB | 6.91 | 122.17 | 110.49 |
| 20 | g | 228 | ILE | N-CA-C | -6.91 | 94.97 | 109.34 |
| 9 | R | 356 | ASN | N-CA-C | -6.91 | 104.16 | 112.59 |
| 19 | m | 234 | GLN | CA-C-N | 6.91 | 133.92 | 121.97 |
| 19 | m | 234 | GLN | C-N-CA | 6.91 | 133.92 | 121.97 |
| 5 | K | 449 | ASP | N-CA-CB | 6.91 | 120.82 | 109.98 |
| 8 | N | 717 | VAL | CA-C-O | 6.91 | 128.17 | 120.85 |
| 20 | n | 1125 | SER | CA-C-N | 6.91 | 134.73 | 121.54 |
| 20 | n | 1125 | SER | C-N-CA | 6.91 | 134.73 | 121.54 |
| 6 | C | 302 | ASP | N-CA-C | -6.90 | 104.17 | 112.59 |
| 7 | M | 1597 | LEU | CA-C-N | 6.90 | 132.66 | 122.86 |
| 7 | M | 1597 | LEU | C-N-CA | 6.90 | 132.66 | 122.86 |
| 8 | P | 1462 | ASN | OD1-CG-ND2 | -6.90 | 115.70 | 122.60 |
| 9 | Q | 54 | PHE | N-CA-CB | 6.90 | 120.02 | 110.01 |
| 14 | h | 368 | VAL | CA-C-N | 6.90 | 130.22 | 120.28 |
| 14 | h | 368 | VAL | C-N-CA | 6.90 | 130.22 | 120.28 |
| 5 | K | 443 | LEU | N-CA-CB | 6.90 | 120.26 | 110.12 |
| 15 | i | 288 | SER | N-CA-CB | 6.90 | 120.48 | 110.20 |
| 15 | b | 599 | SER | CA-C-N | 6.90 | 126.53 | 119.56 |
| 15 | b | 599 | SER | C-N-CA | 6.90 | 126.53 | 119.56 |
| 5 | H | 528 | GLU | CB-CA-C | -6.90 | 99.34 | 110.79 |
| 14 | h | 759 | MET | CG-SD-CE | -6.90 | 85.72 | 100.90 |
| 1 | 0 | 852 | PHE | N-CA-C | 6.90 | 118.88 | 111.36 |
| 6 | I | 300 | ASP | CA-CB-CG | 6.90 | 119.50 | 112.60 |
| 7 | M | 1070 | TYR | N-CA-C | -6.90 | 103.89 | 112.72 |
| 8 | N | 182 | PHE | N-CA-C | -6.90 | 105.40 | 113.88 |
| 7 | O | 604 | GLU | O-C-N | 6.90 | 129.43 | 122.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | Q | 710 | ASN | N-CA-C | -6.90 | 104.75 | 113.72 |
| 1 | Y | 217 | VAL | N-CA-CB | 6.90 | 122.34 | 110.96 |
| 2 | 1 | 1101 | TYR | N-CA-C | -6.90 | 105.02 | 113.50 |
| 8 | N | 50 | ASN | N-CA-C | -6.90 | 103.98 | 112.88 |
| 9 | R | 786 | ILE | CA-C-O | -6.89 | 113.54 | 120.85 |
| 15 | i | 414 | SER | CA-C-N | 6.89 | 130.08 | 120.29 |
| 15 | i | 414 | SER | C-N-CA | 6.89 | 130.08 | 120.29 |
| 15 | i | 588 | ASP | CA-C-O | 6.89 | 125.98 | 120.19 |
| 16 | j | 382 | LEU | CA-C-N | 6.89 | 129.52 | 120.28 |
| 16 | j | 382 | LEU | C-N-CA | 6.89 | 129.52 | 120.28 |
| 15 | b | 200 | ASN | CA-CB-CG | 6.89 | 119.50 | 112.60 |
| 16 | c | 632 | GLU | CA-C-N | 6.89 | 130.79 | 120.31 |
| 16 | c | 632 | GLU | C-N-CA | 6.89 | 130.79 | 120.31 |
| 5 | H | 459 | LEU | O-C-N | 6.89 | 130.75 | 122.27 |
| 7 | O | 1105 | PHE | CA-C-N | 6.89 | 130.37 | 120.79 |
| 7 | O | 1105 | PHE | C-N-CA | 6.89 | 130.37 | 120.79 |
| 9 | T | 160 | GLY | CA-C-N | 6.89 | 129.25 | 120.56 |
| 9 | T | 160 | GLY | C-N-CA | 6.89 | 129.25 | 120.56 |
| 20 | g | 840 | PRO | N-CA-C | -6.89 | 100.17 | 111.68 |
| 8 | P | 1160 | ILE | CA-C-O | -6.89 | 114.07 | 118.69 |
| 16 | j | 463 | ARG | N-CA-C | -6.89 | 97.18 | 108.41 |
| 8 | N | 839 | ILE | CA-C-N | 6.89 | 132.22 | 120.72 |
| 8 | N | 839 | ILE | C-N-CA | 6.89 | 132.22 | 120.72 |
| 12 | v | 382 | GLN | CA-C-N | 6.89 | 131.93 | 122.77 |
| 12 | v | 382 | GLN | C-N-CA | 6.89 | 131.93 | 122.77 |
| 14 | h | 923 | LEU | N-CA-CB | 6.89 | 120.17 | 110.04 |
| 12 | u | 243 | VAL | CA-C-N | 6.89 | 129.24 | 120.56 |
| 12 | u | 243 | VAL | C-N-CA | 6.89 | 129.24 | 120.56 |
| 20 | g | 755 | GLN | N-CA-C | -6.89 | 96.13 | 110.80 |
| 4 | J | 666 | ASP | CA-C-N | 6.88 | 129.39 | 120.44 |
| 4 | J | 666 | ASP | C-N-CA | 6.88 | 129.39 | 120.44 |
| 7 | O | 667 | SER | N-CA-CB | 6.88 | 122.13 | 110.49 |
| 8 | P | 1165 | ILE | N-CA-C | -6.88 | 105.93 | 113.43 |
| 13 | w | 1288 | ILE | CB-CA-C | -6.88 | 102.84 | 112.14 |
| 14 | h | 291 | LEU | N-CA-C | -6.88 | 97.65 | 109.15 |
| 16 | j | 428 | ASN | OD1-CG-ND2 | -6.88 | 115.72 | 122.60 |
| 18 | l | 130 | ASN | CA-CB-CG | -6.88 | 105.72 | 112.60 |
| 15 | b | 288 | SER | N-CA-C | 6.88 | 119.81 | 111.82 |
| 5 | E | 510 | VAL | CA-C-O | 6.88 | 128.15 | 120.85 |
| 1 | Y | 641 | VAL | N-CA-C | -6.88 | 97.82 | 107.80 |
| 1 | Y | 1381 | SER | N-CA-CB | 6.88 | 120.06 | 110.56 |
| 6 | F | 470 | LEU | O-C-N | 6.88 | 130.09 | 122.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | I | 369 | LEU | N-CA-C | -6.88 | 91.73 | 111.00 |
| 9 | R | 285 | TYR | CB-CG-CD2 | -6.88 | 110.48 | 120.80 |
| 10 | U | 274 | GLY | N-CA-C | -6.88 | 101.21 | 111.19 |
| 2 | 1 | 1285 | VAL | CA-C-N | 6.88 | 130.19 | 120.28 |
| 2 | 1 | 1285 | VAL | C-N-CA | 6.88 | 130.19 | 120.28 |
| 11 | X | 290 | HIS | CG-CD2-NE2 | 6.88 | 114.08 | 107.20 |
| 2 | Z | 1048 | MET | N-CA-CB | 6.88 | 120.34 | 110.16 |
| 13 | w | 1273 | GLN | CA-C-N | 6.88 | 129.38 | 120.44 |
| 13 | w | 1273 | GLN | C-N-CA | 6.88 | 129.38 | 120.44 |
| 4 | y | 800 | HIS | CA-C-N | 6.88 | 129.38 | 120.44 |
| 4 | y | 800 | HIS | C-N-CA | 6.88 | 129.38 | 120.44 |
| 14 | h | 515 | GLY | N-CA-C | 6.88 | 122.80 | 113.99 |
| 17 | d | 217 | LEU | N-CA-CB | 6.88 | 122.11 | 110.49 |
| 2 | Z | 1181 | THR | N-CA-C | -6.88 | 103.02 | 112.03 |
| 12 | u | 258 | LYS | CA-C-N | 6.88 | 129.38 | 120.44 |
| 12 | u | 258 | LYS | C-N-CA | 6.88 | 129.38 | 120.44 |
| 14 | h | 16 | GLU | N-CA-C | -6.88 | 100.23 | 110.06 |
| 20 | g | 144 | ALA | N-CA-CB | 6.88 | 122.11 | 110.49 |
| 5 | B | 524 | ASN | CB-CA-C | -6.88 | 100.09 | 110.88 |
| 7 | M | 1381 | LEU | N-CA-C | -6.88 | 103.84 | 111.82 |
| 9 | Q | 549 | ASP | CA-CB-CG | -6.88 | 105.72 | 112.60 |
| 9 | R | 475 | SER | N-CA-C | -6.88 | 104.64 | 113.16 |
| 15 | b | 457 | TYR | O-C-N | -6.88 | 115.64 | 123.48 |
| 17 | d | 213 | SER | N-CA-C | 6.88 | 117.51 | 109.60 |
| 2 | 1 | 1059 | PHE | N-CA-C | 6.87 | 118.85 | 111.36 |
| 7 | M | 1170 | PHE | CA-CB-CG | -6.87 | 106.93 | 113.80 |
| 8 | P | 1471 | GLU | CA-C-N | 6.87 | 129.88 | 120.67 |
| 8 | P | 1471 | GLU | C-N-CA | 6.87 | 129.88 | 120.67 |
| 9 | S | 439 | HIS | CE1-NE2-CD2 | -6.87 | 102.13 | 109.00 |
| 2 | Z | 880 | SER | N-CA-C | -6.87 | 103.79 | 112.93 |
| 14 | h | 895 | CYS | O-C-N | -6.87 | 114.99 | 122.07 |
| 15 | b | 679 | ASP | CB-CA-C | -6.87 | 107.17 | 117.07 |
| 16 | c | 273 | VAL | N-CA-CB | 6.87 | 119.89 | 110.54 |
| 6 | F | 341 | ASP | N-CA-CB | 6.87 | 120.03 | 110.07 |
| 7 | M | 1249 | ILE | CA-C-N | 6.87 | 129.37 | 120.44 |
| 7 | M | 1249 | ILE | C-N-CA | 6.87 | 129.37 | 120.44 |
| 9 | R | 430 | LEU | N-CA-C | -6.87 | 104.43 | 114.39 |
| 1 | Y | 1325 | PHE | CA-C-O | -6.87 | 113.14 | 120.42 |
| 20 | n | 702 | ASP | CA-CB-CG | 6.87 | 119.47 | 112.60 |
| 16 | c | 450 | CYS | CA-C-N | 6.87 | 129.82 | 120.54 |
| 16 | c | 450 | CYS | C-N-CA | 6.87 | 129.82 | 120.54 |
| 7 | M | 1442 | TRP | CB-CG-CD2 | 6.87 | 136.42 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 521 | SER | N-CA-CB | 6.87 | 120.14 | 110.04 |
| 18 | e | 188 | LEU | N-CA-CB | 6.87 | 122.10 | 110.49 |
| 2 | Z | 871 | VAL | N-CA-C | -6.87 | 106.31 | 112.90 |
| 12 | u | 176 | ASP | N-CA-CB | 6.87 | 122.10 | 110.49 |
| 2 | 1 | 1050 | SER | N-CA-C | -6.87 | 100.32 | 110.48 |
| 8 | P | 676 | LEU | N-CA-C | 6.87 | 119.35 | 111.11 |
| 8 | N | 643 | GLU | CA-C-N | 6.87 | 129.21 | 120.56 |
| 8 | N | 643 | GLU | C-N-CA | 6.87 | 129.21 | 120.56 |
| 19 | f | 330 | ARG | NE-CZ-NH1 | 6.87 | 128.37 | 121.50 |
| 1 | 0 | 229 | LYS | N-CA-C | -6.86 | 104.00 | 114.16 |
| 1 | 0 | 982 | GLU | CA-C-O | -6.86 | 112.08 | 119.97 |
| 7 | M | 143 | ASN | CA-CB-CG | 6.86 | 119.46 | 112.60 |
| 8 | P | 412 | ILE | N-CA-C | -6.86 | 105.39 | 113.42 |
| 1 | Y | 1198 | ASN | OD1-CG-ND2 | 6.86 | 129.46 | 122.60 |
| 2 | Z | 650 | LYS | CA-C-N | 6.86 | 130.16 | 120.28 |
| 2 | Z | 650 | LYS | C-N-CA | 6.86 | 130.16 | 120.28 |
| 15 | i | 184 | CYS | O-C-N | 6.86 | 130.71 | 122.27 |
| 7 | M | 1049 | LEU | N-CA-CB | 6.86 | 120.32 | 110.16 |
| 5 | B | 381 | GLU | N-CA-C | 6.86 | 118.84 | 111.36 |
| 15 | i | 606 | ILE | N-CA-CB | 6.86 | 120.56 | 111.64 |
| 20 | n | 323 | LEU | N-CA-C | -6.86 | 104.53 | 113.17 |
| 1 | 0 | 1425 | LYS | N-CA-C | -6.86 | 103.42 | 111.03 |
| 2 | 1 | 953 | ILE | N-CA-C | -6.86 | 106.34 | 111.90 |
| 7 | M | 83 | LEU | N-CA-CB | 6.86 | 122.08 | 110.49 |
| 9 | R | 813 | CYS | CA-C-N | 6.86 | 129.70 | 120.65 |
| 9 | R | 813 | CYS | C-N-CA | 6.86 | 129.70 | 120.65 |
| 4 | J | 702 | ARG | N-CA-C | -6.86 | 104.73 | 113.23 |
| 8 | P | 1019 | THR | O-C-N | -6.86 | 114.20 | 122.22 |
| 1 | Y | 1265 | ALA | N-CA-C | -6.86 | 104.95 | 113.38 |
| 18 | l | 151 | THR | N-CA-C | -6.86 | 103.81 | 112.93 |
| 16 | c | 171 | SER | N-CA-C | -6.86 | 98.22 | 108.99 |
| 2 | 1 | 279 | ASP | CA-CB-CG | 6.86 | 119.46 | 112.60 |
| 9 | T | 309 | ILE | CA-C-N | 6.86 | 130.73 | 120.31 |
| 9 | T | 309 | ILE | C-N-CA | 6.86 | 130.73 | 120.31 |
| 2 | Z | 262 | ASN | CA-CB-CG | -6.86 | 105.75 | 112.60 |
| 2 | Z | 656 | HIS | CA-CB-CG | 6.86 | 120.66 | 113.80 |
| 15 | i | 639 | ARG | NE-CZ-NH1 | -6.86 | 114.64 | 121.50 |
| 15 | b | 277 | THR | N-CA-C | -6.86 | 102.98 | 112.30 |
| 14 | a | 1014 | TYR | N-CA-C | -6.86 | 97.17 | 108.76 |
| 2 | 1 | 1165 | ASP | O-C-N | -6.85 | 114.69 | 122.09 |
| 7 | M | 913 | TYR | CA-C-N | 6.85 | 129.47 | 120.28 |
| 7 | M | 913 | TYR | C-N-CA | 6.85 | 129.47 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | C | 341 | ASP | CA-CB-CG | 6.85 | 119.45 | 112.60 |
| 7 | M | 1163 | LEU | N-CA-C | 6.85 | 118.75 | 111.28 |
| 9 | T | 356 | ASN | N-CA-CB | 6.85 | 122.07 | 110.49 |
| 19 | m | 662 | PHE | CB-CA-C | 6.85 | 123.83 | 110.67 |
| 14 | a | 473 | VAL | O-C-N | 6.85 | 130.15 | 122.68 |
| 9 | Q | 367 | PHE | N-CA-CB | 6.85 | 122.07 | 110.49 |
| 7 | O | 1458 | LEU | CA-C-N | 6.85 | 129.46 | 120.28 |
| 7 | O | 1458 | LEU | C-N-CA | 6.85 | 129.46 | 120.28 |
| 21 | s | 61 | VAL | N-CA-C | -6.85 | 98.26 | 108.12 |
| 9 | T | 215 | TYR | N-CA-CB | 6.85 | 120.26 | 110.13 |
| 2 | Z | 1200 | LEU | CB-CA-C | -6.85 | 100.18 | 109.42 |
| 15 | i | 241 | GLU | N-CA-C | -6.85 | 104.24 | 112.59 |
| 19 | m | 391 | HIS | CE1-NE2-CD2 | -6.85 | 102.15 | 109.00 |
| 7 | O | 251 | ASP | CA-C-N | 6.85 | 129.84 | 120.46 |
| 7 | O | 251 | ASP | C-N-CA | 6.85 | 129.84 | 120.46 |
| 15 | b | 99 | ASP | N-CA-C | -6.85 | 96.22 | 110.80 |
| 8 | N | 1453 | ILE | CA-C-N | 6.84 | 128.65 | 120.09 |
| 8 | N | 1453 | ILE | C-N-CA | 6.84 | 128.65 | 120.09 |
| 9 | R | 136 | PHE | CA-C-O | -6.84 | 113.63 | 120.82 |
| 18 | l | 5 | ASP | CA-CB-CG | 6.84 | 119.44 | 112.60 |
| 14 | a | 952 | ASN | OD1-CG-ND2 | -6.84 | 115.75 | 122.60 |
| 2 | 1 | 1081 | LEU | O-C-N | -6.84 | 114.28 | 120.71 |
| 4 | z | 629 | PRO | N-CA-CB | 6.84 | 110.53 | 103.00 |
| 14 | h | 1021 | GLY | N-CA-C | -6.84 | 105.45 | 111.95 |
| 7 | M | 761 | LEU | N-CA-CB | 6.84 | 122.05 | 110.49 |
| 7 | O | 358 | LYS | N-CA-C | -6.84 | 103.08 | 113.89 |
| 19 | m | 340 | GLU | N-CA-C | -6.84 | 100.17 | 109.54 |
| 16 | c | 265 | HIS | CE1-NE2-CD2 | -6.84 | 102.16 | 109.00 |
| 7 | M | 979 | LYS | CA-C-N | 6.84 | 129.33 | 120.44 |
| 7 | M | 979 | LYS | C-N-CA | 6.84 | 129.33 | 120.44 |
| 2 | Z | 104 | ARG | NE-CZ-NH1 | 6.84 | 128.34 | 121.50 |
| 9 | Q | 132 | ALA | CA-C-N | 6.84 | 129.44 | 120.28 |
| 9 | Q | 132 | ALA | C-N-CA | 6.84 | 129.44 | 120.28 |
| 8 | N | 1046 | LYS | O-C-N | 6.84 | 130.45 | 122.25 |
| 9 | T | 505 | HIS | CG-CD2-NE2 | 6.84 | 114.04 | 107.20 |
| 12 | v | 443 | LYS | N-CA-C | -6.84 | 103.35 | 113.61 |
| 20 | g | 970 | GLN | CB-CG-CD | -6.84 | 100.98 | 112.60 |
| 14 | a | 953 | LEU | CA-C-N | 6.84 | 129.33 | 120.44 |
| 14 | a | 953 | LEU | C-N-CA | 6.84 | 129.33 | 120.44 |
| 6 | F | 325 | TYR | CA-C-O | -6.83 | 113.64 | 120.82 |
| 19 | m | 389 | VAL | CA-C-O | -6.83 | 111.31 | 119.58 |
| 6 | C | 316 | LEU | N-CA-C | 6.83 | 118.38 | 111.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | J | 721 | LEU | CA-C-N | 6.83 | 130.12 | 120.28 |
| 4 | J | 721 | LEU | C-N-CA | 6.83 | 130.12 | 120.28 |
| 7 | M | 859 | LYS | N-CA-C | -6.83 | 102.55 | 111.71 |
| 8 | P | 1540 | LYS | N-CA-C | -6.83 | 96.24 | 110.80 |
| 17 | k | 62 | ALA | O-C-N | -6.83 | 115.00 | 122.79 |
| 4 | A | 753 | GLU | N-CA-CB | 6.83 | 121.27 | 110.55 |
| 4 | G | 798 | ASN | CA-CB-CG | 6.83 | 119.43 | 112.60 |
| 7 | M | 1591 | ASP | CA-C-N | 6.83 | 130.12 | 120.28 |
| 7 | M | 1591 | ASP | C-N-CA | 6.83 | 130.12 | 120.28 |
| 15 | i | 228 | PHE | N-CA-C | -6.83 | 104.52 | 112.92 |
| 20 | g | 332 | LYS | N-CA-C | -6.83 | 105.08 | 113.41 |
| 8 | P | 1633 | ARG | O-C-N | -6.83 | 112.07 | 123.00 |
| 9 | R | 242 | LEU | N-CA-CB | 6.83 | 120.89 | 110.44 |
| 13 | w | 1393 | ASP | CA-C-N | 6.83 | 127.52 | 119.94 |
| 13 | w | 1393 | ASP | C-N-CA | 6.83 | 127.52 | 119.94 |
| 14 | h | 679 | LEU | N-CA-CB | 6.83 | 121.09 | 110.44 |
| 8 | N | 1409 | ALA | N-CA-C | 6.83 | 118.72 | 111.28 |
| 7 | O | 1089 | ASN | CA-CB-CG | 6.83 | 119.42 | 112.60 |
| 20 | n | 862 | PHE | N-CA-C | -6.83 | 105.23 | 113.97 |
| 8 | P | 1398 | VAL | CA-C-O | -6.82 | 112.25 | 120.78 |
| 1 | Y | 1367 | LEU | CA-C-N | 6.82 | 129.73 | 120.38 |
| 1 | Y | 1367 | LEU | C-N-CA | 6.82 | 129.73 | 120.38 |
| 19 | m | 232 | ASN | N-CA-C | -6.82 | 102.08 | 110.61 |
| 7 | M | 1180 | TYR | CB-CG-CD1 | -6.82 | 110.57 | 120.80 |
| 12 | v | 192 | LEU | CB-CA-C | -6.82 | 99.19 | 110.72 |
| 14 | h | 644 | THR | N-CA-C | -6.82 | 104.99 | 113.38 |
| 6 | L | 342 | GLU | CB-CG-CD | -6.82 | 101.01 | 112.60 |
| 8 | P | 1071 | LYS | CA-C-O | 6.82 | 127.77 | 119.38 |
| 9 | S | 343 | ALA | N-CA-C | -6.82 | 105.11 | 113.50 |
| 9 | S | 824 | MET | O-C-N | 6.82 | 126.63 | 121.65 |
| 13 | x | 1442 | ALA | N-CA-CB | 6.82 | 119.89 | 110.01 |
| 6 | F | 308 | ILE | CA-C-O | -6.82 | 110.82 | 119.95 |
| 7 | O | 259 | PHE | CA-CB-CG | 6.82 | 120.62 | 113.80 |
| 7 | M | 816 | PHE | CA-CB-CG | -6.81 | 106.99 | 113.80 |
| 2 | Z | 1068 | ARG | N-CA-C | -6.81 | 102.27 | 110.44 |
| 20 | g | 435 | SER | N-CA-C | -6.81 | 96.29 | 110.80 |
| 20 | g | 947 | ILE | CA-C-N | 6.81 | 129.96 | 120.29 |
| 20 | g | 947 | ILE | C-N-CA | 6.81 | 129.96 | 120.29 |
| 14 | a | 319 | ILE | N-CA-C | -6.81 | 94.16 | 108.88 |
| 8 | N | 1039 | PHE | N-CA-C | -6.81 | 103.53 | 114.09 |
| 7 | O | 926 | LEU | CA-C-N | 6.81 | 127.66 | 120.03 |
| 7 | O | 926 | LEU | C-N-CA | 6.81 | 127.66 | 120.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 297 | HIS | N-CA-C | -6.81 | 98.67 | 109.23 |
| 2 | 1 | 597 | GLU | CA-C-N | 6.81 | 128.35 | 119.84 |
| 2 | 1 | 597 | GLU | C-N-CA | 6.81 | 128.35 | 119.84 |
| 9 | R | 103 | ILE | N-CA-C | -6.81 | 99.90 | 108.89 |
| 9 | R | 747 | PHE | CA-CB-CG | -6.81 | 106.99 | 113.80 |
| 9 | S | 317 | ASP | CA-CB-CG | 6.81 | 119.41 | 112.60 |
| 2 | Z | 536 | HIS | ND1-CE1-NE2 | 6.81 | 115.21 | 108.40 |
| 13 | x | 1356 | ILE | N-CA-C | 6.81 | 117.57 | 110.62 |
| 14 | h | 226 | CYS | N-CA-C | -6.81 | 97.80 | 108.90 |
| 15 | i | 398 | ILE | CA-C-N | 6.81 | 130.66 | 120.31 |
| 15 | i | 398 | ILE | C-N-CA | 6.81 | 130.66 | 120.31 |
| 15 | b | 109 | SER | CA-C-N | 6.81 | 127.36 | 119.94 |
| 15 | b | 109 | SER | C-N-CA | 6.81 | 127.36 | 119.94 |
| 15 | b | 510 | HIS | CE1-NE2-CD2 | -6.81 | 102.19 | 109.00 |
| 7 | O | 723 | GLU | CA-C-N | 6.81 | 131.45 | 121.31 |
| 7 | O | 723 | GLU | C-N-CA | 6.81 | 131.45 | 121.31 |
| 1 | Y | 1313 | VAL | CA-C-O | -6.81 | 110.83 | 119.95 |
| 13 | w | 1145 | ASN | N-CA-CB | 6.81 | 121.65 | 110.69 |
| 15 | b | 141 | ASN | CA-CB-CG | -6.81 | 105.79 | 112.60 |
| 8 | N | 591 | MET | N-CA-C | -6.80 | 104.13 | 113.18 |
| 15 | i | 629 | VAL | CA-C-O | -6.80 | 113.96 | 121.17 |
| 16 | c | 531 | LYS | CA-C-N | 6.80 | 134.72 | 122.13 |
| 16 | c | 531 | LYS | C-N-CA | 6.80 | 134.72 | 122.13 |
| 7 | M | 182 | ARG | NE-CZ-NH1 | 6.80 | 128.30 | 121.50 |
| 1 | Y | 233 | LEU | CA-C-O | -6.80 | 113.08 | 120.36 |
| 20 | n | 926 | VAL | O-C-N | 6.80 | 128.47 | 121.87 |
| 19 | f | 45 | ALA | N-CA-C | 6.80 | 118.35 | 111.07 |
| 14 | a | 984 | TYR | N-CA-CB | 6.80 | 120.23 | 110.16 |
| 2 | 1 | 598 | PRO | CB-CA-C | 6.80 | 122.78 | 111.56 |
| 7 | M | 729 | MET | N-CA-C | 6.80 | 119.08 | 110.24 |
| 8 | P | 523 | SER | N-CA-CB | 6.80 | 121.98 | 110.49 |
| 9 | S | 470 | GLY | CA-C-N | 6.80 | 128.34 | 119.84 |
| 9 | S | 470 | GLY | C-N-CA | 6.80 | 128.34 | 119.84 |
| 16 | j | 653 | GLU | N-CA-C | -6.80 | 104.73 | 113.16 |
| 18 | e | 245 | ILE | N-CA-CB | 6.80 | 119.25 | 111.90 |
| 1 | 0 | 706 | GLY | CA-C-O | -6.80 | 113.46 | 122.23 |
| 1 | Y | 714 | LYS | N-CA-CB | 6.80 | 122.47 | 110.37 |
| 7 | O | 219 | HIS | ND1-CE1-NE2 | 6.80 | 115.20 | 108.40 |
| 9 | R | 736 | LEU | CA-C-O | 6.80 | 127.96 | 120.82 |
| 9 | S | 551 | ARG | N-CA-C | -6.80 | 105.12 | 113.41 |
| 4 | z | 817 | GLN | O-C-N | 6.80 | 129.90 | 122.15 |
| 2 | 1 | 125 | PHE | CA-CB-CG | -6.80 | 107.00 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | A | 792 | GLN | CA-C-N | 6.80 | 129.28 | 120.44 |
| 4 | A | 792 | GLN | C-N-CA | 6.80 | 129.28 | 120.44 |
| 8 | N | 1425 | TYR | CA-C-N | 6.80 | 129.28 | 120.44 |
| 8 | N | 1425 | TYR | C-N-CA | 6.80 | 129.28 | 120.44 |
| 7 | M | 631 | LEU | N-CA-C | -6.79 | 105.52 | 113.88 |
| 8 | P | 637 | VAL | CA-CB-CG1 | 6.79 | 121.95 | 110.40 |
| 9 | R | 373 | ALA | N-CA-C | -6.79 | 96.98 | 108.26 |
| 1 | 0 | 1472 | ILE | N-CA-C | 6.79 | 117.49 | 110.36 |
| 7 | M | 1590 | LYS | CA-C-N | 6.79 | 130.06 | 120.28 |
| 7 | M | 1590 | LYS | C-N-CA | 6.79 | 130.06 | 120.28 |
| 9 | Q | 42 | ILE | O-C-N | 6.79 | 131.06 | 122.57 |
| 14 | h | 957 | ASP | CA-C-O | -6.79 | 114.04 | 121.31 |
| 15 | b | 392 | GLN | CA-C-N | 6.79 | 126.25 | 118.85 |
| 15 | b | 392 | GLN | C-N-CA | 6.79 | 126.25 | 118.85 |
| 8 | N | 345 | ASP | CA-CB-CG | 6.79 | 119.39 | 112.60 |
| 9 | T | 536 | ASN | CA-CB-CG | 6.79 | 119.39 | 112.60 |
| 19 | m | 240 | HIS | CE1-NE2-CD2 | -6.79 | 102.21 | 109.00 |
| 20 | n | 930 | SER | O-C-N | 6.79 | 129.89 | 122.15 |
| 20 | g | 1136 | THR | N-CA-C | -6.79 | 102.26 | 112.04 |
| 14 | a | 844 | CYS | CA-C-N | -6.79 | 113.56 | 121.71 |
| 14 | a | 844 | CYS | C-N-CA | -6.79 | 113.56 | 121.71 |
| 1 | 0 | 1048 | LYS | CA-C-N | 6.79 | 129.38 | 120.28 |
| 1 | 0 | 1048 | LYS | C-N-CA | 6.79 | 129.38 | 120.28 |
| 8 | N | 1415 | VAL | N-CA-C | -6.79 | 100.18 | 109.55 |
| 8 | N | 1466 | TYR | CA-C-N | 6.79 | 131.98 | 121.19 |
| 8 | N | 1466 | TYR | C-N-CA | 6.79 | 131.98 | 121.19 |
| 9 | Q | 231 | ASN | N-CA-C | -6.79 | 98.85 | 108.96 |
| 1 | Y | 204 | VAL | O-C-N | 6.79 | 129.62 | 123.03 |
| 4 | z | 624 | PRO | N-CA-CB | 6.79 | 110.38 | 103.25 |
| 20 | n | 381 | TYR | N-CA-C | -6.79 | 95.94 | 108.02 |
| 21 | o | 20 | LEU | CA-C-O | -6.79 | 113.36 | 120.55 |
| 20 | g | 393 | THR | N-CA-C | -6.79 | 96.34 | 110.80 |
| 17 | k | 58 | ARG | N-CA-C | -6.79 | 98.78 | 109.50 |
| 18 | l | 70 | ARG | N-CA-C | -6.79 | 98.17 | 108.96 |
| 14 | a | 918 | PHE | CA-C-N | -6.79 | 110.00 | 120.31 |
| 14 | a | 918 | PHE | C-N-CA | -6.79 | 110.00 | 120.31 |
| 6 | F | 299 | ILE | CA-CB-CG1 | 6.78 | 121.93 | 110.40 |
| 4 | J | 664 | SER | N-CA-C | 6.78 | 118.67 | 111.28 |
| 8 | N | 760 | ASN | OD1-CG-ND2 | 6.78 | 129.38 | 122.60 |
| 8 | N | 801 | LYS | N-CA-C | -6.78 | 102.27 | 112.04 |
| 18 | e | 85 | GLU | CB-CG-CD | -6.78 | 101.07 | 112.60 |
| 2 | Z | 503 | SER | CA-C-N | 6.78 | 126.41 | 119.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 503 | SER | C-N-CA | 6.78 | 126.41 | 119.56 |
| 7 | O | 228 | PHE | N-CA-C | -6.78 | 102.92 | 113.02 |
| 8 | P | 1252 | LEU | O-C-N | 6.78 | 129.31 | 122.12 |
| 12 | u | 592 | LEU | CA-C-N | 6.78 | 129.92 | 120.29 |
| 12 | u | 592 | LEU | C-N-CA | 6.78 | 129.92 | 120.29 |
| 2 | 1 | 927 | HIS | CA-CB-CG | 6.78 | 120.58 | 113.80 |
| 8 | N | 144 | ILE | N-CA-C | 6.78 | 117.57 | 110.72 |
| 8 | P | 1065 | THR | N-CA-C | -6.78 | 105.14 | 113.41 |
| 9 | R | 562 | LEU | O-C-N | 6.78 | 129.05 | 122.07 |
| 12 | v | 197 | LEU | N-CA-CB | 6.78 | 121.72 | 110.47 |
| 1 | 0 | 163 | GLU | CB-CA-C | -6.78 | 99.33 | 110.85 |
| 8 | N | 1162 | LEU | N-CA-CB | 6.78 | 121.94 | 110.49 |
| 8 | N | 1460 | LEU | N-CA-C | -6.78 | 105.54 | 113.88 |
| 7 | O | 1614 | SER | N-CA-C | -6.78 | 105.14 | 113.41 |
| 10 | U | 315 | LYS | N-CA-C | -6.78 | 102.92 | 113.02 |
| 2 | 1 | 1280 | ASP | CA-CB-CG | 6.78 | 119.38 | 112.60 |
| 8 | P | 1178 | LYS | CA-C-N | 6.78 | 129.69 | 120.54 |
| 8 | P | 1178 | LYS | C-N-CA | 6.78 | 129.69 | 120.54 |
| 9 | Q | 817 | ALA | N-CA-C | 6.78 | 121.14 | 113.01 |
| 9 | T | 758 | GLN | CA-C-O | 6.78 | 127.76 | 120.24 |
| 20 | n | 805 | ALA | N-CA-C | 6.78 | 119.24 | 111.11 |
| 16 | c | 516 | THR | N-CA-C | -6.78 | 104.58 | 112.92 |
| 7 | M | 103 | LYS | CA-C-O | -6.77 | 113.71 | 120.82 |
| 1 | 0 | 1203 | TYR | N-CA-C | -6.77 | 97.93 | 109.24 |
| 5 | E | 512 | ILE | N-CA-CB | 6.77 | 118.47 | 110.55 |
| 1 | Y | 1167 | SER | N-CA-C | -6.77 | 102.21 | 111.56 |
| 2 | Z | 1182 | ARG | NE-CZ-NH2 | -6.77 | 113.10 | 119.20 |
| 16 | c | 460 | ASN | CA-CB-CG | 6.77 | 119.37 | 112.60 |
| 7 | M | 1248 | LEU | N-CA-C | 6.77 | 118.45 | 111.14 |
| 20 | n | 223 | THR | N-CA-C | -6.77 | 98.80 | 109.50 |
| 5 | K | 510 | VAL | CA-C-N | 6.77 | 129.35 | 120.28 |
| 5 | K | 510 | VAL | C-N-CA | 6.77 | 129.35 | 120.28 |
| 7 | M | 168 | LEU | N-CA-C | -6.77 | 106.22 | 114.75 |
| 2 | Z | 550 | ASN | CA-CB-CG | -6.77 | 105.83 | 112.60 |
| 18 | l | 78 | ASP | CA-CB-CG | 6.77 | 119.37 | 112.60 |
| 19 | f | 552 | ARG | CA-C-N | 6.77 | 130.43 | 120.95 |
| 19 | f | 552 | ARG | C-N-CA | 6.77 | 130.43 | 120.95 |
| 19 | f | 613 | ILE | CA-C-N | 6.77 | 128.30 | 119.84 |
| 19 | f | 613 | ILE | C-N-CA | 6.77 | 128.30 | 119.84 |
| 20 | g | 725 | PHE | CA-CB-CG | -6.77 | 107.03 | 113.80 |
| 14 | a | 162 | VAL | O-C-N | 6.77 | 128.82 | 121.10 |
| 1 | 0 | 631 | GLN | N-CA-C | -6.77 | 103.97 | 111.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 1434 | ILE | CA-CB-CG2 | -6.77 | 99.00 | 110.50 |
| 8 | P | 52 | ILE | CB-CA-C | -6.77 | 105.11 | 111.06 |
| 9 | Q | 596 | ASP | CA-CB-CG | 6.77 | 119.37 | 112.60 |
| 9 | T | 220 | PHE | CA-C-O | 6.77 | 127.92 | 120.82 |
| 12 | u | 633 | GLU | N-CA-C | -6.77 | 103.98 | 111.36 |
| 15 | i | 214 | ARG | NE-CZ-NH2 | -6.77 | 113.11 | 119.20 |
| 4 | J | 686 | ALA | N-CA-CB | 6.77 | 120.07 | 110.12 |
| 7 | O | 734 | LEU | N-CA-C | -6.77 | 96.39 | 110.80 |
| 9 | S | 439 | HIS | ND1-CE1-NE2 | 6.77 | 115.17 | 108.40 |
| 12 | v | 527 | ILE | CA-C-N | 6.77 | 129.24 | 120.44 |
| 12 | v | 527 | ILE | C-N-CA | 6.77 | 129.24 | 120.44 |
| 8 | P | 412 | ILE | CA-C-O | 6.76 | 124.85 | 118.90 |
| 1 | Y | 206 | ASP | N-CA-CB | 6.76 | 121.92 | 110.49 |
| 12 | u | 377 | SER | CA-C-N | 6.76 | 134.46 | 121.54 |
| 12 | u | 377 | SER | C-N-CA | 6.76 | 134.46 | 121.54 |
| 21 | o | 38 | GLU | CA-C-N | 6.76 | 129.34 | 120.28 |
| 21 | o | 38 | GLU | C-N-CA | 6.76 | 129.34 | 120.28 |
| 9 | Q | 754 | ARG | NE-CZ-NH2 | 6.76 | 125.29 | 119.20 |
| 1 | Y | 1488 | VAL | O-C-N | 6.76 | 128.43 | 121.87 |
| 12 | u | 138 | ARG | CA-C-N | 6.76 | 134.46 | 121.54 |
| 12 | u | 138 | ARG | C-N-CA | 6.76 | 134.46 | 121.54 |
| 9 | R | 223 | ASN | CA-C-N | 6.76 | 129.23 | 120.44 |
| 9 | R | 223 | ASN | C-N-CA | 6.76 | 129.23 | 120.44 |
| 17 | k | 254 | PRO | N-CA-CB | 6.76 | 110.35 | 103.25 |
| 20 | n | 342 | GLU | N-CA-C | -6.76 | 105.36 | 112.93 |
| 1 | 0 | 282 | ILE | O-C-N | 6.76 | 130.66 | 122.95 |
| 9 | Q | 588 | VAL | N-CA-C | -6.76 | 106.21 | 112.43 |
| 9 | T | 630 | ARG | N-CA-C | -6.76 | 104.19 | 113.18 |
| 4 | y | 751 | LEU | CA-C-N | 6.76 | 129.23 | 120.44 |
| 4 | y | 751 | LEU | C-N-CA | 6.76 | 129.23 | 120.44 |
| 14 | a | 950 | SER | CA-C-O | -6.76 | 113.74 | 120.70 |
| 2 | 1 | 905 | ARG | N-CA-CB | 6.76 | 120.63 | 110.22 |
| 2 | 1 | 1132 | GLU | CA-C-N | 6.76 | 132.97 | 121.14 |
| 2 | 1 | 1132 | GLU | C-N-CA | 6.76 | 132.97 | 121.14 |
| 10 | U | 250 | ASP | CA-CB-CG | 6.76 | 119.36 | 112.60 |
| 12 | u | 156 | ILE | N-CA-C | -6.76 | 105.94 | 112.29 |
| 4 | z | 810 | ASN | CA-C-N | 6.76 | 129.34 | 120.28 |
| 4 | z | 810 | ASN | C-N-CA | 6.76 | 129.34 | 120.28 |
| 20 | n | 400 | PHE | CA-CB-CG | -6.76 | 107.04 | 113.80 |
| 20 | n | 1037 | LEU | N-CA-CB | 6.76 | 120.16 | 110.16 |
| 15 | b | 698 | LYS | CA-C-N | 6.76 | 129.88 | 120.29 |
| 15 | b | 698 | LYS | C-N-CA | 6.76 | 129.88 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | f | 270 | ALA | CA-C-O | 6.76 | 127.95 | 120.92 |
| 2 | 1 | 914 | GLN | CA-C-N | 6.75 | 134.44 | 121.54 |
| 2 | 1 | 914 | GLN | C-N-CA | 6.75 | 134.44 | 121.54 |
| 14 | h | 600 | ASP | CA-C-N | 6.75 | 134.44 | 121.54 |
| 14 | h | 600 | ASP | C-N-CA | 6.75 | 134.44 | 121.54 |
| 21 | p | 71 | HIS | CE1-NE2-CD2 | -6.75 | 102.25 | 109.00 |
| 15 | b | 432 | ASN | CA-C-N | -6.75 | 114.81 | 123.19 |
| 15 | b | 432 | ASN | C-N-CA | -6.75 | 114.81 | 123.19 |
| 1 | 0 | 613 | GLY | O-C-N | 6.75 | 129.19 | 122.77 |
| 8 | N | 809 | PRO | CA-C-N | 6.75 | 134.44 | 121.54 |
| 8 | N | 809 | PRO | C-N-CA | 6.75 | 134.44 | 121.54 |
| 7 | O | 893 | HIS | CE1-NE2-CD2 | -6.75 | 102.25 | 109.00 |
| 9 | Q | 692 | MET | N-CA-C | -6.75 | 104.79 | 113.16 |
| 2 | Z | 596 | ALA | N-CA-C | -6.75 | 99.26 | 108.38 |
| 2 | Z | 1178 | ARG | N-CA-C | -6.75 | 104.78 | 113.16 |
| 8 | N | 149 | ILE | CA-C-N | 6.75 | 130.00 | 120.28 |
| 8 | N | 149 | ILE | C-N-CA | 6.75 | 130.00 | 120.28 |
| 20 | n | 620 | ASN | CA-CB-CG | -6.75 | 105.85 | 112.60 |
| 16 | c | 422 | PHE | CA-CB-CG | -6.75 | 107.05 | 113.80 |
| 8 | P | 971 | PHE | CA-C-N | 6.75 | 130.34 | 120.82 |
| 8 | P | 971 | PHE | C-N-CA | 6.75 | 130.34 | 120.82 |
| 2 | 1 | 1286 | HIS | CB-CG-CD2 | -6.75 | 122.43 | 131.20 |
| 7 | M | 654 | PHE | CA-C-N | 6.75 | 130.57 | 120.31 |
| 7 | M | 654 | PHE | C-N-CA | 6.75 | 130.57 | 120.31 |
| 7 | O | 8 | PHE | CA-CB-CG | -6.75 | 107.05 | 113.80 |
| 13 | x | 1399 | ILE | CA-C-O | -6.75 | 113.56 | 121.05 |
| 14 | a | 772 | GLN | CA-C-N | 6.75 | 129.32 | 120.28 |
| 14 | a | 772 | GLN | C-N-CA | 6.75 | 129.32 | 120.28 |
| 2 | 1 | 1298 | ASP | CA-CB-CG | 6.75 | 119.35 | 112.60 |
| 8 | P | 766 | GLU | N-CA-C | -6.75 | 104.08 | 112.72 |
| 1 | Y | 902 | SER | N-CA-C | -6.75 | 104.31 | 112.54 |
| 2 | Z | 396 | SER | CA-C-N | 6.75 | 127.71 | 120.83 |
| 2 | Z | 396 | SER | C-N-CA | 6.75 | 127.71 | 120.83 |
| 15 | i | 157 | VAL | CA-CB-CG1 | 6.75 | 121.87 | 110.40 |
| 18 | l | 107 | SER | N-CA-CB | 6.75 | 119.90 | 109.85 |
| 9 | T | 539 | ALA | CA-C-N | 6.75 | 130.56 | 120.31 |
| 9 | T | 539 | ALA | C-N-CA | 6.75 | 130.56 | 120.31 |
| 20 | g | 343 | SER | CA-C-N | 6.75 | 132.20 | 122.35 |
| 20 | g | 343 | SER | C-N-CA | 6.75 | 132.20 | 122.35 |
| 5 | B | 322 | ILE | O-C-N | 6.74 | 128.78 | 121.83 |
| 8 | N | 361 | LYS | CA-C-N | 6.74 | 129.32 | 120.28 |
| 8 | N | 361 | LYS | C-N-CA | 6.74 | 129.32 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | v | 569 | LYS | N-CA-CB | 6.74 | 119.79 | 110.01 |
| 2 | 1 | 824 | SER | CA-C-N | 6.74 | 131.49 | 120.63 |
| 2 | 1 | 824 | SER | C-N-CA | 6.74 | 131.49 | 120.63 |
| 20 | n | 905 | ASN | CA-CB-CG | -6.74 | 105.86 | 112.60 |
| 1 | 0 | 156 | ILE | O-C-N | -6.74 | 113.42 | 121.10 |
| 8 | N | 1235 | LYS | N-CA-C | -6.74 | 103.50 | 113.61 |
| 1 | Y | 160 | ILE | CA-C-N | 6.74 | 129.99 | 120.28 |
| 1 | Y | 160 | ILE | C-N-CA | 6.74 | 129.99 | 120.28 |
| 1 | Y | 1054 | MET | CA-C-N | 6.74 | 129.31 | 120.28 |
| 1 | Y | 1054 | MET | C-N-CA | 6.74 | 129.31 | 120.28 |
| 17 | k | 232 | ILE | N-CA-CB | 6.74 | 119.84 | 111.41 |
| 19 | m | 583 | GLU | CA-C-N | 6.74 | 130.03 | 120.53 |
| 19 | m | 583 | GLU | C-N-CA | 6.74 | 130.03 | 120.53 |
| 19 | f | 169 | LEU | N-CA-C | -6.74 | 96.22 | 108.02 |
| 6 | F | 450 | PHE | N-CA-C | -6.74 | 104.02 | 111.36 |
| 8 | N | 261 | ILE | CA-CB-CG1 | 6.74 | 121.86 | 110.40 |
| 20 | g | 642 | PHE | CA-CB-CG | -6.74 | 107.06 | 113.80 |
| 1 | 0 | 1362 | ASN | N-CA-C | -6.74 | 101.30 | 111.34 |
| 7 | M | 360 | LEU | N-CA-C | -6.74 | 104.40 | 114.64 |
| 9 | R | 833 | ILE | N-CA-C | -6.74 | 104.20 | 110.53 |
| 12 | u | 201 | GLU | CA-C-N | 6.74 | 128.47 | 122.47 |
| 12 | u | 201 | GLU | C-N-CA | 6.74 | 128.47 | 122.47 |
| 14 | h | 910 | GLN | OE1-CD-NE2 | -6.74 | 115.86 | 122.60 |
| 1 | 0 | 1337 | MET | CG-SD-CE | -6.74 | 86.08 | 100.90 |
| 7 | M | 640 | PHE | N-CA-CB | 6.74 | 119.78 | 110.01 |
| 7 | O | 830 | TYR | N-CA-C | 6.74 | 118.62 | 111.28 |
| 12 | u | 129 | LYS | N-CA-CB | 6.74 | 121.87 | 110.49 |
| 4 | z | 800 | HIS | CA-C-N | 6.74 | 129.31 | 120.28 |
| 4 | z | 800 | HIS | C-N-CA | 6.74 | 129.31 | 120.28 |
| 20 | n | 157 | ASP | CA-CB-CG | -6.74 | 105.86 | 112.60 |
| 18 | e | 338 | GLU | N-CA-CB | 6.74 | 121.87 | 110.49 |
| 7 | M | 756 | ILE | CA-C-N | 6.73 | 129.60 | 120.44 |
| 7 | M | 756 | ILE | C-N-CA | 6.73 | 129.60 | 120.44 |
| 2 | Z | 872 | ASN | CA-CB-CG | 6.73 | 119.33 | 112.60 |
| 7 | O | 443 | ILE | N-CA-C | 6.73 | 116.88 | 110.42 |
| 13 | x | 1303 | ILE | N-CA-C | -6.73 | 103.92 | 110.72 |
| 18 | l | 205 | ALA | O-C-N | 6.73 | 129.82 | 122.15 |
| 20 | n | 266 | SER | N-CA-C | -6.73 | 104.38 | 112.59 |
| 9 | Q | 760 | PHE | CA-CB-CG | 6.73 | 120.53 | 113.80 |
| 2 | Z | 192 | HIS | ND1-CE1-NE2 | 6.73 | 115.13 | 108.40 |
| 8 | N | 1445 | THR | CA-C-N | 6.73 | 130.14 | 120.79 |
| 8 | N | 1445 | THR | C-N-CA | 6.73 | 130.14 | 120.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 236 | ALA | CA-C-N | 6.73 | 129.19 | 120.44 |
| 7 | O | 236 | ALA | C-N-CA | 6.73 | 129.19 | 120.44 |
| 8 | P | 1005 | LEU | CA-C-O | -6.73 | 114.23 | 121.56 |
| 8 | P | 1404 | PHE | CA-C-N | 6.73 | 129.60 | 120.38 |
| 8 | P | 1404 | PHE | C-N-CA | 6.73 | 129.60 | 120.38 |
| 15 | i | 387 | THR | N-CA-C | -6.73 | 103.66 | 112.41 |
| 18 | l | 228 | TYR | N-CA-C | -6.73 | 99.63 | 109.18 |
| 16 | c | 772 | LEU | O-C-N | -6.73 | 112.24 | 123.00 |
| 19 | f | 59 | GLU | CA-C-N | 6.73 | 129.84 | 120.29 |
| 19 | f | 59 | GLU | C-N-CA | 6.73 | 129.84 | 120.29 |
| 5 | E | 475 | SER | N-CA-CB | 6.73 | 120.11 | 110.16 |
| 6 | I | 446 | GLU | O-C-N | 6.72 | 129.25 | 122.12 |
| 1 | Y | 1114 | LYS | CA-C-O | -6.72 | 114.25 | 121.45 |
| 1 | Y | 1461 | LYS | N-CA-C | -6.72 | 105.08 | 113.55 |
| 12 | u | 134 | PRO | O-C-N | 6.72 | 130.90 | 122.22 |
| 1 | 0 | 218 | ARG | N-CA-C | -6.72 | 100.80 | 110.08 |
| 2 | 1 | 722 | GLN | CA-C-O | 6.72 | 127.88 | 120.82 |
| 8 | N | 772 | THR | N-CA-C | -6.72 | 103.53 | 113.61 |
| 8 | N | 1098 | ASN | N-CA-CB | 6.72 | 121.85 | 110.49 |
| 8 | N | 1525 | PHE | CA-C-N | 6.72 | 127.44 | 119.98 |
| 8 | N | 1525 | PHE | C-N-CA | 6.72 | 127.44 | 119.98 |
| 1 | Y | 970 | ILE | CA-CB-CG2 | 6.72 | 121.93 | 110.50 |
| 14 | a | 1030 | LEU | N-CA-C | -6.72 | 103.46 | 112.94 |
| 9 | Q | 206 | ASN | CA-CB-CG | 6.72 | 119.32 | 112.60 |
| 1 | 0 | 897 | ILE | CA-C-O | -6.72 | 113.96 | 120.95 |
| 6 | L | 301 | HIS | CE1-NE2-CD2 | -6.72 | 102.28 | 109.00 |
| 7 | M | 185 | PHE | CA-C-O | -6.72 | 113.98 | 120.90 |
| 7 | O | 1071 | ALA | CA-C-N | 6.72 | 126.51 | 119.05 |
| 7 | O | 1071 | ALA | C-N-CA | 6.72 | 126.51 | 119.05 |
| 8 | P | 320 | MET | N-CA-C | -6.72 | 104.66 | 112.92 |
| 9 | R | 669 | ASP | CA-CB-CG | 6.72 | 119.32 | 112.60 |
| 9 | R | 736 | LEU | O-C-N | -6.72 | 115.15 | 122.07 |
| 2 | Z | 116 | TYR | N-CA-C | -6.72 | 103.67 | 114.09 |
| 12 | u | 102 | ASP | CA-C-N | 6.72 | 131.79 | 120.64 |
| 12 | u | 102 | ASP | C-N-CA | 6.72 | 131.79 | 120.64 |
| 14 | h | 757 | GLU | CA-C-N | 6.72 | 129.52 | 120.65 |
| 14 | h | 757 | GLU | C-N-CA | 6.72 | 129.52 | 120.65 |
| 6 | I | 450 | PHE | CA-CB-CG | -6.72 | 107.08 | 113.80 |
| 7 | M | 354 | ARG | NE-CZ-NH2 | -6.72 | 113.15 | 119.20 |
| 20 | n | 332 | LYS | N-CA-CB | 6.72 | 120.69 | 110.28 |
| 19 | f | 328 | LEU | CA-C-O | -6.72 | 113.43 | 120.55 |
| 14 | h | 797 | LEU | N-CA-CB | 6.71 | 121.84 | 110.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 329 | GLY | CA-C-O | -6.71 | 113.15 | 120.40 |
| 12 | u | 134 | PRO | N-CA-C | 6.71 | 122.71 | 113.65 |
| 19 | m | 476 | LEU | CB-CA-C | -6.71 | 96.59 | 109.95 |
| 14 | a | 430 | ASN | OD1-CG-ND2 | -6.71 | 115.89 | 122.60 |
| 4 | D | 690 | GLN | CA-C-O | 6.71 | 127.69 | 120.24 |
| 7 | M | 1489 | ILE | N-CA-CB | 6.71 | 119.67 | 110.54 |
| 8 | N | 1064 | GLU | CA-C-N | 6.71 | 129.27 | 120.28 |
| 8 | N | 1064 | GLU | C-N-CA | 6.71 | 129.27 | 120.28 |
| 7 | O | 976 | ALA | O-C-N | -6.71 | 115.11 | 122.09 |
| 7 | O | 1163 | LEU | CA-C-N | 6.71 | 129.57 | 120.38 |
| 7 | O | 1163 | LEU | C-N-CA | 6.71 | 129.57 | 120.38 |
| 8 | P | 845 | SER | O-C-N | 6.71 | 129.34 | 122.09 |
| 19 | m | 435 | PHE | CA-C-N | 6.71 | 130.37 | 120.90 |
| 19 | m | 435 | PHE | C-N-CA | 6.71 | 130.37 | 120.90 |
| 7 | M | 573 | ASN | CB-CG-ND2 | -6.71 | 106.33 | 116.40 |
| 15 | i | 507 | LEU | CA-C-N | 6.71 | 128.48 | 120.09 |
| 15 | i | 507 | LEU | C-N-CA | 6.71 | 128.48 | 120.09 |
| 17 | d | 41 | GLU | CA-C-O | -6.71 | 111.87 | 119.79 |
| 20 | g | 620 | ASN | CA-CB-CG | 6.71 | 119.31 | 112.60 |
| 5 | K | 318 | GLU | N-CA-CB | 6.71 | 121.83 | 110.49 |
| 9 | S | 475 | SER | CA-C-N | 6.71 | 134.35 | 121.54 |
| 9 | S | 475 | SER | C-N-CA | 6.71 | 134.35 | 121.54 |
| 2 | Z | 592 | SER | O-C-N | -6.71 | 114.94 | 121.85 |
| 21 | s | 9 | PRO | N-CA-C | 6.71 | 121.61 | 111.14 |
| 8 | N | 1080 | GLU | CA-C-N | 6.71 | 131.62 | 120.62 |
| 8 | N | 1080 | GLU | C-N-CA | 6.71 | 131.62 | 120.62 |
| 8 | P | 667 | ASN | CA-CB-CG | -6.71 | 105.89 | 112.60 |
| 11 | X | 293 | HIS | ND1-CE1-NE2 | 6.71 | 115.11 | 108.40 |
| 1 | Y | 608 | ILE | O-C-N | -6.71 | 116.09 | 123.20 |
| 1 | Y | 1257 | GLN | OE1-CD-NE2 | 6.71 | 129.31 | 122.60 |
| 1 | Y | 1348 | ARG | NE-CZ-NH1 | 6.71 | 128.21 | 121.50 |
| 12 | u | 696 | GLU | CB-CA-C | -6.71 | 99.66 | 110.79 |
| 5 | E | 393 | ASP | CA-CB-CG | -6.70 | 105.90 | 112.60 |
| 4 | G | 765 | LEU | N-CA-C | 6.70 | 119.42 | 111.71 |
| 7 | M | 900 | LEU | CA-C-N | 6.70 | 126.74 | 119.90 |
| 7 | M | 900 | LEU | C-N-CA | 6.70 | 126.74 | 119.90 |
| 8 | N | 806 | PHE | CA-C-O | 6.70 | 127.09 | 119.18 |
| 8 | N | 962 | SER | CB-CA-C | -6.70 | 100.95 | 110.34 |
| 2 | Z | 166 | PHE | N-CA-C | 6.70 | 118.98 | 110.33 |
| 13 | w | 1447 | LYS | O-C-N | 6.70 | 128.97 | 122.07 |
| 14 | h | 725 | ARG | O-C-N | 6.70 | 129.89 | 122.11 |
| 7 | O | 1479 | LEU | CA-C-N | 6.70 | 134.65 | 121.58 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1479 | LEU | C-N-CA | 6.70 | 134.65 | 121.58 |
| 17 | k | 263 | SER | CA-C-N | 6.70 | 129.26 | 120.28 |
| 17 | k | 263 | SER | C-N-CA | 6.70 | 129.26 | 120.28 |
| 6 | L | 375 | LYS | CA-C-O | -6.70 | 113.32 | 120.42 |
| 8 | N | 210 | ASN | O-C-N | -6.70 | 114.51 | 122.15 |
| 7 | O | 1434 | SER | CA-C-N | 6.70 | 134.34 | 121.54 |
| 7 | O | 1434 | SER | C-N-CA | 6.70 | 134.34 | 121.54 |
| 9 | R | 812 | GLN | OE1-CD-NE2 | 6.70 | 129.30 | 122.60 |
| 1 | Y | 260 | HIS | CB-CG-CD2 | -6.70 | 122.49 | 131.20 |
| 1 | Y | 454 | ARG | O-C-N | 6.70 | 130.06 | 122.22 |
| 1 | Y | 848 | ILE | CA-C-N | 6.70 | 129.59 | 120.54 |
| 1 | Y | 848 | ILE | C-N-CA | 6.70 | 129.59 | 120.54 |
| 20 | n | 461 | ASP | CA-CB-CG | 6.70 | 119.30 | 112.60 |
| 21 | r | 46 | LYS | CA-C-N | 6.70 | 129.15 | 120.44 |
| 21 | r | 46 | LYS | C-N-CA | 6.70 | 129.15 | 120.44 |
| 18 | e | 120 | HIS | CE1-NE2-CD2 | -6.70 | 102.30 | 109.00 |
| 6 | I | 384 | LEU | CA-C-N | 6.70 | 130.49 | 120.31 |
| 6 | I | 384 | LEU | C-N-CA | 6.70 | 130.49 | 120.31 |
| 7 | O | 1575 | PHE | N-CA-C | -6.70 | 96.53 | 110.80 |
| 9 | R | 301 | ASN | N-CA-C | -6.70 | 104.32 | 113.30 |
| 7 | O | 346 | SER | O-C-N | -6.70 | 114.30 | 122.34 |
| 7 | O | 1241 | LYS | CA-C-N | 6.70 | 131.41 | 120.63 |
| 7 | O | 1241 | LYS | C-N-CA | 6.70 | 131.41 | 120.63 |
| 8 | P | 1480 | GLN | OE1-CD-NE2 | 6.70 | 129.30 | 122.60 |
| 1 | Y | 627 | GLU | CB-CA-C | -6.70 | 100.09 | 110.81 |
| 14 | h | 71 | HIS | CB-CA-C | -6.70 | 100.52 | 110.16 |
| 16 | c | 202 | ARG | CA-C-N | 6.70 | 129.55 | 120.44 |
| 16 | c | 202 | ARG | C-N-CA | 6.70 | 129.55 | 120.44 |
| 2 | 1 | 545 | TYR | N-CA-C | 6.70 | 118.58 | 111.28 |
| 5 | B | 407 | GLU | CB-CG-CD | -6.70 | 101.22 | 112.60 |
| 6 | I | 456 | ARG | NE-CZ-NH2 | 6.70 | 125.23 | 119.20 |
| 8 | N | 103 | MET | N-CA-C | 6.70 | 120.32 | 111.75 |
| 7 | O | 1279 | CYS | CA-C-N | 6.70 | 129.00 | 120.56 |
| 7 | O | 1279 | CYS | C-N-CA | 6.70 | 129.00 | 120.56 |
| 8 | P | 1193 | ASN | N-CA-C | 6.70 | 118.58 | 111.28 |
| 9 | R | 499 | SER | CA-C-N | 6.70 | 130.49 | 120.31 |
| 9 | R | 499 | SER | C-N-CA | 6.70 | 130.49 | 120.31 |
| 10 | U | 358 | LYS | CA-C-N | 6.70 | 131.29 | 121.31 |
| 10 | U | 358 | LYS | C-N-CA | 6.70 | 131.29 | 121.31 |
| 15 | i | 661 | HIS | CA-CB-CG | -6.70 | 107.10 | 113.80 |
| 20 | g | 635 | VAL | N-CA-C | -6.70 | 103.70 | 111.00 |
| 1 | 0 | 223 | THR | CA-C-O | -6.69 | 114.06 | 121.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 860 | ILE | N-CA-C | -6.69 | 106.47 | 112.90 |
| 8 | N | 163 | ASP | O-C-N | -6.69 | 114.09 | 122.19 |
| 7 | O | 352 | ILE | N-CA-C | -6.69 | 94.43 | 108.88 |
| 9 | T | 231 | ASN | N-CA-C | -6.69 | 99.28 | 109.85 |
| 1 | Y | 1158 | HIS | ND1-CE1-NE2 | 6.69 | 115.09 | 108.40 |
| 12 | u | 418 | ALA | N-CA-CB | 6.69 | 121.80 | 110.49 |
| 14 | h | 573 | GLU | N-CA-CB | 6.69 | 120.17 | 110.20 |
| 21 | s | 31 | ALA | N-CA-C | 6.69 | 118.57 | 111.28 |
| 4 | J | 684 | VAL | O-C-N | -6.69 | 115.38 | 121.87 |
| 13 | w | 1276 | ILE | CA-C-N | 6.69 | 130.48 | 120.31 |
| 13 | w | 1276 | ILE | C-N-CA | 6.69 | 130.48 | 120.31 |
| 15 | i | 542 | LEU | N-CA-C | -6.69 | 96.55 | 110.80 |
| 20 | n | 794 | LYS | N-CA-C | -6.69 | 104.33 | 113.30 |
| 20 | n | 1046 | VAL | CA-C-N | 6.69 | 129.79 | 120.29 |
| 20 | n | 1046 | VAL | C-N-CA | 6.69 | 129.79 | 120.29 |
| 21 | p | 36 | GLN | N-CA-C | -6.69 | 104.33 | 113.30 |
| 2 | 1 | 1011 | ILE | O-C-N | -6.69 | 114.88 | 122.04 |
| 8 | N | 932 | LEU | CA-C-O | 6.69 | 126.41 | 119.05 |
| 8 | P | 346 | ILE | CA-C-N | 6.69 | 129.24 | 120.28 |
| 8 | P | 346 | ILE | C-N-CA | 6.69 | 129.24 | 120.28 |
| 8 | P | 1351 | ILE | CA-C-O | 6.69 | 124.79 | 118.90 |
| 2 | Z | 946 | GLU | N-CA-C | -6.69 | 104.26 | 114.16 |
| 15 | b | 98 | LEU | N-CA-C | -6.69 | 96.55 | 110.80 |
| 4 | A | 665 | TRP | CA-CB-CG | 6.69 | 126.31 | 113.60 |
| 7 | M | 1466 | LEU | N-CA-C | 6.69 | 118.65 | 111.36 |
| 8 | N | 411 | PHE | N-CA-C | -6.69 | 103.05 | 113.02 |
| 7 | O | 334 | GLN | N-CA-C | -6.69 | 103.72 | 114.09 |
| 4 | z | 639 | ASP | CA-C-N | 6.69 | 129.13 | 120.44 |
| 4 | z | 639 | ASP | C-N-CA | 6.69 | 129.13 | 120.44 |
| 19 | f | 211 | ILE | N-CA-C | -6.69 | 103.00 | 110.62 |
| 20 | g | 1101 | ARG | NE-CZ-NH2 | -6.69 | 113.18 | 119.20 |
| 2 | 1 | 1066 | ASN | OD1-CG-ND2 | -6.69 | 115.91 | 122.60 |
| 7 | M | 833 | THR | CA-C-O | -6.68 | 113.34 | 121.36 |
| 8 | N | 1201 | ILE | CA-C-O | -6.68 | 114.08 | 121.17 |
| 20 | g | 599 | LYS | CA-C-N | 6.68 | 129.13 | 120.44 |
| 20 | g | 599 | LYS | C-N-CA | 6.68 | 129.13 | 120.44 |
| 20 | g | 1075 | ASP | CA-CB-CG | 6.68 | 119.28 | 112.60 |
| 1 | 0 | 1030 | ASN | OD1-CG-ND2 | -6.68 | 115.92 | 122.60 |
| 9 | Q | 326 | THR | CA-C-N | 6.68 | 131.48 | 123.19 |
| 9 | Q | 326 | THR | C-N-CA | 6.68 | 131.48 | 123.19 |
| 9 | S | 60 | ASN | N-CA-CB | 6.68 | 121.78 | 110.49 |
| 12 | v | 223 | LEU | N-CA-CB | 6.68 | 119.90 | 109.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 18 | l | 2 | GLN | CB-CA-C | -6.68 | 99.94 | 109.96 |
| 21 | r | 51 | VAL | CA-CB-CG1 | 6.68 | 121.76 | 110.40 |
| 18 | l | 324 | ASP | N-CA-C | -6.68 | 104.75 | 113.17 |
| 7 | M | 492 | ARG | CA-C-N | 6.68 | 126.13 | 118.85 |
| 7 | M | 492 | ARG | C-N-CA | 6.68 | 126.13 | 118.85 |
| 8 | N | 1049 | ASP | N-CA-CB | 6.68 | 121.78 | 110.49 |
| 9 | Q | 433 | GLU | CA-C-O | 6.68 | 126.49 | 119.14 |
| 9 | R | 727 | TYR | N-CA-C | -6.68 | 103.47 | 111.69 |
| 11 | X | 294 | ILE | N-CA-C | -6.68 | 98.11 | 107.80 |
| 12 | v | 130 | VAL | CA-C-O | 6.68 | 127.02 | 120.27 |
| 20 | n | 1017 | ILE | N-CA-CB | 6.68 | 120.56 | 111.21 |
| 1 | 0 | 831 | LYS | N-CA-CB | 6.68 | 121.85 | 110.50 |
| 7 | O | 961 | LYS | CA-C-N | 6.68 | 133.50 | 122.62 |
| 7 | O | 961 | LYS | C-N-CA | 6.68 | 133.50 | 122.62 |
| 9 | R | 612 | HIS | ND1-CE1-NE2 | 6.68 | 115.08 | 108.40 |
| 12 | v | 166 | LEU | CA-C-O | 6.68 | 127.83 | 119.95 |
| 6 | I | 333 | ILE | N-CA-C | 6.68 | 119.44 | 111.09 |
| 7 | M | 649 | LEU | CA-C-N | 6.68 | 131.02 | 120.47 |
| 7 | M | 649 | LEU | C-N-CA | 6.68 | 131.02 | 120.47 |
| 7 | O | 900 | LEU | CA-C-O | -6.68 | 114.38 | 119.32 |
| 8 | P | 883 | LYS | CA-C-N | 6.68 | 129.77 | 120.29 |
| 8 | P | 883 | LYS | C-N-CA | 6.68 | 129.77 | 120.29 |
| 11 | V | 282 | ASN | CA-CB-CG | -6.68 | 105.92 | 112.60 |
| 10 | W | 346 | SER | CA-C-O | -6.68 | 114.38 | 119.59 |
| 5 | B | 469 | ARG | NE-CZ-NH1 | 6.67 | 128.17 | 121.50 |
| 5 | E | 375 | ILE | N-CA-C | 6.67 | 116.83 | 110.42 |
| 1 | Y | 1427 | TYR | CB-CG-CD1 | 6.67 | 130.81 | 120.80 |
| 2 | Z | 537 | LYS | CA-C-N | -6.67 | 113.79 | 123.00 |
| 2 | Z | 537 | LYS | C-N-CA | -6.67 | 113.79 | 123.00 |
| 2 | Z | 986 | ARG | NE-CZ-NH1 | -6.67 | 114.83 | 121.50 |
| 2 | 1 | 1247 | ASN | OD1-CG-ND2 | -6.67 | 115.93 | 122.60 |
| 7 | O | 1474 | PHE | CA-C-N | 6.67 | 131.23 | 120.55 |
| 7 | O | 1474 | PHE | C-N-CA | 6.67 | 131.23 | 120.55 |
| 14 | h | 547 | VAL | CA-C-N | 6.67 | 129.76 | 120.29 |
| 14 | h | 547 | VAL | C-N-CA | 6.67 | 129.76 | 120.29 |
| 16 | j | 589 | ASN | OD1-CG-ND2 | 6.67 | 129.27 | 122.60 |
| 1 | 0 | 1004 | PHE | N-CA-C | -6.67 | 104.16 | 112.90 |
| 4 | G | 702 | ARG | CA-C-O | 6.67 | 126.24 | 118.90 |
| 5 | K | 511 | GLU | CA-C-N | 6.67 | 129.60 | 120.46 |
| 5 | K | 511 | GLU | C-N-CA | 6.67 | 129.60 | 120.46 |
| 8 | N | 324 | SER | N-CA-CB | 6.67 | 119.91 | 110.24 |
| 12 | v | 275 | GLU | N-CA-C | -6.67 | 103.93 | 111.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | n | 556 | HIS | CE1-NE2-CD2 | -6.67 | 102.33 | 109.00 |
| 8 | P | 323 | TYR | N-CA-C | -6.67 | 103.59 | 113.40 |
| 21 | s | 19 | LYS | N-CA-C | 6.67 | 118.21 | 111.07 |
| 4 | A | 673 | GLY | CA-C-N | 6.67 | 129.11 | 120.44 |
| 4 | A | 673 | GLY | C-N-CA | 6.67 | 129.11 | 120.44 |
| 5 | E | 359 | ASN | CA-CB-CG | 6.67 | 119.27 | 112.60 |
| 5 | K | 355 | PHE | N-CA-C | -6.67 | 104.72 | 112.92 |
| 8 | P | 507 | PRO | N-CA-C | 6.67 | 118.84 | 110.70 |
| 1 | 0 | 580 | VAL | CA-C-N | 6.67 | 127.66 | 120.13 |
| 1 | 0 | 580 | VAL | C-N-CA | 6.67 | 127.66 | 120.13 |
| 2 | 1 | 659 | SER | N-CA-C | -6.67 | 105.02 | 113.02 |
| 5 | H | 313 | TYR | O-C-N | 6.67 | 131.15 | 122.68 |
| 7 | M | 288 | TRP | CB-CG-CD1 | -6.67 | 116.90 | 126.90 |
| 7 | M | 493 | PRO | CA-C-N | 6.67 | 131.26 | 120.60 |
| 7 | M | 493 | PRO | C-N-CA | 6.67 | 131.26 | 120.60 |
| 8 | N | 780 | HIS | CB-CG-CD2 | -6.67 | 122.54 | 131.20 |
| 9 | Q | 257 | TRP | CA-C-N | 6.67 | 130.44 | 120.31 |
| 9 | Q | 257 | TRP | C-N-CA | 6.67 | 130.44 | 120.31 |
| 9 | S | 485 | SER | N-CA-CB | 6.67 | 120.61 | 110.28 |
| 4 | A | 803 | ALA | CA-C-N | 6.66 | 129.21 | 120.28 |
| 4 | A | 803 | ALA | C-N-CA | 6.66 | 129.21 | 120.28 |
| 7 | M | 1568 | VAL | N-CA-C | -6.66 | 106.74 | 113.47 |
| 8 | P | 426 | SER | N-CA-CB | 6.66 | 121.75 | 110.49 |
| 9 | Q | 371 | PHE | N-CA-C | -6.66 | 104.97 | 113.23 |
| 7 | M | 1352 | GLU | CA-C-N | 6.66 | 129.10 | 120.44 |
| 7 | M | 1352 | GLU | C-N-CA | 6.66 | 129.10 | 120.44 |
| 20 | g | 390 | ILE | N-CA-CB | 6.66 | 118.50 | 110.31 |
| 1 | 0 | 951 | ASP | N-CA-C | -6.66 | 105.72 | 114.31 |
| 2 | 1 | 125 | PHE | N-CA-CB | 6.66 | 121.58 | 110.92 |
| 7 | M | 285 | PHE | CA-CB-CG | -6.66 | 107.14 | 113.80 |
| 8 | P | 1447 | ILE | CA-C-N | 6.66 | 129.10 | 120.44 |
| 8 | P | 1447 | ILE | C-N-CA | 6.66 | 129.10 | 120.44 |
| 20 | n | 981 | ARG | CA-C-N | 6.66 | 131.56 | 120.70 |
| 20 | n | 981 | ARG | C-N-CA | 6.66 | 131.56 | 120.70 |
| 15 | b | 695 | ILE | O-C-N | -6.66 | 115.06 | 122.05 |
| 14 | a | 343 | ASN | N-CA-CB | 6.66 | 122.04 | 110.65 |
| 2 | 1 | 850 | HIS | ND1-CE1-NE2 | 6.66 | 115.06 | 108.40 |
| 7 | O | 1075 | LEU | CA-C-N | 6.66 | 129.50 | 120.38 |
| 7 | O | 1075 | LEU | C-N-CA | 6.66 | 129.50 | 120.38 |
| 1 | Y | 122 | ASP | CA-C-O | 6.66 | 130.03 | 120.51 |
| 19 | f | 351 | ILE | N-CA-C | 6.66 | 117.41 | 110.62 |
| 12 | v | 329 | LYS | N-CA-C | -6.66 | 98.39 | 109.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 17 | d | 94 | VAL | O-C-N | -6.66 | 115.98 | 123.10 |
| 8 | N | 281 | GLN | OE1-CD-NE2 | 6.66 | 129.26 | 122.60 |
| 7 | O | 715 | ASN | O-C-N | -6.66 | 114.56 | 122.15 |
| 9 | R | 536 | ASN | CA-CB-CG | -6.66 | 105.94 | 112.60 |
| 11 | X | 394 | GLN | N-CA-C | 6.66 | 119.54 | 111.82 |
| 12 | v | 225 | LEU | N-CA-CB | 6.66 | 119.72 | 110.07 |
| 13 | w | 1305 | GLN | N-CA-C | 6.66 | 118.53 | 111.28 |
| 5 | B | 335 | TRP | CB-CA-C | 6.65 | 122.16 | 110.85 |
| 13 | x | 1448 | GLN | N-CA-C | 6.65 | 120.66 | 112.54 |
| 20 | n | 658 | PHE | O-C-N | -6.65 | 113.67 | 121.32 |
| 7 | M | 134 | LEU | CA-C-O | 6.65 | 127.32 | 119.67 |
| 7 | M | 1282 | ALA | CA-C-N | 6.65 | 129.09 | 120.44 |
| 7 | M | 1282 | ALA | C-N-CA | 6.65 | 129.09 | 120.44 |
| 2 | Z | 1057 | TYR | CA-C-O | -6.65 | 113.85 | 120.70 |
| 12 | v | 242 | ASP | CA-C-N | 6.65 | 133.94 | 121.97 |
| 12 | v | 242 | ASP | C-N-CA | 6.65 | 133.94 | 121.97 |
| 16 | c | 373 | LYS | N-CA-C | -6.65 | 105.07 | 113.72 |
| 4 | J | 797 | LEU | CA-C-N | 6.65 | 129.09 | 120.44 |
| 4 | J | 797 | LEU | C-N-CA | 6.65 | 129.09 | 120.44 |
| 7 | M | 84 | ASP | CA-CB-CG | 6.65 | 119.25 | 112.60 |
| 12 | v | 437 | LEU | N-CA-C | -6.65 | 98.06 | 108.90 |
| 17 | d | 74 | SER | N-CA-C | -6.65 | 99.40 | 108.38 |
| 4 | A | 805 | ARG | O-C-N | 6.65 | 129.27 | 122.09 |
| 7 | M | 759 | ASP | CA-C-N | 6.65 | 130.84 | 121.66 |
| 7 | M | 759 | ASP | C-N-CA | 6.65 | 130.84 | 121.66 |
| 17 | k | 64 | PRO | O-C-N | 6.65 | 131.07 | 123.03 |
| 19 | m | 399 | ILE | N-CA-C | -6.65 | 104.69 | 110.74 |
| 5 | K | 345 | PRO | N-CA-C | 6.65 | 120.84 | 111.33 |
| 7 | M | 305 | ASP | CA-CB-CG | -6.65 | 105.95 | 112.60 |
| 7 | M | 1592 | ALA | CA-C-N | 6.65 | 129.49 | 120.38 |
| 7 | M | 1592 | ALA | C-N-CA | 6.65 | 129.49 | 120.38 |
| 8 | P | 1534 | TYR | CA-C-O | -6.65 | 113.37 | 120.42 |
| 14 | h | 401 | THR | N-CA-C | 6.65 | 120.01 | 110.24 |
| 17 | d | 203 | HIS | CB-CG-CD2 | -6.65 | 122.56 | 131.20 |
| 2 | 1 | 1080 | VAL | N-CA-CB | 6.65 | 117.60 | 110.62 |
| 7 | M | 736 | PHE | CA-CB-CG | 6.65 | 120.45 | 113.80 |
| 8 | P | 591 | MET | CA-C-N | 6.65 | 131.20 | 120.30 |
| 8 | P | 591 | MET | C-N-CA | 6.65 | 131.20 | 120.30 |
| 8 | P | 801 | LYS | CA-C-N | 6.65 | 129.19 | 120.28 |
| 8 | P | 801 | LYS | C-N-CA | 6.65 | 129.19 | 120.28 |
| 6 | F | 373 | PHE | CA-CB-CG | -6.64 | 107.16 | 113.80 |
| 8 | N | 751 | GLU | CA-C-N | 6.64 | 129.18 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 751 | GLU | C-N-CA | 6.64 | 129.18 | 120.28 |
| 8 | N | 962 | SER | N-CA-CB | 6.64 | 121.28 | 110.32 |
| 9 | S | 136 | PHE | CA-C-N | 6.64 | 129.51 | 120.54 |
| 9 | S | 136 | PHE | C-N-CA | 6.64 | 129.51 | 120.54 |
| 2 | Z | 1200 | LEU | CA-C-O | -6.64 | 112.91 | 119.69 |
| 20 | n | 931 | SER | CA-C-N | 6.64 | 129.72 | 120.29 |
| 20 | n | 931 | SER | C-N-CA | 6.64 | 129.72 | 120.29 |
| 5 | K | 474 | SER | CA-C-N | 6.64 | 129.85 | 120.28 |
| 5 | K | 474 | SER | C-N-CA | 6.64 | 129.85 | 120.28 |
| 7 | M | 929 | TYR | CA-C-N | 6.64 | 131.53 | 120.64 |
| 7 | M | 929 | TYR | C-N-CA | 6.64 | 131.53 | 120.64 |
| 7 | O | 642 | PHE | N-CA-C | 6.64 | 118.52 | 111.28 |
| 8 | P | 1517 | GLU | CA-C-N | 6.64 | 129.72 | 120.29 |
| 8 | P | 1517 | GLU | C-N-CA | 6.64 | 129.72 | 120.29 |
| 9 | T | 607 | ARG | NH1-CZ-NH2 | -6.64 | 110.67 | 119.30 |
| 19 | m | 391 | HIS | ND1-CE1-NE2 | 6.64 | 115.04 | 108.40 |
| 20 | n | 474 | VAL | N-CA-CB | 6.64 | 117.96 | 110.72 |
| 7 | M | 912 | PHE | CA-CB-CG | 6.64 | 120.44 | 113.80 |
| 7 | O | 1237 | TYR | CA-C-O | 6.64 | 128.82 | 120.65 |
| 21 | r | 55 | ASN | CB-CA-C | -6.64 | 97.20 | 110.42 |
| 7 | M | 887 | PHE | CA-CB-CG | 6.64 | 120.44 | 113.80 |
| 9 | R | 607 | ARG | N-CA-C | -6.64 | 104.93 | 113.16 |
| 1 | Y | 185 | THR | N-CA-C | -6.64 | 99.10 | 109.72 |
| 12 | v | 164 | ILE | CA-CB-CG1 | 6.64 | 121.69 | 110.40 |
| 12 | v | 219 | ASN | CA-CB-CG | 6.64 | 119.24 | 112.60 |
| 19 | m | 373 | THR | CA-CB-OG1 | -6.64 | 99.64 | 109.60 |
| 17 | d | 170 | SER | CA-C-N | 6.64 | 130.78 | 120.75 |
| 17 | d | 170 | SER | C-N-CA | 6.64 | 130.78 | 120.75 |
| 7 | M | 159 | LYS | N-CA-CB | 6.64 | 119.64 | 110.01 |
| 9 | Q | 288 | ASN | OD1-CG-ND2 | 6.64 | 129.24 | 122.60 |
| 1 | Y | 1202 | VAL | N-CA-C | -6.64 | 106.32 | 112.43 |
| 14 | h | 798 | LYS | O-C-N | 6.64 | 131.42 | 122.59 |
| 20 | g | 128 | ASP | CA-CB-CG | -6.64 | 105.96 | 112.60 |
| 1 | 0 | 209 | HIS | CA-CB-CG | 6.64 | 120.44 | 113.80 |
| 5 | E | 339 | MET | CB-CA-C | -6.64 | 99.57 | 110.85 |
| 8 | P | 85 | ASN | CA-CB-CG | 6.64 | 119.24 | 112.60 |
| 16 | c | 768 | ASN | N-CA-C | -6.64 | 100.55 | 110.24 |
| 20 | g | 273 | GLY | CA-C-N | 6.64 | 128.14 | 119.84 |
| 20 | g | 273 | GLY | C-N-CA | 6.64 | 128.14 | 119.84 |
| 6 | L | 386 | ASP | CA-CB-CG | 6.63 | 119.23 | 112.60 |
| 8 | P | 1469 | LEU | O-C-N | 6.63 | 129.26 | 122.09 |
| 1 | Y | 272 | ASP | CA-CB-CG | 6.63 | 119.23 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | u | 441 | SER | N-CA-C | -6.63 | 99.51 | 108.86 |
| 4 | z | 818 | ILE | CB-CA-C | -6.63 | 103.19 | 112.14 |
| 15 | i | 109 | SER | CA-C-N | 6.63 | 127.34 | 119.98 |
| 15 | i | 109 | SER | C-N-CA | 6.63 | 127.34 | 119.98 |
| 4 | A | 744 | ALA | N-CA-CB | 6.63 | 121.70 | 110.49 |
| 7 | M | 29 | LEU | O-C-N | -6.63 | 114.47 | 120.71 |
| 20 | g | 1152 | THR | N-CA-C | -6.63 | 107.06 | 114.62 |
| 8 | P | 815 | LEU | N-CA-C | -6.63 | 103.79 | 112.41 |
| 9 | T | 502 | ASP | CA-C-N | 6.63 | 129.17 | 120.28 |
| 9 | T | 502 | ASP | C-N-CA | 6.63 | 129.17 | 120.28 |
| 1 | Y | 626 | ASN | OD1-CG-ND2 | 6.63 | 129.23 | 122.60 |
| 2 | Z | 1189 | LYS | CA-C-N | 6.63 | 129.17 | 120.28 |
| 2 | Z | 1189 | LYS | C-N-CA | 6.63 | 129.17 | 120.28 |
| 12 | v | 259 | LEU | N-CA-CB | 6.63 | 119.63 | 110.01 |
| 15 | i | 412 | LEU | N-CA-C | -6.63 | 100.58 | 110.06 |
| 20 | g | 761 | ASN | N-CA-CB | 6.63 | 121.70 | 110.49 |
| 7 | M | 1240 | HIS | CB-CG-ND1 | 6.63 | 132.65 | 122.70 |
| 7 | O | 479 | GLU | CA-C-N | 6.63 | 129.16 | 120.28 |
| 7 | O | 479 | GLU | C-N-CA | 6.63 | 129.16 | 120.28 |
| 4 | A | 695 | GLN | CA-C-N | 6.63 | 129.70 | 120.29 |
| 4 | A | 695 | GLN | C-N-CA | 6.63 | 129.70 | 120.29 |
| 8 | N | 400 | PHE | CA-CB-CG | 6.63 | 120.43 | 113.80 |
| 8 | N | 977 | ALA | N-CA-CB | 6.63 | 121.69 | 110.49 |
| 7 | O | 1308 | GLN | N-CA-C | 6.63 | 118.50 | 111.28 |
| 1 | Y | 148 | PHE | O-C-N | -6.63 | 116.30 | 123.26 |
| 4 | y | 640 | LEU | N-CA-C | 6.63 | 118.50 | 111.28 |
| 19 | m | 323 | THR | CA-C-N | 6.63 | 131.64 | 120.64 |
| 19 | m | 323 | THR | C-N-CA | 6.63 | 131.64 | 120.64 |
| 19 | f | 289 | HIS | CB-CG-CD2 | -6.63 | 122.58 | 131.20 |
| 1 | 0 | 611 | LEU | N-CA-C | 6.63 | 118.50 | 111.28 |
| 1 | Y | 1066 | PHE | CA-CB-CG | -6.63 | 107.17 | 113.80 |
| 12 | v | 689 | ILE | CB-CA-C | -6.63 | 103.19 | 112.14 |
| 15 | b | 136 | PHE | N-CA-C | 6.63 | 118.50 | 111.28 |
| 8 | P | 895 | HIS | ND1-CE1-NE2 | 6.62 | 115.03 | 108.40 |
| 12 | v | 217 | LEU | N-CA-CB | 6.62 | 120.92 | 111.65 |
| 14 | h | 138 | LEU | N-CA-C | -6.62 | 104.78 | 114.39 |
| 5 | K | 530 | ASP | CA-C-O | 6.62 | 127.52 | 120.70 |
| 7 | M | 108 | LEU | CA-C-N | 6.62 | 129.16 | 120.28 |
| 7 | M | 108 | LEU | C-N-CA | 6.62 | 129.16 | 120.28 |
| 7 | O | 980 | ASP | CA-CB-CG | -6.62 | 105.98 | 112.60 |
| 1 | Y | 374 | LYS | N-CA-C | -6.62 | 104.43 | 113.30 |
| 20 | n | 376 | THR | N-CA-C | -6.62 | 99.42 | 109.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | q | 86 | PHE | N-CA-C | -6.62 | 96.97 | 108.69 |
| 2 | 1 | 930 | THR | CA-C-N | 6.62 | 134.19 | 121.54 |
| 2 | 1 | 930 | THR | C-N-CA | 6.62 | 134.19 | 121.54 |
| 5 | H | 405 | ASN | OD1-CG-ND2 | -6.62 | 115.98 | 122.60 |
| 9 | Q | 405 | ASP | CA-C-N | 6.62 | 126.21 | 119.19 |
| 9 | Q | 405 | ASP | C-N-CA | 6.62 | 126.21 | 119.19 |
| 1 | Y | 201 | TYR | N-CA-C | -6.62 | 98.59 | 108.99 |
| 4 | z | 692 | LYS | CA-C-N | 6.62 | 129.82 | 120.42 |
| 4 | z | 692 | LYS | C-N-CA | 6.62 | 129.82 | 120.42 |
| 4 | z | 796 | ILE | N-CA-C | 6.62 | 117.37 | 110.62 |
| 20 | n | 998 | ASN | OD1-CG-ND2 | 6.62 | 129.22 | 122.60 |
| 2 | 1 | 286 | LEU | N-CA-C | -6.62 | 99.88 | 110.14 |
| 8 | P | 771 | LEU | N-CA-C | -6.62 | 104.06 | 111.28 |
| 9 | T | 642 | LEU | CA-C-N | 6.62 | 129.45 | 120.38 |
| 9 | T | 642 | LEU | C-N-CA | 6.62 | 129.45 | 120.38 |
| 14 | h | 15 | TYR | CA-CB-CG | 6.62 | 125.81 | 113.90 |
| 2 | 1 | 964 | VAL | CA-C-N | 6.62 | 128.63 | 120.22 |
| 2 | 1 | 964 | VAL | C-N-CA | 6.62 | 128.63 | 120.22 |
| 7 | O | 607 | ILE | CA-C-N | 6.62 | 129.04 | 120.44 |
| 7 | O | 607 | ILE | C-N-CA | 6.62 | 129.04 | 120.44 |
| 8 | P | 69 | ASN | CA-CB-CG | 6.62 | 119.22 | 112.60 |
| 1 | Y | 257 | PHE | CA-CB-CG | -6.62 | 107.18 | 113.80 |
| 14 | h | 338 | ARG | N-CA-CB | 6.62 | 120.02 | 110.03 |
| 7 | M | 1518 | PHE | CA-CB-CG | -6.62 | 107.18 | 113.80 |
| 9 | Q | 457 | TYR | CA-CB-CG | -6.62 | 101.99 | 113.90 |
| 1 | Y | 468 | PRO | N-CA-CB | 6.62 | 109.50 | 103.08 |
| 6 | C | 404 | ASP | N-CA-C | -6.62 | 104.69 | 112.89 |
| 8 | N | 866 | ARG | N-CA-CB | 6.62 | 121.67 | 110.49 |
| 8 | N | 1500 | LEU | CA-C-N | 6.62 | 130.37 | 120.31 |
| 8 | N | 1500 | LEU | C-N-CA | 6.62 | 130.37 | 120.31 |
| 7 | O | 1587 | LEU | CA-C-N | 6.62 | 128.89 | 120.56 |
| 7 | O | 1587 | LEU | C-N-CA | 6.62 | 128.89 | 120.56 |
| 13 | x | 1222 | GLU | CB-CA-C | -6.62 | 99.81 | 110.79 |
| 14 | a | 900 | VAL | CA-C-O | 6.62 | 126.30 | 119.35 |
| 2 | 1 | 1179 | ASN | CA-CB-CG | 6.61 | 119.21 | 112.60 |
| 7 | O | 1184 | LEU | N-CA-C | -6.61 | 104.52 | 112.59 |
| 12 | u | 212 | LEU | CA-C-N | 6.61 | 127.00 | 119.92 |
| 12 | u | 212 | LEU | C-N-CA | 6.61 | 127.00 | 119.92 |
| 2 | 1 | 1213 | LEU | CA-C-O | -6.61 | 111.87 | 119.14 |
| 7 | O | 1311 | GLN | N-CA-C | -6.61 | 102.52 | 112.04 |
| 8 | P | 1603 | SER | CA-C-N | 6.61 | 129.04 | 120.44 |
| 8 | P | 1603 | SER | C-N-CA | 6.61 | 129.04 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 17 | k | 146 | ILE | N-CA-C | -6.61 | 104.57 | 111.58 |
| 14 | a | 441 | GLU | CA-C-N | 6.61 | 129.43 | 120.44 |
| 14 | a | 441 | GLU | C-N-CA | 6.61 | 129.43 | 120.44 |
| 5 | E | 467 | LYS | N-CA-CB | 6.61 | 119.59 | 110.01 |
| 7 | O | 754 | ASP | CA-C-N | 6.61 | 129.03 | 120.44 |
| 7 | O | 754 | ASP | C-N-CA | 6.61 | 129.03 | 120.44 |
| 2 | Z | 840 | THR | CA-CB-OG1 | 6.61 | 119.52 | 109.60 |
| 20 | g | 717 | CYS | CA-C-N | 6.61 | 131.79 | 121.35 |
| 20 | g | 717 | CYS | C-N-CA | 6.61 | 131.79 | 121.35 |
| 8 | P | 299 | ASN | CA-CB-CG | 6.61 | 119.21 | 112.60 |
| 9 | T | 20 | LYS | CA-C-N | 6.61 | 130.35 | 120.31 |
| 9 | T | 20 | LYS | C-N-CA | 6.61 | 130.35 | 120.31 |
| 11 | V | 300 | VAL | CA-C-N | 6.61 | 132.04 | 122.85 |
| 11 | V | 300 | VAL | C-N-CA | 6.61 | 132.04 | 122.85 |
| 14 | h | 894 | GLU | CA-C-N | 6.61 | 129.03 | 120.44 |
| 14 | h | 894 | GLU | C-N-CA | 6.61 | 129.03 | 120.44 |
| 5 | B | 378 | HIS | CB-CG-ND1 | 6.61 | 132.61 | 122.70 |
| 4 | D | 802 | ASP | CA-C-O | 6.61 | 126.68 | 119.15 |
| 7 | M | 861 | GLN | CA-C-N | 6.61 | 129.13 | 120.28 |
| 7 | M | 861 | GLN | C-N-CA | 6.61 | 129.13 | 120.28 |
| 13 | x | 1227 | VAL | N-CA-CB | 6.61 | 118.28 | 110.55 |
| 19 | m | 617 | ILE | CA-C-N | 6.61 | 129.03 | 120.44 |
| 19 | m | 617 | ILE | C-N-CA | 6.61 | 129.03 | 120.44 |
| 4 | D | 818 | ILE | N-CA-C | -6.61 | 105.10 | 113.22 |
| 6 | L | 350 | PHE | CB-CG-CD2 | -6.61 | 109.47 | 120.70 |
| 8 | N | 454 | ASN | N-CA-C | 6.61 | 120.94 | 113.01 |
| 8 | P | 718 | PHE | CB-CG-CD2 | -6.61 | 109.47 | 120.70 |
| 9 | R | 343 | ALA | N-CA-C | -6.61 | 98.95 | 108.07 |
| 9 | T | 159 | PHE | CA-C-O | -6.61 | 113.55 | 120.55 |
| 9 | T | 551 | ARG | N-CA-C | 6.61 | 118.14 | 111.07 |
| 2 | Z | 401 | ASN | N-CA-C | -6.61 | 103.85 | 114.09 |
| 9 | T | 222 | PHE | N-CA-C | 6.60 | 118.48 | 111.28 |
| 12 | v | 243 | VAL | CA-C-N | 6.60 | 129.84 | 120.53 |
| 12 | v | 243 | VAL | C-N-CA | 6.60 | 129.84 | 120.53 |
| 1 | 0 | 681 | THR | N-CA-CB | 6.60 | 119.83 | 110.12 |
| 7 | M | 1288 | ASN | CA-C-N | 6.60 | 129.50 | 120.46 |
| 7 | M | 1288 | ASN | C-N-CA | 6.60 | 129.50 | 120.46 |
| 12 | u | 186 | GLU | N-CA-CB | 6.60 | 121.65 | 110.49 |
| 18 | e | 13 | HIS | CA-CB-CG | -6.60 | 107.20 | 113.80 |
| 18 | e | 345 | ILE | N-CA-CB | 6.60 | 120.22 | 111.64 |
| 9 | R | 139 | PHE | N-CA-C | 6.60 | 118.13 | 111.07 |
| 2 | Z | 400 | SER | CA-C-O | -6.60 | 114.16 | 120.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 926 | ASN | OD1-CG-ND2 | 6.60 | 129.20 | 122.60 |
| 16 | c | 345 | THR | N-CA-C | -6.60 | 104.39 | 114.16 |
| 7 | M | 1613 | VAL | N-CA-CB | 6.60 | 120.11 | 112.39 |
| 20 | n | 980 | ILE | CA-C-N | 6.60 | 131.23 | 122.06 |
| 20 | n | 980 | ILE | C-N-CA | 6.60 | 131.23 | 122.06 |
| 20 | g | 326 | PHE | CA-CB-CG | 6.60 | 120.40 | 113.80 |
| 6 | I | 279 | GLN | CA-C-N | 6.60 | 129.12 | 120.28 |
| 6 | I | 279 | GLN | C-N-CA | 6.60 | 129.12 | 120.28 |
| 2 | Z | 246 | ILE | CA-CB-CG2 | -6.60 | 99.29 | 110.50 |
| 20 | n | 111 | HIS | CE1-NE2-CD2 | -6.60 | 102.40 | 109.00 |
| 20 | g | 390 | ILE | N-CA-C | -6.60 | 101.05 | 109.30 |
| 8 | N | 1025 | ASN | CA-C-N | 6.60 | 130.74 | 121.24 |
| 8 | N | 1025 | ASN | C-N-CA | 6.60 | 130.74 | 121.24 |
| 9 | R | 410 | ALA | N-CA-CB | 6.60 | 119.57 | 110.01 |
| 2 | 1 | 679 | SER | CA-C-O | -6.59 | 111.08 | 120.51 |
| 2 | 1 | 1325 | LEU | CA-C-N | 6.59 | 129.12 | 120.28 |
| 2 | 1 | 1325 | LEU | C-N-CA | 6.59 | 129.12 | 120.28 |
| 8 | P | 1042 | SER | CA-C-N | 6.59 | 132.53 | 122.37 |
| 8 | P | 1042 | SER | C-N-CA | 6.59 | 132.53 | 122.37 |
| 9 | R | 835 | ILE | CA-CB-CG1 | 6.59 | 121.61 | 110.40 |
| 9 | T | 141 | ASN | CA-C-N | 6.59 | 129.01 | 120.44 |
| 9 | T | 141 | ASN | C-N-CA | 6.59 | 129.01 | 120.44 |
| 16 | c | 136 | LYS | CA-C-N | 6.59 | 129.12 | 120.28 |
| 16 | c | 136 | LYS | C-N-CA | 6.59 | 129.12 | 120.28 |
| 7 | M | 1455 | THR | CA-CB-CG2 | -6.59 | 99.29 | 110.50 |
| 7 | O | 1304 | HIS | CA-C-N | 6.59 | 129.01 | 120.44 |
| 7 | O | 1304 | HIS | C-N-CA | 6.59 | 129.01 | 120.44 |
| 9 | S | 437 | TRP | CB-CG-CD2 | 6.59 | 136.03 | 126.80 |
| 1 | Y | 1484 | ILE | CA-C-N | 6.59 | 129.11 | 120.28 |
| 1 | Y | 1484 | ILE | C-N-CA | 6.59 | 129.11 | 120.28 |
| 17 | k | 258 | TRP | CA-C-N | 6.59 | 130.07 | 120.71 |
| 17 | k | 258 | TRP | C-N-CA | 6.59 | 130.07 | 120.71 |
| 19 | m | 357 | SER | CA-C-N | 6.59 | 129.78 | 120.42 |
| 19 | m | 357 | SER | C-N-CA | 6.59 | 129.78 | 120.42 |
| 19 | f | 287 | HIS | CE1-NE2-CD2 | -6.59 | 102.41 | 109.00 |
| 7 | M | 713 | PHE | CA-C-N | 6.59 | 129.65 | 120.29 |
| 7 | M | 713 | PHE | C-N-CA | 6.59 | 129.65 | 120.29 |
| 13 | x | 1390 | LEU | N-CA-C | -6.59 | 103.91 | 112.68 |
| 16 | j | 380 | SER | CA-C-N | 6.59 | 129.77 | 120.28 |
| 16 | j | 380 | SER | C-N-CA | 6.59 | 129.77 | 120.28 |
| 16 | j | 491 | LEU | O-C-N | 6.59 | 129.66 | 122.15 |
| 19 | m | 390 | THR | CA-C-N | 6.59 | 129.11 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | m | 390 | THR | C-N-CA | 6.59 | 129.11 | 120.28 |
| 14 | a | 542 | ASP | CA-CB-CG | 6.59 | 119.19 | 112.60 |
| 7 | M | 1139 | ILE | N-CA-C | -6.59 | 106.88 | 113.20 |
| 9 | R | 137 | ASP | N-CA-C | 6.59 | 118.46 | 111.28 |
| 9 | S | 710 | ASN | N-CA-C | -6.59 | 104.82 | 112.92 |
| 2 | Z | 653 | LYS | CA-C-N | 6.59 | 129.41 | 120.38 |
| 2 | Z | 653 | LYS | C-N-CA | 6.59 | 129.41 | 120.38 |
| 15 | i | 517 | ASP | CA-C-O | -6.59 | 113.25 | 120.30 |
| 6 | L | 328 | GLN | CA-C-N | 6.59 | 129.11 | 120.28 |
| 6 | L | 328 | GLN | C-N-CA | 6.59 | 129.11 | 120.28 |
| 8 | P | 910 | ALA | CA-C-O | -6.59 | 111.13 | 120.16 |
| 12 | u | 329 | LYS | N-CA-C | -6.59 | 98.50 | 109.24 |
| 16 | c | 466 | SER | N-CA-C | -6.59 | 102.31 | 110.41 |
| 6 | I | 292 | HIS | CE1-NE2-CD2 | -6.59 | 102.41 | 109.00 |
| 7 | O | 1177 | VAL | CA-C-N | 6.59 | 129.40 | 120.38 |
| 7 | O | 1177 | VAL | C-N-CA | 6.59 | 129.40 | 120.38 |
| 8 | P | 499 | LEU | N-CA-C | -6.59 | 98.47 | 109.07 |
| 8 | P | 853 | LYS | CA-C-N | 6.59 | 129.41 | 120.38 |
| 8 | P | 853 | LYS | C-N-CA | 6.59 | 129.41 | 120.38 |
| 8 | P | 1252 | LEU | CA-C-N | 6.59 | 129.00 | 120.44 |
| 8 | P | 1252 | LEU | C-N-CA | 6.59 | 129.00 | 120.44 |
| 1 | Y | 1330 | PHE | CA-CB-CG | 6.59 | 120.39 | 113.80 |
| 12 | v | 600 | GLU | CA-C-N | 6.59 | 129.11 | 120.28 |
| 12 | v | 600 | GLU | C-N-CA | 6.59 | 129.11 | 120.28 |
| 14 | h | 431 | LYS | CA-C-N | -6.59 | 114.15 | 123.11 |
| 14 | h | 431 | LYS | C-N-CA | -6.59 | 114.15 | 123.11 |
| 14 | h | 484 | TYR | N-CA-C | -6.59 | 97.54 | 108.34 |
| 15 | i | 239 | VAL | CA-C-N | 6.59 | 132.06 | 122.77 |
| 15 | i | 239 | VAL | C-N-CA | 6.59 | 132.06 | 122.77 |
| 16 | c | 489 | HIS | CB-CG-ND1 | 6.59 | 132.58 | 122.70 |
| 20 | g | 991 | LEU | O-C-N | -6.59 | 113.37 | 122.20 |
| 14 | a | 109 | THR | CA-CB-OG1 | 6.59 | 119.48 | 109.60 |
| 1 | 0 | 164 | PHE | CA-CB-CG | -6.58 | 107.22 | 113.80 |
| 18 | l | 10 | ASP | CA-C-N | 6.58 | 130.47 | 121.05 |
| 18 | l | 10 | ASP | C-N-CA | 6.58 | 130.47 | 121.05 |
| 21 | p | 66 | GLY | N-CA-C | -6.58 | 100.64 | 110.71 |
| 8 | N | 350 | ALA | N-CA-C | 6.58 | 118.46 | 111.28 |
| 8 | N | 729 | HIS | CE1-NE2-CD2 | -6.58 | 102.42 | 109.00 |
| 7 | O | 281 | PHE | CA-C-N | 6.58 | 129.76 | 120.28 |
| 7 | O | 281 | PHE | C-N-CA | 6.58 | 129.76 | 120.28 |
| 7 | O | 910 | ARG | CA-C-N | 6.58 | 129.64 | 120.29 |
| 7 | O | 910 | ARG | C-N-CA | 6.58 | 129.64 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | T | 143 | ASN | N-CA-C | 6.58 | 118.11 | 111.07 |
| 14 | h | 297 | LEU | N-CA-C | -6.58 | 99.58 | 108.86 |
| 18 | l | 192 | ILE | CB-CA-C | 6.58 | 118.78 | 111.08 |
| 16 | c | 385 | LEU | O-C-N | -6.58 | 115.14 | 122.12 |
| 4 | J | 688 | HIS | CA-CB-CG | -6.58 | 107.22 | 113.80 |
| 6 | L | 443 | VAL | CA-CB-CG1 | 6.58 | 121.59 | 110.40 |
| 7 | M | 859 | LYS | CA-C-N | 6.58 | 132.26 | 121.99 |
| 7 | M | 859 | LYS | C-N-CA | 6.58 | 132.26 | 121.99 |
| 8 | P | 672 | VAL | CA-C-O | -6.58 | 113.36 | 120.47 |
| 1 | Y | 356 | ILE | N-CA-C | -6.58 | 98.95 | 108.36 |
| 2 | 1 | 594 | TYR | CA-C-N | 6.58 | 132.56 | 122.23 |
| 2 | 1 | 594 | TYR | C-N-CA | 6.58 | 132.56 | 122.23 |
| 2 | 1 | 1077 | SER | CA-C-O | 6.58 | 129.16 | 121.46 |
| 21 | t | 19 | LYS | CA-C-N | 6.58 | 129.63 | 120.29 |
| 21 | t | 19 | LYS | C-N-CA | 6.58 | 129.63 | 120.29 |
| 7 | M | 470 | ASP | CA-CB-CG | 6.58 | 119.18 | 112.60 |
| 7 | M | 1459 | LEU | N-CA-CB | -6.58 | 100.45 | 110.12 |
| 7 | M | 1461 | ASP | CA-C-N | 6.58 | 129.38 | 120.44 |
| 7 | M | 1461 | ASP | C-N-CA | 6.58 | 129.38 | 120.44 |
| 7 | O | 844 | VAL | CA-C-N | 6.58 | 129.39 | 120.38 |
| 7 | O | 844 | VAL | C-N-CA | 6.58 | 129.39 | 120.38 |
| 12 | u | 421 | GLU | N-CA-C | -6.58 | 102.65 | 113.50 |
| 17 | k | 128 | VAL | CB-CA-C | -6.58 | 104.18 | 111.35 |
| 16 | c | 588 | GLN | N-CA-C | 6.58 | 118.53 | 111.36 |
| 8 | N | 664 | LEU | N-CA-C | -6.58 | 105.41 | 113.50 |
| 8 | N | 915 | ASP | N-CA-CB | 6.58 | 121.61 | 110.49 |
| 18 | e | 175 | PRO | CA-C-N | 6.58 | 134.10 | 121.54 |
| 18 | e | 175 | PRO | C-N-CA | 6.58 | 134.10 | 121.54 |
| 20 | g | 1145 | ASN | CA-C-N | 6.58 | 130.05 | 120.71 |
| 20 | g | 1145 | ASN | C-N-CA | 6.58 | 130.05 | 120.71 |
| 2 | Z | 496 | THR | CA-CB-CG2 | 6.58 | 121.68 | 110.50 |
| 20 | n | 855 | LYS | CA-C-O | 6.58 | 127.60 | 119.78 |
| 20 | g | 728 | ALA | N-CA-C | 6.58 | 118.53 | 111.36 |
| 4 | A | 640 | LEU | CA-C-N | 6.57 | 129.75 | 120.42 |
| 4 | A | 640 | LEU | C-N-CA | 6.57 | 129.75 | 120.42 |
| 7 | M | 1154 | ARG | NE-CZ-NH2 | 6.57 | 125.11 | 119.20 |
| 8 | N | 198 | MET | CA-C-N | 6.57 | 130.88 | 121.55 |
| 8 | N | 198 | MET | C-N-CA | 6.57 | 130.88 | 121.55 |
| 7 | O | 1388 | CYS | CA-C-N | 6.57 | 128.84 | 120.56 |
| 7 | O | 1388 | CYS | C-N-CA | 6.57 | 128.84 | 120.56 |
| 7 | O | 642 | PHE | CA-C-N | 6.57 | 129.09 | 120.28 |
| 7 | O | 642 | PHE | C-N-CA | 6.57 | 129.09 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 13 | x | 1280 | GLN | CA-C-N | 6.57 | 129.09 | 120.28 |
| 13 | x | 1280 | GLN | C-N-CA | 6.57 | 129.09 | 120.28 |
| 15 | i | 161 | ARG | NE-CZ-NH1 | -6.57 | 114.93 | 121.50 |
| 4 | D | 800 | HIS | CE1-NE2-CD2 | -6.57 | 102.43 | 109.00 |
| 8 | N | 794 | ILE | CA-CB-CG1 | 6.57 | 121.57 | 110.40 |
| 8 | N | 994 | ILE | CA-CB-CG1 | 6.57 | 121.57 | 110.40 |
| 7 | O | 1585 | PRO | N-CA-CB | 6.57 | 110.56 | 103.33 |
| 8 | P | 57 | THR | N-CA-CB | 6.57 | 121.59 | 110.49 |
| 9 | Q | 18 | ALA | CA-C-O | -6.57 | 113.93 | 120.70 |
| 11 | X | 276 | TYR | CA-C-N | 6.57 | 126.59 | 119.89 |
| 11 | X | 276 | TYR | C-N-CA | 6.57 | 126.59 | 119.89 |
| 1 | Y | 634 | SER | N-CA-C | -6.57 | 98.53 | 108.52 |
| 14 | h | 101 | SER | CA-C-N | 6.57 | 129.62 | 120.29 |
| 14 | h | 101 | SER | C-N-CA | 6.57 | 129.62 | 120.29 |
| 15 | b | 302 | THR | N-CA-C | -6.57 | 105.57 | 112.93 |
| 14 | a | 164 | HIS | CE1-NE2-CD2 | -6.57 | 102.43 | 109.00 |
| 7 | O | 711 | GLN | N-CA-CB | 6.57 | 119.53 | 110.01 |
| 9 | S | 305 | ILE | CB-CA-C | -6.57 | 103.41 | 112.02 |
| 9 | T | 615 | ASP | CA-C-N | 6.57 | 129.38 | 120.38 |
| 9 | T | 615 | ASP | C-N-CA | 6.57 | 129.38 | 120.38 |
| 13 | x | 1352 | VAL | O-C-N | -6.57 | 115.47 | 121.91 |
| 17 | d | 76 | ASP | CA-CB-CG | 6.57 | 119.17 | 112.60 |
| 1 | 0 | 965 | GLU | N-CA-C | 6.57 | 118.23 | 111.14 |
| 5 | E | 347 | THR | O-C-N | -6.57 | 115.65 | 123.27 |
| 7 | M | 628 | LYS | CA-C-N | 6.57 | 129.08 | 120.28 |
| 7 | M | 628 | LYS | C-N-CA | 6.57 | 129.08 | 120.28 |
| 9 | Q | 806 | LEU | O-C-N | 6.57 | 128.84 | 122.07 |
| 1 | Y | 1196 | ILE | O-C-N | -6.57 | 115.27 | 121.90 |
| 12 | v | 630 | TRP | O-C-N | 6.57 | 129.08 | 122.12 |
| 5 | B | 449 | ASP | CA-CB-CG | 6.57 | 119.17 | 112.60 |
| 5 | H | 449 | ASP | CA-C-N | 6.57 | 126.15 | 119.19 |
| 5 | H | 449 | ASP | C-N-CA | 6.57 | 126.15 | 119.19 |
| 6 | L | 276 | GLU | CA-C-N | 6.57 | 131.58 | 120.29 |
| 6 | L | 276 | GLU | C-N-CA | 6.57 | 131.58 | 120.29 |
| 7 | M | 449 | LEU | CA-C-N | 6.57 | 128.97 | 120.44 |
| 7 | M | 449 | LEU | C-N-CA | 6.57 | 128.97 | 120.44 |
| 7 | M | 1200 | PRO | CA-C-O | 6.57 | 128.52 | 121.03 |
| 7 | O | 202 | ASP | N-CA-C | -6.57 | 104.20 | 112.93 |
| 8 | P | 104 | SER | CA-C-N | 6.57 | 129.61 | 120.29 |
| 8 | P | 104 | SER | C-N-CA | 6.57 | 129.61 | 120.29 |
| 1 | Y | 161 | LEU | CA-C-N | 6.57 | 129.08 | 120.28 |
| 1 | Y | 161 | LEU | C-N-CA | 6.57 | 129.08 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 23 | ASP | CA-C-O | 6.56 | 126.81 | 118.54 |
| 20 | n | 328 | HIS | CG-CD2-NE2 | 6.56 | 113.76 | 107.20 |
| 9 | R | 638 | TYR | CA-C-N | 6.56 | 129.40 | 120.54 |
| 9 | R | 638 | TYR | C-N-CA | 6.56 | 129.40 | 120.54 |
| 9 | S | 745 | LEU | CA-C-N | 6.56 | 126.52 | 119.76 |
| 9 | S | 745 | LEU | C-N-CA | 6.56 | 126.52 | 119.76 |
| 9 | T | 39 | LEU | O-C-N | 6.56 | 131.32 | 122.59 |
| 11 | X | 287 | HIS | CE1-NE2-CD2 | -6.56 | 102.44 | 109.00 |
| 15 | i | 518 | ASP | N-CA-CB | 6.56 | 121.58 | 110.49 |
| 18 | l | 219 | SER | CA-C-N | 6.56 | 131.16 | 122.30 |
| 18 | l | 219 | SER | C-N-CA | 6.56 | 131.16 | 122.30 |
| 14 | a | 484 | TYR | CA-C-O | 6.56 | 128.19 | 120.58 |
| 20 | n | 128 | ASP | CA-CB-CG | 6.56 | 119.16 | 112.60 |
| 17 | d | 232 | ILE | N-CA-C | -6.56 | 98.41 | 107.99 |
| 5 | E | 329 | HIS | ND1-CE1-NE2 | 6.56 | 114.96 | 108.40 |
| 7 | M | 184 | ASP | CA-C-N | 6.56 | 129.55 | 120.63 |
| 7 | M | 184 | ASP | C-N-CA | 6.56 | 129.55 | 120.63 |
| 7 | M | 698 | ASN | OD1-CG-ND2 | -6.56 | 116.04 | 122.60 |
| 2 | Z | 1006 | THR | CA-CB-OG1 | 6.56 | 119.44 | 109.60 |
| 14 | h | 471 | ILE | N-CA-CB | -6.56 | 104.82 | 111.90 |
| 16 | j | 346 | GLY | CA-C-N | 6.56 | 134.27 | 121.41 |
| 16 | j | 346 | GLY | C-N-CA | 6.56 | 134.27 | 121.41 |
| 18 | e | 3 | PRO | CA-C-O | -6.56 | 114.08 | 121.43 |
| 9 | S | 797 | SER | N-CA-C | -6.56 | 105.41 | 113.41 |
| 7 | M | 497 | CYS | CA-C-O | -6.56 | 112.43 | 119.97 |
| 15 | i | 84 | ALA | O-C-N | 6.56 | 131.67 | 123.15 |
| 7 | M | 104 | VAL | CA-C-N | 6.55 | 129.06 | 120.28 |
| 7 | M | 104 | VAL | C-N-CA | 6.55 | 129.06 | 120.28 |
| 9 | Q | 69 | ALA | CB-CA-C | -6.55 | 100.54 | 110.90 |
| 9 | S | 215 | TYR | N-CA-CB | 6.55 | 119.86 | 110.16 |
| 16 | j | 446 | ASP | CA-C-N | 6.55 | 129.44 | 120.46 |
| 16 | j | 446 | ASP | C-N-CA | 6.55 | 129.44 | 120.46 |
| 17 | d | 19 | TYR | CA-C-N | 6.55 | 129.72 | 120.28 |
| 17 | d | 19 | TYR | C-N-CA | 6.55 | 129.72 | 120.28 |
| 14 | a | 236 | VAL | CA-CB-CG2 | 6.55 | 121.54 | 110.40 |
| 8 | P | 505 | VAL | N-CA-C | -6.55 | 106.59 | 111.90 |
| 2 | Z | 982 | GLU | N-CA-C | 6.55 | 119.25 | 111.71 |
| 15 | b | 696 | GLU | CA-C-N | 6.55 | 128.96 | 120.44 |
| 15 | b | 696 | GLU | C-N-CA | 6.55 | 128.96 | 120.44 |
| 1 | 0 | 1352 | ASN | CA-CB-CG | 6.55 | 119.15 | 112.60 |
| 1 | Y | 236 | THR | CA-C-N | 6.55 | 129.71 | 120.28 |
| 1 | Y | 236 | THR | C-N-CA | 6.55 | 129.71 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 975 | ILE | CB-CA-C | -6.55 | 105.22 | 111.05 |
| 13 | x | 1234 | ASN | CA-C-N | 6.55 | 129.05 | 120.28 |
| 13 | x | 1234 | ASN | C-N-CA | 6.55 | 129.05 | 120.28 |
| 20 | g | 1040 | LEU | CA-C-O | 6.55 | 127.36 | 120.42 |
| 4 | A | 649 | THR | CA-C-N | 6.55 | 129.59 | 120.29 |
| 4 | A | 649 | THR | C-N-CA | 6.55 | 129.59 | 120.29 |
| 7 | M | 1188 | THR | CB-CA-C | -6.55 | 97.39 | 110.42 |
| 8 | P | 187 | PHE | N-CA-C | 6.55 | 119.24 | 111.71 |
| 9 | R | 800 | GLY | CA-C-O | 6.55 | 127.50 | 120.30 |
| 2 | Z | 769 | HIS | CE1-NE2-CD2 | -6.55 | 102.45 | 109.00 |
| 16 | j | 367 | GLU | N-CA-CB | 6.55 | 120.41 | 109.94 |
| 20 | g | 351 | ILE | N-CA-CB | 6.55 | 118.87 | 111.21 |
| 1 | 0 | 1465 | ILE | N-CA-C | -6.54 | 100.83 | 108.82 |
| 8 | N | 304 | ASN | N-CA-CB | 6.54 | 121.63 | 110.50 |
| 18 | l | 114 | VAL | CA-CB-CG1 | 6.54 | 121.53 | 110.40 |
| 2 | 1 | 147 | PRO | CA-C-O | -6.54 | 113.97 | 121.36 |
| 8 | P | 1555 | VAL | N-CA-CB | 6.54 | 118.21 | 110.55 |
| 9 | R | 81 | GLU | CA-C-O | -6.54 | 113.46 | 120.92 |
| 4 | y | 629 | PRO | N-CA-CB | 6.54 | 110.20 | 103.00 |
| 20 | g | 637 | ASN | N-CA-CB | 6.54 | 121.55 | 110.49 |
| 14 | a | 828 | LEU | O-C-N | 6.54 | 128.84 | 122.03 |
| 4 | G | 775 | THR | CA-C-N | 6.54 | 134.03 | 121.54 |
| 4 | G | 775 | THR | C-N-CA | 6.54 | 134.03 | 121.54 |
| 7 | M | 456 | ALA | O-C-N | 6.54 | 129.06 | 122.12 |
| 7 | M | 509 | GLY | CA-C-O | -6.54 | 113.78 | 120.45 |
| 7 | M | 559 | ALA | CA-C-N | 6.54 | 129.88 | 120.79 |
| 7 | M | 559 | ALA | C-N-CA | 6.54 | 129.88 | 120.79 |
| 19 | f | 403 | SER | CA-C-N | 6.54 | 131.71 | 123.14 |
| 19 | f | 403 | SER | C-N-CA | 6.54 | 131.71 | 123.14 |
| 9 | R | 662 | SER | CA-C-N | 6.54 | 128.94 | 120.44 |
| 9 | R | 662 | SER | C-N-CA | 6.54 | 128.94 | 120.44 |
| 6 | F | 465 | LYS | CA-C-N | 6.54 | 129.04 | 120.28 |
| 6 | F | 465 | LYS | C-N-CA | 6.54 | 129.04 | 120.28 |
| 7 | M | 423 | LEU | CA-C-O | -6.54 | 114.19 | 121.51 |
| 8 | P | 1438 | ILE | CA-C-N | 6.54 | 129.04 | 120.28 |
| 8 | P | 1438 | ILE | C-N-CA | 6.54 | 129.04 | 120.28 |
| 9 | R | 156 | MET | CA-C-N | 6.54 | 128.94 | 120.44 |
| 9 | R | 156 | MET | C-N-CA | 6.54 | 128.94 | 120.44 |
| 2 | Z | 1267 | ASN | N-CA-CB | 6.54 | 121.54 | 110.49 |
| 9 | Q | 424 | ASN | CA-CB-CG | 6.54 | 119.14 | 112.60 |
| 17 | k | 290 | GLU | CA-C-N | 6.54 | 126.89 | 119.83 |
| 17 | k | 290 | GLU | C-N-CA | 6.54 | 126.89 | 119.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 634 | ILE | O-C-N | 6.54 | 128.50 | 121.90 |
| 7 | O | 1250 | LYS | CA-C-N | 6.54 | 129.04 | 120.28 |
| 7 | O | 1250 | LYS | C-N-CA | 6.54 | 129.04 | 120.28 |
| 4 | y | 802 | ASP | CA-C-N | 6.54 | 129.04 | 120.28 |
| 4 | y | 802 | ASP | C-N-CA | 6.54 | 129.04 | 120.28 |
| 14 | h | 331 | ILE | N-CA-CB | 6.54 | 119.58 | 110.56 |
| 14 | h | 685 | GLU | O-C-N | 6.54 | 129.60 | 122.15 |
| 16 | j | 343 | TRP | CD2-CE2-CZ2 | -6.54 | 115.86 | 122.40 |
| 16 | c | 604 | ASP | CA-CB-CG | 6.54 | 119.14 | 112.60 |
| 2 | 1 | 720 | PHE | CA-CB-CG | -6.53 | 107.27 | 113.80 |
| 7 | O | 702 | LYS | N-CA-C | -6.53 | 100.22 | 108.45 |
| 9 | Q | 771 | ILE | N-CA-CB | 6.53 | 114.62 | 110.50 |
| 2 | Z | 662 | LEU | CA-C-N | 6.53 | 128.94 | 120.44 |
| 2 | Z | 662 | LEU | C-N-CA | 6.53 | 128.94 | 120.44 |
| 14 | h | 871 | HIS | CB-CG-CD2 | -6.53 | 122.71 | 131.20 |
| 21 | s | 25 | LEU | N-CA-CB | 6.53 | 119.83 | 110.16 |
| 17 | d | 275 | ASP | CA-CB-CG | 6.53 | 119.13 | 112.60 |
| 18 | e | 56 | SER | CA-C-N | 6.53 | 134.02 | 121.54 |
| 18 | e | 56 | SER | C-N-CA | 6.53 | 134.02 | 121.54 |
| 16 | j | 224 | MET | CA-C-N | 6.53 | 130.03 | 120.82 |
| 16 | j | 224 | MET | C-N-CA | 6.53 | 130.03 | 120.82 |
| 20 | n | 362 | ILE | N-CA-C | -6.53 | 98.71 | 108.12 |
| 21 | t | 79 | PHE | CA-CB-CG | 6.53 | 120.33 | 113.80 |
| 20 | g | 579 | ILE | N-CA-C | -6.53 | 95.75 | 109.34 |
| 7 | M | 755 | TYR | CA-C-O | -6.53 | 114.14 | 121.00 |
| 8 | N | 999 | GLN | N-CA-C | 6.53 | 119.23 | 111.33 |
| 1 | Y | 373 | SER | CA-C-N | 6.53 | 132.61 | 122.49 |
| 1 | Y | 373 | SER | C-N-CA | 6.53 | 132.61 | 122.49 |
| 15 | i | 121 | ASP | O-C-N | -6.53 | 114.92 | 122.89 |
| 6 | C | 402 | ASP | CA-C-O | -6.53 | 113.97 | 120.82 |
| 8 | N | 1440 | GLY | CA-C-N | 6.53 | 131.14 | 120.63 |
| 8 | N | 1440 | GLY | C-N-CA | 6.53 | 131.14 | 120.63 |
| 1 | Y | 1332 | ASP | N-CA-C | -6.53 | 96.89 | 110.80 |
| 12 | v | 49 | LEU | N-CA-CB | 6.53 | 121.01 | 111.54 |
| 8 | N | 520 | ILE | CA-C-O | -6.53 | 113.64 | 119.71 |
| 8 | P | 1344 | PHE | N-CA-CB | 6.53 | 121.52 | 110.49 |
| 9 | R | 300 | THR | N-CA-C | -6.53 | 98.80 | 108.79 |
| 19 | m | 528 | HIS | CB-CA-C | -6.53 | 100.36 | 110.81 |
| 14 | a | 89 | HIS | N-CA-C | -6.53 | 103.74 | 112.94 |
| 2 | 1 | 120 | GLY | O-C-N | 6.53 | 129.85 | 122.67 |
| 5 | B | 334 | GLU | CA-C-N | 6.53 | 129.56 | 120.29 |
| 5 | B | 334 | GLU | C-N-CA | 6.53 | 129.56 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | F | 347 | THR | CA-C-O | 6.53 | 127.34 | 120.42 |
| 7 | M | 291 | GLU | N-CA-C | -6.53 | 103.97 | 114.09 |
| 7 | O | 950 | GLU | O-C-N | -6.53 | 115.53 | 123.30 |
| 7 | O | 1295 | ALA | N-CA-C | 6.53 | 118.05 | 111.07 |
| 10 | U | 264 | ASN | OD1-CG-ND2 | 6.53 | 129.12 | 122.60 |
| 19 | m | 166 | THR | CA-C-O | 6.53 | 128.54 | 119.80 |
| 20 | n | 372 | SER | N-CA-C | -6.53 | 97.64 | 108.34 |
| 17 | d | 139 | ILE | CA-C-O | 6.53 | 127.40 | 120.48 |
| 1 | 0 | 292 | ASN | OD1-CG-ND2 | -6.52 | 116.08 | 122.60 |
| 6 | I | 327 | LYS | N-CA-C | 6.52 | 118.05 | 111.07 |
| 9 | R | 341 | LEU | CA-C-N | 6.52 | 132.42 | 122.37 |
| 9 | R | 341 | LEU | C-N-CA | 6.52 | 132.42 | 122.37 |
| 1 | Y | 1235 | PHE | CA-CB-CG | -6.52 | 107.28 | 113.80 |
| 2 | Z | 1350 | TRP | CA-C-O | 6.52 | 127.29 | 119.59 |
| 19 | m | 509 | HIS | N-CA-C | 6.52 | 118.39 | 111.28 |
| 15 | b | 306 | TRP | CA-CB-CG | 6.52 | 126.00 | 113.60 |
| 4 | A | 710 | PHE | CA-CB-CG | 6.52 | 120.32 | 113.80 |
| 7 | M | 758 | ASN | CA-C-N | 6.52 | 128.92 | 120.44 |
| 7 | M | 758 | ASN | C-N-CA | 6.52 | 128.92 | 120.44 |
| 9 | R | 209 | ARG | N-CA-C | 6.52 | 119.39 | 111.82 |
| 9 | S | 579 | LEU | N-CA-C | 6.52 | 119.39 | 111.82 |
| 12 | u | 278 | LEU | CA-C-N | 6.52 | 131.18 | 120.94 |
| 12 | u | 278 | LEU | C-N-CA | 6.52 | 131.18 | 120.94 |
| 13 | w | 1221 | VAL | CA-C-N | 6.52 | 129.02 | 120.28 |
| 13 | w | 1221 | VAL | C-N-CA | 6.52 | 129.02 | 120.28 |
| 7 | O | 227 | ASP | CA-C-O | 6.52 | 121.72 | 117.94 |
| 9 | Q | 86 | PHE | CA-C-N | 6.52 | 128.78 | 120.56 |
| 9 | Q | 86 | PHE | C-N-CA | 6.52 | 128.78 | 120.56 |
| 15 | b | 236 | GLY | O-C-N | 6.52 | 129.84 | 122.34 |
| 6 | L | 454 | ALA | CA-C-N | 6.52 | 129.31 | 120.44 |
| 6 | L | 454 | ALA | C-N-CA | 6.52 | 129.31 | 120.44 |
| 8 | N | 1620 | THR | CA-C-N | 6.52 | 129.02 | 120.28 |
| 8 | N | 1620 | THR | C-N-CA | 6.52 | 129.02 | 120.28 |
| 7 | O | 330 | SER | N-CA-C | -6.52 | 99.55 | 109.85 |
| 1 | Y | 1406 | HIS | ND1-CE1-NE2 | 6.52 | 114.92 | 108.40 |
| 20 | n | 926 | VAL | CA-C-O | -6.52 | 114.17 | 120.95 |
| 1 | 0 | 1089 | LEU | N-CA-C | -6.52 | 104.64 | 112.59 |
| 2 | 1 | 1167 | ALA | CA-C-O | -6.52 | 113.64 | 120.55 |
| 7 | O | 605 | ALA | O-C-N | -6.52 | 115.36 | 122.07 |
| 8 | P | 387 | LEU | CA-C-O | 6.52 | 127.08 | 119.32 |
| 9 | Q | 606 | GLU | N-CA-C | -6.52 | 105.36 | 113.38 |
| 17 | k | 52 | HIS | CB-CG-CD2 | -6.52 | 122.73 | 131.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 923 | HIS | CA-CB-CG | 6.52 | 120.32 | 113.80 |
| 1 | 0 | 1363 | PHE | CA-CB-CG | -6.52 | 107.28 | 113.80 |
| 9 | R | 483 | LEU | CA-C-N | 6.52 | 129.54 | 120.29 |
| 9 | R | 483 | LEU | C-N-CA | 6.52 | 129.54 | 120.29 |
| 20 | n | 1065 | VAL | CA-CB-CG1 | 6.52 | 121.48 | 110.40 |
| 21 | q | 50 | ASP | CA-C-N | 6.52 | 129.39 | 120.46 |
| 21 | q | 50 | ASP | C-N-CA | 6.52 | 129.39 | 120.46 |
| 21 | t | 54 | GLY | N-CA-C | -6.52 | 104.47 | 112.68 |
| 2 | 1 | 997 | PHE | CA-CB-CG | -6.51 | 107.29 | 113.80 |
| 7 | M | 1378 | ASP | CA-C-N | 6.51 | 127.33 | 120.03 |
| 7 | M | 1378 | ASP | C-N-CA | 6.51 | 127.33 | 120.03 |
| 8 | N | 766 | GLU | N-CA-C | -6.51 | 105.25 | 113.72 |
| 2 | Z | 642 | SER | N-CA-CB | 6.51 | 119.70 | 110.12 |
| 14 | h | 675 | LEU | CA-C-N | 6.51 | 128.91 | 120.44 |
| 14 | h | 675 | LEU | C-N-CA | 6.51 | 128.91 | 120.44 |
| 16 | j | 489 | HIS | CA-C-O | 6.51 | 127.48 | 119.79 |
| 20 | n | 855 | LYS | O-C-N | -6.51 | 114.34 | 122.35 |
| 14 | a | 641 | ASP | CA-C-N | 6.51 | 129.96 | 120.71 |
| 14 | a | 641 | ASP | C-N-CA | 6.51 | 129.96 | 120.71 |
| 2 | Z | 728 | VAL | N-CA-C | -6.51 | 105.98 | 112.17 |
| 16 | c | 409 | LYS | CB-CG-CD | 6.51 | 126.28 | 111.30 |
| 20 | g | 668 | ASN | N-CA-C | -6.51 | 104.10 | 111.07 |
| 4 | J | 697 | LEU | N-CA-C | -6.51 | 105.26 | 113.72 |
| 7 | O | 1082 | ILE | CA-C-O | -6.51 | 114.27 | 121.17 |
| 20 | n | 734 | SER | N-CA-C | -6.51 | 104.52 | 114.16 |
| 16 | c | 129 | ASN | CA-CB-CG | -6.51 | 106.09 | 112.60 |
| 2 | 1 | 721 | SER | CA-C-N | 6.51 | 128.90 | 120.44 |
| 2 | 1 | 721 | SER | C-N-CA | 6.51 | 128.90 | 120.44 |
| 2 | 1 | 965 | GLY | CA-C-N | 6.51 | 129.00 | 120.28 |
| 2 | 1 | 965 | GLY | C-N-CA | 6.51 | 129.00 | 120.28 |
| 5 | K | 300 | ASP | CA-CB-CG | 6.51 | 119.11 | 112.60 |
| 1 | Y | 1363 | PHE | N-CA-C | -6.51 | 104.11 | 111.14 |
| 20 | n | 173 | ILE | N-CA-C | -6.51 | 95.80 | 109.34 |
| 17 | d | 95 | HIS | CG-CD2-NE2 | 6.51 | 113.71 | 107.20 |
| 1 | 0 | 841 | TYR | N-CA-C | -6.51 | 104.82 | 112.89 |
| 12 | v | 249 | VAL | N-CA-CB | 6.51 | 118.17 | 110.55 |
| 14 | h | 84 | LEU | CA-C-N | 6.51 | 132.70 | 122.94 |
| 14 | h | 84 | LEU | C-N-CA | 6.51 | 132.70 | 122.94 |
| 21 | t | 49 | LEU | CA-C-N | 6.51 | 129.00 | 120.28 |
| 21 | t | 49 | LEU | C-N-CA | 6.51 | 129.00 | 120.28 |
| 1 | 0 | 1368 | SER | N-CA-CB | 6.51 | 121.49 | 110.49 |
| 8 | P | 997 | VAL | N-CA-CB | 6.51 | 120.90 | 112.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | T | 87 | ILE | CB-CA-C | -6.51 | 103.52 | 112.04 |
| 12 | v | 399 | GLU | N-CA-C | 6.51 | 121.05 | 113.18 |
| 13 | x | 1402 | LEU | CB-CA-C | -6.51 | 99.79 | 110.85 |
| 13 | x | 1434 | PHE | CA-CB-CG | -6.51 | 107.29 | 113.80 |
| 20 | n | 939 | LEU | N-CA-C | -6.51 | 99.22 | 109.50 |
| 15 | b | 550 | HIS | CA-C-O | -6.51 | 114.41 | 121.44 |
| 2 | Z | 945 | CYS | N-CA-C | -6.50 | 101.61 | 111.56 |
| 4 | D | 723 | SER | N-CA-C | -6.50 | 105.34 | 113.28 |
| 8 | N | 515 | ASN | OD1-CG-ND2 | 6.50 | 129.10 | 122.60 |
| 8 | N | 801 | LYS | CA-C-N | 6.50 | 130.57 | 120.82 |
| 8 | N | 801 | LYS | C-N-CA | 6.50 | 130.57 | 120.82 |
| 12 | v | 425 | ASN | OD1-CG-ND2 | -6.50 | 116.10 | 122.60 |
| 12 | v | 608 | LYS | CA-C-O | 6.50 | 127.45 | 120.10 |
| 14 | h | 139 | PHE | CB-CG-CD1 | 6.50 | 131.75 | 120.70 |
| 20 | n | 264 | ASN | N-CA-C | -6.50 | 99.15 | 109.23 |
| 16 | c | 161 | THR | N-CA-C | -6.50 | 99.09 | 109.76 |
| 19 | f | 318 | PRO | CA-C-O | -6.50 | 114.01 | 121.36 |
| 9 | T | 28 | SER | CA-C-O | 6.50 | 127.65 | 120.63 |
| 9 | T | 713 | ILE | CA-C-N | 6.50 | 128.89 | 120.44 |
| 9 | T | 713 | ILE | C-N-CA | 6.50 | 128.89 | 120.44 |
| 10 | W | 283 | ILE | CB-CA-C | -6.50 | 103.45 | 111.32 |
| 11 | X | 295 | MET | CA-C-N | 6.50 | 132.13 | 121.86 |
| 11 | X | 295 | MET | C-N-CA | 6.50 | 132.13 | 121.86 |
| 15 | i | 286 | SER | CA-C-O | 6.50 | 127.46 | 120.24 |
| 19 | m | 182 | LYS | CA-C-O | -6.50 | 113.94 | 120.90 |
| 19 | m | 648 | ASP | CA-CB-CG | 6.50 | 119.10 | 112.60 |
| 20 | g | 215 | GLU | O-C-N | -6.50 | 114.26 | 120.70 |
| 2 | Z | 997 | PHE | CA-C-O | -6.50 | 114.00 | 120.82 |
| 12 | u | 114 | TYR | N-CA-C | -6.50 | 99.28 | 108.96 |
| 20 | n | 366 | ILE | N-CA-C | -6.50 | 97.83 | 107.51 |
| 17 | d | 125 | VAL | N-CA-C | -6.50 | 98.84 | 108.85 |
| 20 | g | 670 | THR | N-CA-C | -6.50 | 104.12 | 111.14 |
| 7 | M | 627 | VAL | N-CA-C | 6.50 | 117.25 | 110.62 |
| 7 | M | 1405 | PHE | CB-CG-CD1 | 6.50 | 131.75 | 120.70 |
| 9 | S | 673 | PRO | CA-C-O | -6.50 | 114.24 | 121.32 |
| 4 | D | 654 | HIS | ND1-CE1-NE2 | 6.50 | 114.90 | 108.40 |
| 5 | K | 378 | HIS | CA-C-N | 6.50 | 129.65 | 120.42 |
| 5 | K | 378 | HIS | C-N-CA | 6.50 | 129.65 | 120.42 |
| 5 | K | 469 | ARG | N-CA-C | 6.50 | 119.18 | 111.71 |
| 7 | O | 284 | TYR | N-CA-C | 6.50 | 119.18 | 111.71 |
| 11 | V | 364 | SER | CA-C-O | 6.50 | 127.64 | 120.82 |
| 1 | Y | 1407 | ILE | N-CA-C | -6.50 | 99.23 | 108.58 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 811 | LEU | CA-C-O | 6.50 | 127.44 | 120.55 |
| 18 | l | 135 | ARG | N-CA-CB | 6.50 | 121.25 | 110.47 |
| 2 | 1 | 182 | LEU | N-CA-C | -6.50 | 96.65 | 108.02 |
| 7 | M | 144 | ILE | CA-C-N | 6.50 | 128.88 | 120.44 |
| 7 | M | 144 | ILE | C-N-CA | 6.50 | 128.88 | 120.44 |
| 1 | 0 | 1157 | PHE | O-C-N | -6.49 | 115.50 | 122.19 |
| 2 | 1 | 1204 | ASP | N-CA-CB | 6.49 | 120.10 | 110.49 |
| 7 | O | 526 | PHE | CA-CB-CG | 6.49 | 120.29 | 113.80 |
| 14 | h | 14 | TYR | N-CA-C | -6.49 | 103.78 | 112.94 |
| 20 | n | 1094 | TYR | CA-C-N | 6.49 | 130.95 | 120.30 |
| 20 | n | 1094 | TYR | C-N-CA | 6.49 | 130.95 | 120.30 |
| 19 | m | 597 | TYR | N-CA-C | -6.49 | 104.41 | 112.72 |
| 1 | 0 | 1321 | ALA | N-CA-C | 6.49 | 118.35 | 111.28 |
| 4 | z | 698 | GLN | N-CA-C | 6.49 | 118.01 | 111.07 |
| 19 | f | 341 | HIS | CA-C-O | -6.49 | 113.95 | 120.64 |
| 1 | 0 | 612 | SER | CA-C-N | 6.49 | 130.85 | 121.44 |
| 1 | 0 | 612 | SER | C-N-CA | 6.49 | 130.85 | 121.44 |
| 7 | O | 443 | ILE | CA-C-O | 6.49 | 128.05 | 121.17 |
| 1 | Y | 1063 | SER | CA-C-N | 6.49 | 131.51 | 121.19 |
| 1 | Y | 1063 | SER | C-N-CA | 6.49 | 131.51 | 121.19 |
| 19 | m | 59 | GLU | CA-C-N | 6.49 | 128.88 | 120.44 |
| 19 | m | 59 | GLU | C-N-CA | 6.49 | 128.88 | 120.44 |
| 20 | n | 974 | ARG | NE-CZ-NH2 | -6.49 | 113.36 | 119.20 |
| 14 | a | 1012 | SER | CA-C-N | 6.49 | 133.93 | 121.54 |
| 14 | a | 1012 | SER | C-N-CA | 6.49 | 133.93 | 121.54 |
| 14 | h | 858 | ILE | N-CA-C | -6.49 | 99.38 | 108.27 |
| 17 | k | 251 | GLU | N-CA-C | -6.49 | 99.44 | 109.24 |
| 20 | n | 649 | PHE | O-C-N | -6.49 | 113.20 | 122.41 |
| 20 | n | 744 | LYS | N-CA-C | -6.49 | 105.01 | 113.12 |
| 1 | 0 | 516 | LEU | N-CA-C | -6.49 | 98.77 | 109.80 |
| 1 | 0 | 1200 | LEU | CA-C-N | 6.49 | 133.03 | 122.65 |
| 1 | 0 | 1200 | LEU | C-N-CA | 6.49 | 133.03 | 122.65 |
| 5 | B | 360 | GLN | N-CA-CB | 6.49 | 119.65 | 110.12 |
| 8 | P | 216 | TYR | O-C-N | 6.49 | 129.09 | 122.09 |
| 14 | h | 215 | SER | CB-CA-C | -6.49 | 97.05 | 109.95 |
| 2 | 1 | 388 | MET | N-CA-C | -6.48 | 104.06 | 112.23 |
| 7 | M | 335 | ASP | CA-C-N | 6.48 | 128.87 | 120.44 |
| 7 | M | 335 | ASP | C-N-CA | 6.48 | 128.87 | 120.44 |
| 7 | O | 1137 | ASN | N-CA-CB | 6.48 | 121.52 | 110.50 |
| 8 | P | 517 | LEU | CA-C-N | 6.48 | 133.93 | 121.54 |
| 8 | P | 517 | LEU | C-N-CA | 6.48 | 133.93 | 121.54 |
| 14 | a | 813 | CYS | CA-C-N | 6.48 | 130.17 | 120.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | a | 813 | CYS | C-N-CA | 6.48 | 130.17 | 120.31 |
| 7 | O | 1476 | LEU | CA-C-N | 6.48 | 128.97 | 120.28 |
| 7 | O | 1476 | LEU | C-N-CA | 6.48 | 128.97 | 120.28 |
| 9 | Q | 800 | GLY | CA-C-N | 6.48 | 131.67 | 120.58 |
| 9 | Q | 800 | GLY | C-N-CA | 6.48 | 131.67 | 120.58 |
| 9 | S | 654 | ILE | O-C-N | -6.48 | 114.53 | 122.18 |
| 9 | T | 305 | ILE | CA-C-N | 6.48 | 134.02 | 121.18 |
| 9 | T | 305 | ILE | C-N-CA | 6.48 | 134.02 | 121.18 |
| 10 | W | 340 | ILE | CB-CA-C | 6.48 | 117.78 | 111.23 |
| 8 | P | 1308 | TYR | CA-C-N | 6.48 | 128.19 | 120.09 |
| 8 | P | 1308 | TYR | C-N-CA | 6.48 | 128.19 | 120.09 |
| 9 | R | 285 | TYR | CB-CG-CD1 | 6.48 | 130.52 | 120.80 |
| 9 | R | 600 | ILE | N-CA-C | -6.48 | 100.40 | 108.05 |
| 2 | Z | 1130 | ARG | NE-CZ-NH2 | 6.48 | 125.03 | 119.20 |
| 20 | n | 782 | ASP | N-CA-C | 6.48 | 118.00 | 111.07 |
| 15 | b | 504 | ILE | N-CA-C | -6.48 | 105.25 | 113.22 |
| 6 | F | 369 | LEU | N-CA-CB | 6.48 | 121.51 | 110.50 |
| 4 | G | 706 | GLU | CA-C-O | 6.48 | 127.16 | 119.06 |
| 2 | Z | 676 | LYS | N-CA-CB | 6.48 | 121.90 | 110.37 |
| 12 | u | 698 | ASN | CA-C-N | 6.48 | 128.96 | 120.28 |
| 12 | u | 698 | ASN | C-N-CA | 6.48 | 128.96 | 120.28 |
| 15 | b | 65 | MET | CG-SD-CE | -6.48 | 86.65 | 100.90 |
| 2 | 1 | 580 | THR | N-CA-C | -6.48 | 98.42 | 109.24 |
| 4 | A | 716 | THR | CA-C-N | 6.48 | 130.16 | 120.31 |
| 4 | A | 716 | THR | C-N-CA | 6.48 | 130.16 | 120.31 |
| 7 | O | 143 | ASN | CA-CB-CG | 6.48 | 119.08 | 112.60 |
| 1 | Y | 248 | ASP | N-CA-C | -6.48 | 99.48 | 109.52 |
| 12 | v | 312 | ASN | N-CA-C | -6.48 | 97.85 | 108.41 |
| 20 | n | 840 | PRO | N-CA-CB | 6.48 | 108.99 | 103.35 |
| 20 | g | 792 | LEU | N-CA-C | -6.48 | 103.45 | 112.45 |
| 4 | G | 791 | ILE | CA-C-O | -6.48 | 114.22 | 120.95 |
| 7 | M | 709 | PHE | CA-C-N | 6.48 | 128.86 | 120.44 |
| 7 | M | 709 | PHE | C-N-CA | 6.48 | 128.86 | 120.44 |
| 8 | N | 887 | VAL | CA-C-O | 6.48 | 125.11 | 118.96 |
| 8 | N | 1247 | PHE | CA-C-N | 6.48 | 130.15 | 120.31 |
| 8 | N | 1247 | PHE | C-N-CA | 6.48 | 130.15 | 120.31 |
| 9 | Q | 771 | ILE | O-C-N | -6.48 | 115.47 | 120.07 |
| 17 | d | 219 | ARG | NE-CZ-NH1 | 6.48 | 127.98 | 121.50 |
| 2 | 1 | 769 | HIS | CA-C-O | -6.47 | 111.95 | 119.59 |
| 7 | O | 305 | ASP | N-CA-C | 6.47 | 118.34 | 111.28 |
| 8 | P | 356 | HIS | ND1-CE1-NE2 | 6.47 | 114.88 | 108.40 |
| 14 | h | 1010 | PHE | N-CA-C | -6.47 | 102.77 | 110.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | q | 54 | GLY | CA-C-N | 6.47 | 133.91 | 121.54 |
| 21 | q | 54 | GLY | C-N-CA | 6.47 | 133.91 | 121.54 |
| 14 | a | 61 | LEU | CA-C-N | 6.47 | 133.91 | 121.54 |
| 14 | a | 61 | LEU | C-N-CA | 6.47 | 133.91 | 121.54 |
| 2 | 1 | 136 | THR | N-CA-CB | 6.47 | 121.89 | 110.37 |
| 5 | E | 420 | ALA | N-CA-C | -6.47 | 105.51 | 113.41 |
| 7 | M | 1288 | ASN | N-CA-CB | 6.47 | 120.24 | 110.14 |
| 8 | N | 497 | ILE | CA-C-N | 6.47 | 133.90 | 121.54 |
| 8 | N | 497 | ILE | C-N-CA | 6.47 | 133.90 | 121.54 |
| 2 | Z | 1112 | ALA | N-CA-C | 6.47 | 118.42 | 111.36 |
| 4 | z | 756 | ASN | CA-C-N | 6.47 | 128.85 | 120.44 |
| 4 | z | 756 | ASN | C-N-CA | 6.47 | 128.85 | 120.44 |
| 4 | z | 811 | SER | CA-C-O | -6.47 | 113.69 | 120.55 |
| 19 | m | 587 | TYR | N-CA-CB | 6.47 | 119.58 | 109.94 |
| 10 | U | 347 | PRO | CB-CA-C | 6.47 | 119.32 | 110.52 |
| 1 | Y | 651 | LYS | CA-C-O | -6.47 | 114.08 | 121.72 |
| 1 | Y | 1069 | ASN | N-CA-C | 6.47 | 120.27 | 112.38 |
| 2 | Z | 791 | GLU | N-CA-C | -6.47 | 104.87 | 112.89 |
| 6 | C | 388 | CYS | N-CA-CB | 6.47 | 119.73 | 110.16 |
| 7 | M | 194 | SER | CA-C-O | -6.47 | 113.69 | 120.55 |
| 12 | v | 564 | LEU | N-CA-C | 6.47 | 118.33 | 111.28 |
| 13 | x | 1455 | ASN | N-CA-CB | 6.47 | 121.42 | 110.49 |
| 15 | i | 356 | SER | N-CA-C | 6.47 | 117.99 | 111.07 |
| 20 | n | 356 | CYS | N-CA-CB | 6.47 | 121.42 | 110.49 |
| 15 | b | 390 | TRP | N-CA-C | -6.47 | 103.55 | 112.03 |
| 16 | c | 585 | ASN | OD1-CG-ND2 | -6.47 | 116.13 | 122.60 |
| 20 | g | 951 | LEU | N-CA-C | -6.47 | 104.32 | 111.82 |
| 14 | a | 908 | LEU | N-CA-C | 6.47 | 118.87 | 111.11 |
| 1 | 0 | 1177 | ILE | N-CA-C | -6.47 | 105.26 | 113.22 |
| 19 | m | 113 | ASN | N-CA-C | -6.47 | 97.87 | 108.41 |
| 7 | M | 966 | LEU | CA-C-N | 6.47 | 129.23 | 120.44 |
| 7 | M | 966 | LEU | C-N-CA | 6.47 | 129.23 | 120.44 |
| 7 | M | 971 | SER | O-C-N | 6.47 | 128.97 | 122.12 |
| 7 | M | 1361 | PHE | CA-C-O | 6.47 | 125.57 | 118.65 |
| 12 | u | 204 | ASP | O-C-N | -6.47 | 115.88 | 123.25 |
| 16 | j | 165 | VAL | CA-C-O | 6.47 | 126.31 | 119.91 |
| 18 | e | 34 | LYS | N-CA-CB | 6.47 | 120.06 | 110.49 |
| 8 | N | 555 | PHE | O-C-N | 6.46 | 130.97 | 122.95 |
| 8 | P | 722 | SER | CA-C-N | 6.46 | 133.21 | 122.54 |
| 8 | P | 722 | SER | C-N-CA | 6.46 | 133.21 | 122.54 |
| 9 | S | 92 | THR | O-C-N | 6.46 | 128.73 | 122.07 |
| 9 | T | 817 | ALA | CA-C-N | 6.46 | 128.22 | 120.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | T | 817 | ALA | C-N-CA | 6.46 | 128.22 | 120.14 |
| 12 | u | 647 | SER | CA-C-N | 6.46 | 128.84 | 120.44 |
| 12 | u | 647 | SER | C-N-CA | 6.46 | 128.84 | 120.44 |
| 18 | l | 11 | LEU | CA-C-O | 6.46 | 128.01 | 120.96 |
| 20 | n | 350 | SER | N-CA-CB | 6.46 | 119.98 | 110.35 |
| 16 | c | 458 | ARG | N-CA-C | -6.46 | 105.52 | 113.41 |
| 14 | a | 948 | ILE | N-CA-CB | 6.46 | 120.28 | 110.58 |
| 1 | 0 | 122 | ASP | N-CA-CB | 6.46 | 121.41 | 110.49 |
| 20 | n | 988 | VAL | N-CA-CB | 6.46 | 118.11 | 110.55 |
| 15 | b | 556 | ILE | CA-CB-CG2 | 6.46 | 121.49 | 110.50 |
| 1 | 0 | 1160 | HIS | N-CA-C | 6.46 | 118.40 | 111.36 |
| 7 | M | 1385 | PHE | O-C-N | -6.46 | 115.42 | 122.07 |
| 8 | N | 1395 | ILE | CB-CA-C | -6.46 | 103.42 | 112.14 |
| 13 | x | 1280 | GLN | N-CA-C | 6.46 | 118.40 | 111.36 |
| 19 | m | 474 | ASN | CA-C-N | 6.46 | 129.31 | 120.46 |
| 19 | m | 474 | ASN | C-N-CA | 6.46 | 129.31 | 120.46 |
| 19 | f | 287 | HIS | CG-CD2-NE2 | 6.46 | 113.66 | 107.20 |
| 20 | g | 517 | PRO | CA-C-N | 6.46 | 126.09 | 119.56 |
| 20 | g | 517 | PRO | C-N-CA | 6.46 | 126.09 | 119.56 |
| 20 | g | 985 | ASN | CA-CB-CG | 6.46 | 119.06 | 112.60 |
| 8 | P | 1538 | ASP | CA-CB-CG | 6.46 | 119.06 | 112.60 |
| 19 | m | 634 | PHE | CA-C-N | 6.46 | 133.88 | 121.54 |
| 19 | m | 634 | PHE | C-N-CA | 6.46 | 133.88 | 121.54 |
| 18 | e | 84 | TRP | N-CA-CB | 6.46 | 121.30 | 110.77 |
| 7 | M | 1155 | ASN | N-CA-C | 6.46 | 120.62 | 112.87 |
| 8 | N | 1082 | PHE | N-CA-C | -6.46 | 105.56 | 113.50 |
| 8 | N | 1407 | ILE | CA-CB-CG2 | -6.46 | 99.52 | 110.50 |
| 8 | N | 1538 | ASP | CA-CB-CG | -6.46 | 106.14 | 112.60 |
| 5 | K | 384 | THR | CA-C-N | 6.46 | 129.46 | 120.29 |
| 5 | K | 384 | THR | C-N-CA | 6.46 | 129.46 | 120.29 |
| 8 | N | 770 | HIS | N-CA-C | -6.46 | 105.56 | 113.50 |
| 2 | Z | 106 | ARG | N-CA-C | -6.46 | 105.03 | 113.17 |
| 15 | i | 52 | THR | N-CA-C | -6.46 | 97.89 | 108.41 |
| 15 | i | 622 | GLN | N-CA-C | -6.46 | 104.71 | 112.59 |
| 20 | g | 303 | HIS | CA-C-N | 6.46 | 126.68 | 119.90 |
| 20 | g | 303 | HIS | C-N-CA | 6.46 | 126.68 | 119.90 |
| 7 | M | 1216 | PHE | CA-CB-CG | -6.46 | 107.34 | 113.80 |
| 7 | O | 182 | ARG | CA-C-N | 6.46 | 128.83 | 120.44 |
| 7 | O | 182 | ARG | C-N-CA | 6.46 | 128.83 | 120.44 |
| 2 | Z | 91 | LEU | N-CA-C | 6.46 | 117.98 | 111.07 |
| 12 | v | 55 | HIS | CG-CD2-NE2 | 6.46 | 113.66 | 107.20 |
| 12 | v | 342 | TYR | CA-C-O | 6.46 | 128.39 | 121.16 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 18 | l | 185 | VAL | N-CA-C | -6.46 | 98.22 | 107.77 |
| 9 | Q | 317 | ASP | CA-CB-CG | 6.45 | 119.05 | 112.60 |
| 2 | Z | 501 | ILE | N-CA-C | -6.45 | 98.33 | 107.75 |
| 13 | w | 1281 | MET | CB-CA-C | -6.45 | 100.08 | 110.79 |
| 20 | g | 1119 | GLN | CA-C-N | 6.45 | 129.30 | 120.46 |
| 20 | g | 1119 | GLN | C-N-CA | 6.45 | 129.30 | 120.46 |
| 9 | R | 833 | ILE | N-CA-CB | 6.45 | 118.83 | 110.57 |
| 9 | T | 612 | HIS | ND1-CE1-NE2 | 6.45 | 114.85 | 108.40 |
| 1 | Y | 1441 | ASN | CA-CB-CG | 6.45 | 119.05 | 112.60 |
| 2 | Z | 1208 | ASP | CA-CB-CG | 6.45 | 119.05 | 112.60 |
| 14 | h | 883 | GLU | N-CA-CB | 6.45 | 121.17 | 110.85 |
| 7 | O | 145 | LEU | CA-C-N | 6.45 | 128.92 | 120.28 |
| 7 | O | 145 | LEU | C-N-CA | 6.45 | 128.92 | 120.28 |
| 7 | O | 1149 | SER | CA-C-N | 6.45 | 128.92 | 120.28 |
| 7 | O | 1149 | SER | C-N-CA | 6.45 | 128.92 | 120.28 |
| 8 | P | 375 | TYR | N-CA-C | -6.45 | 105.45 | 113.38 |
| 9 | R | 322 | ILE | CA-CB-CG1 | 6.45 | 121.37 | 110.40 |
| 1 | Y | 1281 | THR | N-CA-C | -6.45 | 105.33 | 113.72 |
| 2 | Z | 1096 | ASN | N-CA-CB | 6.45 | 119.33 | 109.98 |
| 19 | f | 113 | ASN | N-CA-C | -6.45 | 98.01 | 108.52 |
| 1 | 0 | 157 | PRO | CA-C-N | 6.45 | 128.92 | 120.28 |
| 1 | 0 | 157 | PRO | C-N-CA | 6.45 | 128.92 | 120.28 |
| 1 | 0 | 1060 | TYR | O-C-N | 6.45 | 128.47 | 121.12 |
| 1 | 0 | 1473 | HIS | CA-CB-CG | -6.45 | 107.35 | 113.80 |
| 5 | B | 309 | ARG | NE-CZ-NH2 | -6.45 | 113.40 | 119.20 |
| 6 | C | 356 | GLN | N-CA-C | -6.45 | 97.07 | 110.80 |
| 8 | P | 904 | LEU | O-C-N | 6.45 | 128.96 | 122.12 |
| 9 | Q | 348 | GLU | CA-C-N | 6.45 | 131.49 | 120.72 |
| 9 | Q | 348 | GLU | C-N-CA | 6.45 | 131.49 | 120.72 |
| 16 | c | 615 | ASN | N-CA-C | -6.45 | 105.17 | 113.16 |
| 20 | g | 627 | GLU | N-CA-C | -6.45 | 100.41 | 109.69 |
| 6 | L | 374 | GLN | CA-C-N | 6.45 | 129.44 | 120.29 |
| 6 | L | 374 | GLN | C-N-CA | 6.45 | 129.44 | 120.29 |
| 7 | M | 228 | PHE | CA-CB-CG | 6.45 | 120.25 | 113.80 |
| 1 | 0 | 665 | ASN | CA-C-O | -6.45 | 114.38 | 119.99 |
| 4 | D | 774 | ASN | CA-CB-CG | -6.45 | 106.15 | 112.60 |
| 8 | N | 717 | VAL | N-CA-C | 6.45 | 117.23 | 110.72 |
| 7 | O | 1286 | PHE | CA-CB-CG | 6.45 | 120.25 | 113.80 |
| 8 | P | 1525 | PHE | N-CA-C | -6.45 | 102.78 | 111.87 |
| 9 | Q | 796 | SER | CA-C-N | 6.45 | 129.44 | 120.29 |
| 9 | Q | 796 | SER | C-N-CA | 6.45 | 129.44 | 120.29 |
| 9 | T | 122 | LEU | N-CA-CB | 6.45 | 119.36 | 110.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 905 | LEU | CA-C-N | 6.45 | 128.82 | 120.44 |
| 14 | h | 905 | LEU | C-N-CA | 6.45 | 128.82 | 120.44 |
| 17 | d | 137 | SER | O-C-N | -6.45 | 116.09 | 121.44 |
| 20 | g | 831 | LEU | N-CA-CB | 6.45 | 120.25 | 109.94 |
| 7 | M | 74 | ALA | N-CA-CB | 6.44 | 119.59 | 110.12 |
| 7 | M | 613 | LEU | N-CA-C | 6.44 | 118.30 | 111.28 |
| 9 | T | 776 | ILE | CA-C-N | 6.44 | 128.68 | 120.56 |
| 9 | T | 776 | ILE | C-N-CA | 6.44 | 128.68 | 120.56 |
| 14 | h | 139 | PHE | CA-CB-CG | -6.44 | 107.36 | 113.80 |
| 20 | g | 510 | ASN | CA-CB-CG | -6.44 | 106.16 | 112.60 |
| 20 | g | 674 | ASN | OD1-CG-ND2 | 6.44 | 129.04 | 122.60 |
| 6 | F | 358 | LEU | N-CA-C | -6.44 | 106.63 | 114.75 |
| 6 | I | 450 | PHE | CB-CA-C | 6.44 | 121.48 | 110.79 |
| 7 | M | 487 | PHE | N-CA-C | 6.44 | 118.30 | 111.28 |
| 1 | Y | 382 | ILE | CA-C-N | 6.44 | 133.84 | 121.54 |
| 1 | Y | 382 | ILE | C-N-CA | 6.44 | 133.84 | 121.54 |
| 13 | w | 1112 | SER | N-CA-C | -6.44 | 104.85 | 114.64 |
| 4 | J | 755 | LEU | N-CA-C | -6.44 | 105.55 | 113.41 |
| 7 | M | 462 | LEU | N-CA-CB | 6.44 | 119.63 | 109.71 |
| 8 | N | 696 | GLY | O-C-N | 6.44 | 131.07 | 122.70 |
| 9 | R | 581 | LEU | CA-C-O | -6.44 | 114.27 | 120.90 |
| 9 | T | 628 | ALA | CA-C-O | -6.44 | 113.72 | 120.55 |
| 2 | Z | 666 | SER | N-CA-C | 6.44 | 118.18 | 111.03 |
| 20 | n | 239 | LYS | CA-C-O | -6.44 | 113.66 | 119.59 |
| 14 | a | 979 | GLU | CA-C-O | -6.44 | 113.72 | 120.55 |
| 13 | w | 1388 | GLU | N-CA-C | 6.44 | 118.30 | 111.28 |
| 2 | 1 | 1331 | ASN | N-CA-C | 6.44 | 121.30 | 113.38 |
| 7 | M | 1054 | SER | N-CA-C | 6.44 | 118.30 | 111.28 |
| 8 | N | 824 | LEU | CA-C-N | 6.44 | 133.56 | 121.97 |
| 8 | N | 824 | LEU | C-N-CA | 6.44 | 133.56 | 121.97 |
| 8 | N | 896 | PHE | N-CA-C | -6.44 | 99.96 | 109.81 |
| 8 | P | 1334 | ASP | CA-CB-CG | 6.44 | 119.04 | 112.60 |
| 13 | x | 1347 | GLN | N-CA-C | -6.44 | 105.56 | 113.41 |
| 15 | i | 459 | ASN | N-CA-C | -6.44 | 99.54 | 109.52 |
| 16 | j | 188 | VAL | CA-C-N | 6.44 | 128.81 | 120.44 |
| 16 | j | 188 | VAL | C-N-CA | 6.44 | 128.81 | 120.44 |
| 19 | m | 100 | ASN | N-CA-CB | 6.44 | 120.76 | 110.46 |
| 21 | t | 38 | GLU | N-CA-C | 6.44 | 117.96 | 111.07 |
| 16 | c | 250 | THR | N-CA-C | -6.44 | 99.52 | 109.24 |
| 2 | 1 | 861 | GLN | CA-C-O | 6.44 | 127.37 | 120.55 |
| 6 | L | 394 | ILE | O-C-N | -6.44 | 115.63 | 121.87 |
| 9 | S | 214 | ASN | CA-C-N | 6.44 | 129.43 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | S | 214 | ASN | C-N-CA | 6.44 | 129.43 | 120.29 |
| 7 | M | 189 | GLU | CA-C-O | -6.43 | 112.83 | 120.10 |
| 8 | N | 395 | SER | CA-C-N | 6.43 | 129.55 | 120.28 |
| 8 | N | 395 | SER | C-N-CA | 6.43 | 129.55 | 120.28 |
| 1 | Y | 153 | VAL | O-C-N | -6.43 | 116.31 | 123.26 |
| 12 | v | 273 | GLN | CA-C-N | 6.43 | 129.77 | 120.38 |
| 12 | v | 273 | GLN | C-N-CA | 6.43 | 129.77 | 120.38 |
| 4 | y | 772 | VAL | CA-C-N | 6.43 | 128.81 | 120.44 |
| 4 | y | 772 | VAL | C-N-CA | 6.43 | 128.81 | 120.44 |
| 21 | s | 38 | GLU | CA-C-N | 6.43 | 128.90 | 120.28 |
| 21 | s | 38 | GLU | C-N-CA | 6.43 | 128.90 | 120.28 |
| 14 | a | 924 | ARG | NE-CZ-NH2 | -6.43 | 113.41 | 119.20 |
| 6 | L | 444 | ILE | O-C-N | 6.43 | 130.63 | 121.82 |
| 7 | M | 1188 | THR | CA-CB-OG1 | -6.43 | 99.95 | 109.60 |
| 17 | k | 86 | ASN | CA-CB-CG | 6.43 | 119.03 | 112.60 |
| 20 | n | 146 | MET | CG-SD-CE | -6.43 | 86.75 | 100.90 |
| 7 | O | 1004 | ASP | CA-C-N | 6.43 | 128.80 | 120.44 |
| 7 | O | 1004 | ASP | C-N-CA | 6.43 | 128.80 | 120.44 |
| 1 | Y | 256 | VAL | CG1-CB-CG2 | 6.43 | 124.95 | 110.80 |
| 4 | z | 798 | ASN | CA-C-N | 6.43 | 128.80 | 120.44 |
| 4 | z | 798 | ASN | C-N-CA | 6.43 | 128.80 | 120.44 |
| 20 | n | 1092 | PRO | N-CA-CB | 6.43 | 110.34 | 103.52 |
| 1 | 0 | 263 | VAL | CA-C-N | 6.43 | 126.46 | 119.90 |
| 1 | 0 | 263 | VAL | C-N-CA | 6.43 | 126.46 | 119.90 |
| 6 | C | 327 | LYS | N-CA-CB | 6.43 | 119.57 | 110.12 |
| 7 | O | 493 | PRO | CA-C-N | 6.43 | 129.77 | 120.38 |
| 7 | O | 493 | PRO | C-N-CA | 6.43 | 129.77 | 120.38 |
| 8 | P | 111 | HIS | CG-CD2-NE2 | 6.43 | 113.63 | 107.20 |
| 12 | v | 168 | LYS | N-CA-CB | 6.43 | 120.18 | 110.02 |
| 13 | w | 1221 | VAL | N-CA-CB | -6.43 | 103.03 | 110.55 |
| 4 | y | 748 | ALA | CA-C-N | 6.43 | 129.22 | 120.54 |
| 4 | y | 748 | ALA | C-N-CA | 6.43 | 129.22 | 120.54 |
| 16 | j | 776 | GLN | CA-C-N | 6.43 | 127.39 | 120.83 |
| 16 | j | 776 | GLN | C-N-CA | 6.43 | 127.39 | 120.83 |
| 21 | t | 74 | GLY | N-CA-C | -6.43 | 105.74 | 115.00 |
| 14 | a | 835 | ASN | CA-C-N | 6.43 | 133.82 | 121.54 |
| 14 | a | 835 | ASN | C-N-CA | 6.43 | 133.82 | 121.54 |
| 9 | S | 593 | ILE | N-CA-C | -6.43 | 99.22 | 108.48 |
| 14 | h | 605 | ILE | N-CA-C | 6.43 | 116.59 | 110.42 |
| 6 | F | 315 | LEU | CA-C-N | 6.43 | 129.18 | 120.44 |
| 6 | F | 315 | LEU | C-N-CA | 6.43 | 129.18 | 120.44 |
| 8 | N | 426 | SER | N-CA-C | -6.43 | 103.61 | 112.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 1346 | LYS | N-CA-CB | 6.42 | 120.09 | 110.65 |
| 1 | 0 | 251 | THR | CA-C-N | 6.42 | 131.94 | 122.82 |
| 1 | 0 | 251 | THR | C-N-CA | 6.42 | 131.94 | 122.82 |
| 2 | 1 | 989 | ASN | OD1-CG-ND2 | 6.42 | 129.02 | 122.60 |
| 7 | M | 925 | HIS | CA-C-N | 6.42 | 128.79 | 120.44 |
| 7 | M | 925 | HIS | C-N-CA | 6.42 | 128.79 | 120.44 |
| 9 | T | 743 | ASP | CA-CB-CG | 6.42 | 119.02 | 112.60 |
| 7 | M | 825 | ILE | O-C-N | -6.42 | 116.31 | 120.42 |
| 17 | k | 14 | ASP | CA-C-O | -6.42 | 113.83 | 120.89 |
| 17 | k | 144 | HIS | CE1-NE2-CD2 | -6.42 | 102.58 | 109.00 |
| 14 | a | 204 | TYR | N-CA-C | -6.42 | 104.69 | 113.30 |
| 2 | 1 | 773 | PHE | CA-C-N | 6.42 | 129.17 | 120.63 |
| 2 | 1 | 773 | PHE | C-N-CA | 6.42 | 129.17 | 120.63 |
| 2 | 1 | 225 | ALA | N-CA-CB | 6.42 | 120.63 | 110.55 |
| 7 | M | 35 | LEU | CA-C-N | 6.42 | 133.80 | 121.54 |
| 7 | M | 35 | LEU | C-N-CA | 6.42 | 133.80 | 121.54 |
| 8 | N | 1345 | SER | N-CA-C | -6.42 | 104.64 | 113.18 |
| 7 | O | 647 | THR | O-C-N | -6.42 | 117.36 | 121.85 |
| 9 | R | 39 | LEU | N-CA-CB | 6.42 | 121.37 | 110.71 |
| 4 | y | 725 | VAL | CA-C-O | -6.42 | 114.28 | 120.95 |
| 16 | j | 538 | ILE | CA-C-O | 6.42 | 127.65 | 120.85 |
| 20 | n | 742 | LEU | N-CA-C | -6.42 | 104.71 | 112.54 |
| 7 | M | 193 | LEU | CA-C-N | 6.42 | 128.88 | 120.28 |
| 7 | M | 193 | LEU | C-N-CA | 6.42 | 128.88 | 120.28 |
| 12 | u | 59 | PHE | CA-CB-CG | 6.42 | 120.22 | 113.80 |
| 14 | h | 942 | ILE | CA-C-N | 6.42 | 129.40 | 120.29 |
| 14 | h | 942 | ILE | C-N-CA | 6.42 | 129.40 | 120.29 |
| 20 | n | 159 | ASP | N-CA-CB | 6.42 | 121.33 | 110.49 |
| 2 | 1 | 1173 | LEU | CA-C-N | 6.42 | 130.87 | 120.60 |
| 2 | 1 | 1173 | LEU | C-N-CA | 6.42 | 130.87 | 120.60 |
| 7 | M | 76 | SER | N-CA-C | 6.42 | 118.35 | 111.36 |
| 16 | j | 434 | LEU | CA-C-O | 6.42 | 127.35 | 120.10 |
| 2 | 1 | 874 | ASN | N-CA-C | -6.41 | 104.61 | 112.88 |
| 8 | N | 1509 | GLN | N-CA-C | -6.41 | 102.92 | 113.50 |
| 8 | P | 564 | LEU | CA-C-O | -6.41 | 113.62 | 120.42 |
| 13 | x | 1287 | ASN | CA-C-N | 6.41 | 129.25 | 120.46 |
| 13 | x | 1287 | ASN | C-N-CA | 6.41 | 129.25 | 120.46 |
| 14 | h | 157 | ASP | CA-CB-CG | 6.41 | 119.01 | 112.60 |
| 20 | n | 642 | PHE | CA-CB-CG | -6.41 | 107.39 | 113.80 |
| 7 | O | 523 | ARG | CA-C-N | 6.41 | 129.70 | 120.79 |
| 7 | O | 523 | ARG | C-N-CA | 6.41 | 129.70 | 120.79 |
| 7 | O | 1085 | LYS | N-CA-C | 6.41 | 118.27 | 111.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1378 | ASP | CA-C-N | 6.41 | 127.21 | 120.03 |
| 7 | O | 1378 | ASP | C-N-CA | 6.41 | 127.21 | 120.03 |
| 8 | P | 1197 | VAL | CB-CA-C | -6.41 | 103.37 | 112.22 |
| 14 | a | 668 | TYR | N-CA-C | -6.41 | 105.28 | 113.23 |
| 7 | M | 190 | TYR | CA-CB-CG | 6.41 | 125.44 | 113.90 |
| 7 | M | 259 | PHE | CA-CB-CG | 6.41 | 120.21 | 113.80 |
| 7 | O | 219 | HIS | CE1-NE2-CD2 | -6.41 | 102.59 | 109.00 |
| 8 | P | 942 | PRO | N-CA-CB | 6.41 | 109.98 | 103.25 |
| 9 | T | 128 | LEU | N-CA-C | 6.41 | 118.27 | 111.28 |
| 2 | Z | 856 | ASN | OD1-CG-ND2 | 6.41 | 129.01 | 122.60 |
| 8 | P | 1082 | PHE | CA-C-N | 6.41 | 130.95 | 120.63 |
| 8 | P | 1082 | PHE | C-N-CA | 6.41 | 130.95 | 120.63 |
| 10 | W | 284 | LYS | CA-CB-CG | -6.41 | 101.28 | 114.10 |
| 2 | Z | 1349 | ASP | CA-C-O | -6.41 | 111.50 | 119.38 |
| 1 | 0 | 1440 | ASP | N-CA-C | -6.41 | 97.16 | 110.80 |
| 2 | 1 | 713 | ALA | CA-C-N | 6.41 | 129.38 | 120.29 |
| 2 | 1 | 713 | ALA | C-N-CA | 6.41 | 129.38 | 120.29 |
| 4 | A | 807 | LEU | CA-C-N | 6.41 | 130.04 | 120.31 |
| 4 | A | 807 | LEU | C-N-CA | 6.41 | 130.04 | 120.31 |
| 21 | p | 25 | LEU | CA-C-N | 6.41 | 129.15 | 120.44 |
| 21 | p | 25 | LEU | C-N-CA | 6.41 | 129.15 | 120.44 |
| 14 | a | 591 | MET | CA-C-O | 6.41 | 126.27 | 119.03 |
| 14 | a | 871 | HIS | CE1-NE2-CD2 | -6.41 | 102.59 | 109.00 |
| 9 | S | 829 | TYR | N-CA-C | -6.40 | 104.16 | 112.23 |
| 20 | n | 719 | ASN | CA-C-O | 6.40 | 126.45 | 119.15 |
| 7 | M | 305 | ASP | CA-C-O | 6.40 | 126.18 | 119.14 |
| 8 | N | 599 | THR | N-CA-C | 6.40 | 121.93 | 111.37 |
| 7 | O | 866 | GLN | CA-C-N | 6.40 | 129.69 | 120.79 |
| 7 | O | 866 | GLN | C-N-CA | 6.40 | 129.69 | 120.79 |
| 7 | O | 1385 | PHE | CA-CB-CG | -6.40 | 107.40 | 113.80 |
| 1 | Y | 768 | PRO | N-CA-C | 6.40 | 122.29 | 113.65 |
| 19 | m | 210 | MET | CA-C-N | 6.40 | 128.63 | 120.56 |
| 19 | m | 210 | MET | C-N-CA | 6.40 | 128.63 | 120.56 |
| 19 | f | 329 | ASN | CA-CB-CG | -6.40 | 106.20 | 112.60 |
| 2 | 1 | 1165 | ASP | N-CA-C | 6.40 | 118.05 | 111.14 |
| 9 | Q | 309 | ILE | CA-C-N | 6.40 | 128.76 | 120.44 |
| 9 | Q | 309 | ILE | C-N-CA | 6.40 | 128.76 | 120.44 |
| 2 | Z | 1212 | PRO | N-CA-C | -6.40 | 108.02 | 114.68 |
| 12 | v | 444 | THR | N-CA-CB | 6.40 | 122.32 | 110.99 |
| 13 | x | 1402 | LEU | N-CA-CB | 6.40 | 119.63 | 110.16 |
| 18 | l | 109 | GLY | CA-C-O | -6.40 | 116.89 | 121.88 |
| 20 | n | 556 | HIS | CB-CG-CD2 | -6.40 | 122.88 | 131.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | n | 817 | THR | CA-C-N | 6.40 | 128.76 | 120.44 |
| 20 | n | 817 | THR | C-N-CA | 6.40 | 128.76 | 120.44 |
| 4 | J | 685 | MET | CA-C-N | 6.40 | 128.85 | 120.28 |
| 4 | J | 685 | MET | C-N-CA | 6.40 | 128.85 | 120.28 |
| 1 | Y | 646 | SER | CA-C-O | 6.40 | 127.92 | 120.75 |
| 20 | n | 688 | THR | N-CA-C | 6.40 | 119.51 | 110.23 |
| 1 | 0 | 1113 | ILE | N-CA-CB | 6.40 | 121.78 | 111.23 |
| 5 | B | 311 | PHE | CA-CB-CG | -6.40 | 107.40 | 113.80 |
| 8 | P | 1170 | ASP | N-CA-C | -6.40 | 104.09 | 112.41 |
| 9 | Q | 206 | ASN | CA-C-N | 6.40 | 129.46 | 121.85 |
| 9 | Q | 206 | ASN | C-N-CA | 6.40 | 129.46 | 121.85 |
| 9 | Q | 434 | ASP | CA-C-N | 6.40 | 128.76 | 120.44 |
| 9 | Q | 434 | ASP | C-N-CA | 6.40 | 128.76 | 120.44 |
| 9 | Q | 724 | ARG | CA-C-N | 6.40 | 129.14 | 120.44 |
| 9 | Q | 724 | ARG | C-N-CA | 6.40 | 129.14 | 120.44 |
| 9 | S | 629 | ARG | NE-CZ-NH2 | 6.40 | 124.96 | 119.20 |
| 10 | W | 266 | ILE | CA-C-N | 6.40 | 129.22 | 120.46 |
| 10 | W | 266 | ILE | C-N-CA | 6.40 | 129.22 | 120.46 |
| 20 | n | 386 | PHE | CA-CB-CG | -6.40 | 107.40 | 113.80 |
| 20 | n | 884 | HIS | CE1-NE2-CD2 | -6.40 | 102.60 | 109.00 |
| 20 | g | 135 | ALA | CA-C-N | 6.40 | 127.22 | 120.12 |
| 20 | g | 135 | ALA | C-N-CA | 6.40 | 127.22 | 120.12 |
| 1 | 0 | 1394 | VAL | CA-C-N | 6.40 | 129.18 | 120.54 |
| 1 | 0 | 1394 | VAL | C-N-CA | 6.40 | 129.18 | 120.54 |
| 8 | N | 899 | GLN | N-CA-C | -6.40 | 104.73 | 113.30 |
| 12 | u | 559 | GLU | CA-C-N | 6.40 | 128.75 | 120.44 |
| 12 | u | 559 | GLU | C-N-CA | 6.40 | 128.75 | 120.44 |
| 13 | x | 1141 | PRO | N-CA-CB | 6.40 | 110.04 | 103.00 |
| 17 | d | 54 | GLY | CA-C-N | 6.40 | 127.83 | 119.84 |
| 17 | d | 54 | GLY | C-N-CA | 6.40 | 127.83 | 119.84 |
| 7 | M | 516 | ARG | N-CA-C | -6.39 | 98.84 | 109.46 |
| 7 | M | 541 | LEU | CA-C-N | 6.39 | 130.41 | 120.82 |
| 7 | M | 541 | LEU | C-N-CA | 6.39 | 130.41 | 120.82 |
| 7 | M | 1385 | PHE | CA-C-N | 6.39 | 129.14 | 120.38 |
| 7 | M | 1385 | PHE | C-N-CA | 6.39 | 129.14 | 120.38 |
| 16 | j | 401 | SER | N-CA-CB | 6.39 | 120.19 | 110.28 |
| 15 | b | 289 | ILE | CA-C-N | 6.39 | 131.40 | 120.72 |
| 15 | b | 289 | ILE | C-N-CA | 6.39 | 131.40 | 120.72 |
| 7 | O | 502 | ASP | CA-CB-CG | -6.39 | 106.21 | 112.60 |
| 8 | P | 693 | MET | N-CA-C | -6.39 | 102.77 | 110.44 |
| 14 | h | 975 | ARG | CA-C-N | 6.39 | 133.75 | 121.54 |
| 14 | h | 975 | ARG | C-N-CA | 6.39 | 133.75 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 18 | l | 30 | ASP | N-CA-C | -6.39 | 105.06 | 112.92 |
| 9 | R | 163 | ILE | CB-CA-C | -6.39 | 103.51 | 112.14 |
| 12 | v | 424 | PRO | CB-CA-C | -6.39 | 103.83 | 112.97 |
| 12 | v | 636 | ASN | CA-C-O | 6.39 | 127.32 | 119.97 |
| 2 | 1 | 155 | SER | CB-CA-C | -6.39 | 98.81 | 110.63 |
| 6 | C | 273 | ILE | CA-C-N | 6.39 | 128.84 | 120.28 |
| 6 | C | 273 | ILE | C-N-CA | 6.39 | 128.84 | 120.28 |
| 8 | N | 69 | ASN | OD1-CG-ND2 | -6.39 | 116.21 | 122.60 |
| 7 | O | 631 | LEU | CA-C-N | 6.39 | 128.84 | 120.28 |
| 7 | O | 631 | LEU | C-N-CA | 6.39 | 128.84 | 120.28 |
| 8 | P | 1470 | LEU | N-CA-C | 6.39 | 120.33 | 112.54 |
| 14 | h | 263 | SER | N-CA-C | -6.39 | 99.33 | 109.23 |
| 14 | h | 988 | GLN | N-CA-C | 6.39 | 118.24 | 111.28 |
| 20 | g | 959 | ASN | CA-CB-CG | 6.39 | 118.99 | 112.60 |
| 2 | Z | 792 | SER | N-CA-C | 6.39 | 117.91 | 111.07 |
| 18 | l | 175 | PRO | N-CA-CB | 6.39 | 108.88 | 102.17 |
| 2 | 1 | 765 | PHE | CA-CB-CG | 6.39 | 120.19 | 113.80 |
| 7 | O | 488 | PHE | CA-CB-CG | 6.39 | 120.19 | 113.80 |
| 9 | S | 147 | ASP | CA-C-N | 6.39 | 130.82 | 120.60 |
| 9 | S | 147 | ASP | C-N-CA | 6.39 | 130.82 | 120.60 |
| 9 | T | 462 | PHE | N-CA-C | -6.39 | 102.84 | 112.04 |
| 8 | N | 1489 | PRO | CA-C-N | 6.38 | 129.08 | 120.65 |
| 8 | N | 1489 | PRO | C-N-CA | 6.38 | 129.08 | 120.65 |
| 9 | Q | 415 | ILE | O-C-N | 6.38 | 128.49 | 122.23 |
| 9 | Q | 695 | ILE | N-CA-C | -6.38 | 107.64 | 113.71 |
| 11 | V | 347 | TYR | CA-C-N | 6.38 | 127.82 | 119.84 |
| 11 | V | 347 | TYR | C-N-CA | 6.38 | 127.82 | 119.84 |
| 21 | t | 30 | ASP | CA-C-N | 6.38 | 128.84 | 120.28 |
| 21 | t | 30 | ASP | C-N-CA | 6.38 | 128.84 | 120.28 |
| 4 | D | 752 | ASP | CA-CB-CG | 6.38 | 118.98 | 112.60 |
| 5 | H | 385 | GLN | N-CA-C | -6.38 | 104.54 | 112.90 |
| 20 | g | 531 | LEU | CA-C-N | 6.38 | 128.83 | 120.28 |
| 20 | g | 531 | LEU | C-N-CA | 6.38 | 128.83 | 120.28 |
| 7 | M | 443 | ILE | CA-C-O | -6.38 | 114.31 | 120.95 |
| 7 | M | 1272 | LEU | N-CA-CB | -6.38 | 99.65 | 110.50 |
| 9 | T | 254 | LEU | CA-C-N | 6.38 | 128.83 | 120.28 |
| 9 | T | 254 | LEU | C-N-CA | 6.38 | 128.83 | 120.28 |
| 9 | T | 358 | ALA | CA-C-O | 6.38 | 125.48 | 118.65 |
| 4 | z | 650 | GLU | CA-C-N | 6.38 | 128.83 | 120.28 |
| 4 | z | 650 | GLU | C-N-CA | 6.38 | 128.83 | 120.28 |
| 17 | d | 101 | SER | N-CA-C | 6.38 | 119.73 | 110.28 |
| 17 | d | 144 | HIS | CE1-NE2-CD2 | -6.38 | 102.62 | 109.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 874 | PHE | N-CA-CB | 6.38 | 119.50 | 110.12 |
| 14 | a | 136 | SER | CA-C-N | 6.38 | 128.83 | 120.28 |
| 14 | a | 136 | SER | C-N-CA | 6.38 | 128.83 | 120.28 |
| 11 | V | 353 | GLU | N-CA-C | -6.38 | 102.76 | 111.56 |
| 4 | D | 657 | GLN | CB-CG-CD | -6.38 | 101.76 | 112.60 |
| 7 | M | 1302 | VAL | N-CA-C | 6.38 | 116.54 | 110.42 |
| 7 | M | 1501 | SER | CB-CA-C | -6.38 | 96.43 | 109.38 |
| 8 | N | 575 | SER | N-CA-C | 6.38 | 118.31 | 111.36 |
| 8 | N | 979 | ASN | CA-C-N | 6.38 | 131.98 | 122.99 |
| 8 | N | 979 | ASN | C-N-CA | 6.38 | 131.98 | 122.99 |
| 7 | O | 1293 | ASN | N-CA-CB | 6.38 | 119.60 | 110.16 |
| 8 | P | 447 | LEU | CA-C-N | 6.38 | 133.45 | 121.97 |
| 8 | P | 447 | LEU | C-N-CA | 6.38 | 133.45 | 121.97 |
| 9 | Q | 535 | ALA | CA-C-N | 6.38 | 128.73 | 120.44 |
| 9 | Q | 535 | ALA | C-N-CA | 6.38 | 128.73 | 120.44 |
| 1 | Y | 122 | ASP | CA-CB-CG | -6.38 | 106.22 | 112.60 |
| 20 | g | 513 | ASP | CA-CB-CG | 6.38 | 118.98 | 112.60 |
| 2 | 1 | 237 | PHE | CA-C-O | 6.38 | 127.47 | 120.71 |
| 7 | M | 484 | SER | CA-CB-OG | 6.38 | 123.85 | 111.10 |
| 7 | O | 683 | SER | N-CA-C | -6.38 | 98.60 | 108.42 |
| 2 | Z | 208 | LYS | CA-C-N | 6.38 | 126.33 | 119.76 |
| 2 | Z | 208 | LYS | C-N-CA | 6.38 | 126.33 | 119.76 |
| 20 | n | 618 | LEU | N-CA-C | -6.38 | 104.20 | 112.68 |
| 15 | b | 609 | GLN | N-CA-C | -6.38 | 97.97 | 108.49 |
| 17 | d | 255 | ASP | N-CA-C | -6.38 | 99.03 | 108.79 |
| 14 | a | 673 | CYS | CA-C-O | 6.38 | 127.31 | 120.10 |
| 2 | 1 | 753 | GLU | CA-C-O | -6.38 | 112.64 | 119.97 |
| 8 | N | 1046 | LYS | N-CA-C | -6.38 | 106.14 | 114.04 |
| 2 | Z | 125 | PHE | N-CA-C | 6.38 | 119.97 | 111.30 |
| 17 | d | 48 | THR | CA-C-N | 6.38 | 130.90 | 122.42 |
| 17 | d | 48 | THR | C-N-CA | 6.38 | 130.90 | 122.42 |
| 14 | a | 1032 | ASP | N-CA-C | -6.38 | 105.26 | 114.12 |
| 1 | 0 | 783 | ASP | CA-CB-CG | 6.37 | 118.97 | 112.60 |
| 1 | 0 | 986 | THR | CA-CB-CG2 | 6.37 | 121.34 | 110.50 |
| 10 | W | 322 | LEU | N-CA-C | -6.37 | 104.81 | 112.59 |
| 12 | v | 352 | GLU | CB-CA-C | -6.37 | 99.73 | 109.99 |
| 14 | h | 1024 | VAL | N-CA-C | 6.37 | 116.52 | 110.53 |
| 20 | n | 623 | LEU | N-CA-C | -6.37 | 105.66 | 113.50 |
| 15 | b | 645 | ALA | CB-CA-C | -6.37 | 99.67 | 109.29 |
| 2 | 1 | 405 | LYS | CA-C-N | 6.37 | 130.74 | 121.18 |
| 2 | 1 | 405 | LYS | C-N-CA | 6.37 | 130.74 | 121.18 |
| 7 | M | 31 | ASP | CA-C-O | 6.37 | 127.17 | 120.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 485 | THR | N-CA-C | -6.37 | 105.44 | 113.72 |
| 14 | h | 385 | SER | CA-C-N | 6.37 | 128.82 | 120.28 |
| 14 | h | 385 | SER | C-N-CA | 6.37 | 128.82 | 120.28 |
| 15 | b | 223 | TYR | N-CA-C | -6.37 | 104.82 | 112.59 |
| 15 | b | 254 | LEU | N-CA-C | -6.37 | 104.76 | 113.30 |
| 20 | g | 305 | THR | CA-C-N | 6.37 | 129.88 | 120.90 |
| 20 | g | 305 | THR | C-N-CA | 6.37 | 129.88 | 120.90 |
| 5 | E | 522 | TYR | CA-C-N | 6.37 | 128.81 | 120.28 |
| 5 | E | 522 | TYR | C-N-CA | 6.37 | 128.81 | 120.28 |
| 14 | h | 556 | ASN | CA-C-N | 6.37 | 128.81 | 120.28 |
| 14 | h | 556 | ASN | C-N-CA | 6.37 | 128.81 | 120.28 |
| 20 | n | 225 | MET | N-CA-C | -6.37 | 104.29 | 113.21 |
| 21 | s | 56 | THR | CA-CB-CG2 | -6.37 | 99.67 | 110.50 |
| 2 | 1 | 875 | ILE | N-CA-C | -6.37 | 106.92 | 113.10 |
| 6 | F | 301 | HIS | CE1-NE2-CD2 | -6.37 | 102.63 | 109.00 |
| 5 | H | 391 | GLU | N-CA-C | 6.37 | 119.03 | 111.71 |
| 5 | K | 507 | ASN | OD1-CG-ND2 | 6.37 | 128.97 | 122.60 |
| 7 | M | 345 | ARG | N-CA-CB | -6.37 | 101.36 | 110.79 |
| 12 | v | 320 | ASP | CA-C-N | 6.37 | 129.99 | 120.31 |
| 12 | v | 320 | ASP | C-N-CA | 6.37 | 129.99 | 120.31 |
| 14 | a | 889 | LEU | N-CA-C | -6.37 | 104.77 | 113.30 |
| 7 | O | 1430 | LEU | CA-C-O | 6.37 | 127.05 | 119.60 |
| 9 | S | 679 | ASP | CA-CB-CG | -6.37 | 106.23 | 112.60 |
| 7 | M | 162 | ILE | N-CA-CB | 6.37 | 118.00 | 110.55 |
| 7 | O | 284 | TYR | CA-C-N | 6.37 | 129.45 | 120.28 |
| 7 | O | 284 | TYR | C-N-CA | 6.37 | 129.45 | 120.28 |
| 8 | P | 1160 | ILE | N-CA-CB | 6.37 | 115.42 | 110.45 |
| 14 | a | 494 | PHE | N-CA-C | -6.37 | 104.71 | 113.18 |
| 1 | 0 | 949 | PHE | CA-CB-CG | 6.36 | 120.16 | 113.80 |
| 4 | A | 658 | TYR | O-C-N | -6.36 | 114.44 | 122.27 |
| 4 | G | 678 | GLN | CB-CG-CD | 6.36 | 123.42 | 112.60 |
| 9 | T | 150 | GLN | N-CA-C | -6.36 | 105.27 | 114.12 |
| 14 | h | 193 | HIS | CE1-NE2-CD2 | -6.36 | 102.64 | 109.00 |
| 15 | i | 246 | TRP | CD2-CE2-CZ2 | -6.36 | 116.04 | 122.40 |
| 21 | t | 59 | VAL | CA-CB-CG2 | -6.36 | 99.58 | 110.40 |
| 16 | c | 318 | LEU | N-CA-C | -6.36 | 104.77 | 113.30 |
| 7 | M | 158 | ILE | CA-C-N | 6.36 | 128.71 | 120.44 |
| 7 | M | 158 | ILE | C-N-CA | 6.36 | 128.71 | 120.44 |
| 9 | S | 548 | SER | CA-C-N | 6.36 | 129.26 | 122.26 |
| 9 | S | 548 | SER | C-N-CA | 6.36 | 129.26 | 122.26 |
| 9 | S | 662 | SER | N-CA-CB | 6.36 | 119.47 | 110.12 |
| 2 | Z | 642 | SER | N-CA-C | 6.36 | 118.22 | 111.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | G | 725 | VAL | CA-C-N | 6.36 | 133.42 | 121.97 |
| 4 | G | 725 | VAL | C-N-CA | 6.36 | 133.42 | 121.97 |
| 8 | P | 975 | GLN | CA-C-N | 6.36 | 130.15 | 121.05 |
| 8 | P | 975 | GLN | C-N-CA | 6.36 | 130.15 | 121.05 |
| 9 | T | 638 | TYR | N-CA-C | -6.36 | 103.97 | 111.03 |
| 9 | T | 821 | GLN | CB-CA-C | 6.36 | 121.69 | 110.37 |
| 20 | n | 540 | HIS | CB-CG-CD2 | -6.36 | 122.93 | 131.20 |
| 20 | n | 1001 | ASP | CA-C-N | 6.36 | 129.32 | 120.29 |
| 20 | n | 1001 | ASP | C-N-CA | 6.36 | 129.32 | 120.29 |
| 21 | t | 22 | GLU | O-C-N | -6.36 | 115.38 | 122.12 |
| 16 | c | 477 | PHE | CA-CB-CG | -6.36 | 107.44 | 113.80 |
| 20 | g | 137 | ARG | N-CA-C | -6.36 | 105.56 | 113.38 |
| 4 | J | 769 | ILE | N-CA-C | 6.36 | 117.11 | 110.62 |
| 8 | P | 1465 | LEU | CA-C-O | -6.36 | 112.07 | 119.64 |
| 9 | T | 744 | LEU | N-CA-C | -6.36 | 103.97 | 112.94 |
| 12 | u | 233 | MET | CA-CB-CG | -6.36 | 101.38 | 114.10 |
| 1 | 0 | 1157 | PHE | N-CA-C | -6.36 | 105.17 | 114.39 |
| 2 | 1 | 565 | ASP | O-C-N | -6.36 | 115.73 | 123.30 |
| 6 | F | 292 | HIS | CG-CD2-NE2 | 6.36 | 113.56 | 107.20 |
| 5 | H | 289 | GLN | CA-C-N | 6.36 | 129.86 | 120.90 |
| 5 | H | 289 | GLN | C-N-CA | 6.36 | 129.86 | 120.90 |
| 8 | N | 1258 | SER | CA-C-N | 6.36 | 128.80 | 120.28 |
| 8 | N | 1258 | SER | C-N-CA | 6.36 | 128.80 | 120.28 |
| 1 | Y | 1010 | LEU | N-CA-CB | 6.36 | 122.83 | 110.88 |
| 7 | M | 1116 | VAL | CA-C-O | -6.36 | 113.72 | 120.39 |
| 21 | o | 66 | GLY | N-CA-C | -6.36 | 99.40 | 110.71 |
| 20 | n | 91 | ASP | N-CA-C | -6.35 | 98.26 | 109.06 |
| 20 | n | 1093 | GLU | N-CA-C | 6.35 | 120.29 | 112.54 |
| 20 | g | 754 | ASN | O-C-N | 6.35 | 131.29 | 121.63 |
| 8 | N | 134 | ARG | N-CA-C | -6.35 | 103.86 | 113.89 |
| 16 | j | 423 | GLN | OE1-CD-NE2 | -6.35 | 116.25 | 122.60 |
| 21 | t | 58 | HIS | CA-CB-CG | -6.35 | 107.45 | 113.80 |
| 2 | 1 | 355 | HIS | CE1-NE2-CD2 | -6.35 | 102.65 | 109.00 |
| 6 | C | 308 | ILE | CA-C-O | -6.35 | 111.44 | 119.95 |
| 7 | O | 1530 | GLU | N-CA-C | 6.35 | 117.86 | 111.07 |
| 8 | P | 675 | TYR | CA-C-O | -6.35 | 113.75 | 120.55 |
| 8 | P | 1615 | ARG | NE-CZ-NH2 | -6.35 | 113.48 | 119.20 |
| 19 | f | 189 | LEU | N-CA-CB | 6.35 | 119.45 | 110.12 |
| 2 | 1 | 1095 | SER | CA-C-N | 6.35 | 129.26 | 120.63 |
| 2 | 1 | 1095 | SER | C-N-CA | 6.35 | 129.26 | 120.63 |
| 7 | M | 1442 | TRP | CB-CG-CD1 | -6.35 | 117.38 | 126.90 |
| 7 | O | 152 | HIS | CA-CB-CG | 6.35 | 120.15 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 941 | SER | CA-C-N | 6.35 | 129.08 | 120.38 |
| 7 | O | 941 | SER | C-N-CA | 6.35 | 129.08 | 120.38 |
| 1 | Y | 1088 | PHE | N-CA-C | -6.35 | 99.30 | 109.96 |
| 12 | v | 662 | LEU | CA-C-N | 6.35 | 128.69 | 120.44 |
| 12 | v | 662 | LEU | C-N-CA | 6.35 | 128.69 | 120.44 |
| 14 | a | 578 | ASP | CA-CB-CG | 6.35 | 118.95 | 112.60 |
| 14 | a | 606 | LYS | N-CA-CB | 6.35 | 121.22 | 110.49 |
| 8 | N | 782 | VAL | N-CA-CB | 6.35 | 119.90 | 112.35 |
| 8 | P | 1554 | LEU | CA-C-N | 6.35 | 128.56 | 120.56 |
| 8 | P | 1554 | LEU | C-N-CA | 6.35 | 128.56 | 120.56 |
| 13 | x | 1432 | LYS | N-CA-C | 6.35 | 117.86 | 111.07 |
| 16 | j | 220 | ALA | N-CA-C | -6.35 | 104.09 | 113.61 |
| 20 | n | 411 | ASN | CA-CB-CG | -6.35 | 106.25 | 112.60 |
| 14 | a | 295 | ASN | CA-CB-CG | 6.35 | 118.95 | 112.60 |
| 1 | 0 | 712 | ASP | N-CA-CB | 6.34 | 119.37 | 110.04 |
| 1 | 0 | 1483 | PRO | N-CA-C | -6.34 | 105.93 | 113.86 |
| 7 | M | 170 | ASN | N-CA-C | -6.34 | 105.17 | 113.17 |
| 9 | R | 686 | VAL | CA-C-N | 6.34 | 128.78 | 120.28 |
| 9 | R | 686 | VAL | C-N-CA | 6.34 | 128.78 | 120.28 |
| 14 | h | 143 | ASN | N-CA-C | -6.34 | 99.86 | 109.95 |
| 15 | i | 158 | PHE | CA-CB-CG | 6.34 | 120.14 | 113.80 |
| 15 | b | 103 | GLU | CA-C-N | 6.34 | 128.69 | 120.44 |
| 15 | b | 103 | GLU | C-N-CA | 6.34 | 128.69 | 120.44 |
| 20 | g | 257 | TRP | N-CA-C | -6.34 | 99.96 | 110.17 |
| 14 | a | 422 | ARG | O-C-N | 6.34 | 130.49 | 121.92 |
| 12 | v | 288 | ASN | N-CA-CB | 6.34 | 121.66 | 110.37 |
| 9 | Q | 407 | TYR | CB-CG-CD1 | -6.34 | 111.29 | 120.80 |
| 9 | S | 507 | ALA | CA-C-N | 6.34 | 128.55 | 120.56 |
| 9 | S | 507 | ALA | C-N-CA | 6.34 | 128.55 | 120.56 |
| 13 | w | 1398 | GLU | CA-C-N | 6.34 | 128.55 | 120.56 |
| 13 | w | 1398 | GLU | C-N-CA | 6.34 | 128.55 | 120.56 |
| 20 | g | 102 | HIS | CA-CB-CG | -6.34 | 107.46 | 113.80 |
| 20 | g | 1006 | TYR | CA-C-N | 6.34 | 133.65 | 121.54 |
| 20 | g | 1006 | TYR | C-N-CA | 6.34 | 133.65 | 121.54 |
| 14 | a | 501 | THR | CA-CB-CG2 | -6.34 | 99.72 | 110.50 |
| 4 | G | 676 | ILE | CA-C-N | 6.34 | 131.42 | 120.58 |
| 4 | G | 676 | ILE | C-N-CA | 6.34 | 131.42 | 120.58 |
| 4 | G | 685 | MET | CA-C-N | 6.34 | 129.29 | 120.29 |
| 4 | G | 685 | MET | C-N-CA | 6.34 | 129.29 | 120.29 |
| 7 | M | 108 | LEU | N-CA-CB | 6.34 | 119.44 | 110.12 |
| 7 | O | 1363 | ILE | N-CA-C | -6.34 | 106.00 | 113.42 |
| 19 | m | 49 | LEU | CA-C-O | -6.34 | 113.83 | 120.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 309 | ASP | CA-CB-CG | 6.34 | 118.94 | 112.60 |
| 7 | M | 664 | LEU | N-CA-C | -6.34 | 99.41 | 109.23 |
| 7 | M | 1339 | ILE | N-CA-C | -6.34 | 104.86 | 111.58 |
| 7 | O | 122 | ASN | OD1-CG-ND2 | -6.34 | 116.26 | 122.60 |
| 9 | S | 692 | MET | CA-C-N | 6.34 | 130.00 | 119.35 |
| 9 | S | 692 | MET | C-N-CA | 6.34 | 130.00 | 119.35 |
| 18 | l | 200 | GLY | N-CA-C | 6.34 | 123.67 | 114.10 |
| 6 | C | 285 | GLN | N-CA-C | 6.34 | 118.27 | 111.36 |
| 6 | C | 441 | SER | CA-C-O | 6.34 | 127.07 | 119.59 |
| 14 | h | 688 | PHE | CA-C-N | 6.34 | 133.83 | 121.41 |
| 14 | h | 688 | PHE | C-N-CA | 6.34 | 133.83 | 121.41 |
| 14 | a | 426 | ILE | N-CA-CB | -6.34 | 103.80 | 111.21 |
| 1 | 0 | 1302 | LEU | N-CA-C | -6.33 | 99.44 | 109.07 |
| 9 | Q | 293 | ASN | CA-CB-CG | -6.33 | 106.27 | 112.60 |
| 9 | T | 315 | LYS | CA-C-N | 6.33 | 133.64 | 121.54 |
| 9 | T | 315 | LYS | C-N-CA | 6.33 | 133.64 | 121.54 |
| 1 | 0 | 890 | SER | N-CA-CB | 6.33 | 119.16 | 109.91 |
| 7 | O | 259 | PHE | CA-C-N | 6.33 | 128.67 | 120.44 |
| 7 | O | 259 | PHE | C-N-CA | 6.33 | 128.67 | 120.44 |
| 7 | O | 1409 | ALA | CA-C-N | 6.33 | 128.67 | 120.44 |
| 7 | O | 1409 | ALA | C-N-CA | 6.33 | 128.67 | 120.44 |
| 1 | Y | 944 | LEU | N-CA-C | -6.33 | 105.86 | 113.97 |
| 4 | D | 748 | ALA | CA-C-O | -6.33 | 113.71 | 120.42 |
| 5 | H | 530 | ASP | N-CA-CB | 6.33 | 119.53 | 110.16 |
| 9 | R | 143 | ASN | CA-C-N | 6.33 | 128.67 | 120.44 |
| 9 | R | 143 | ASN | C-N-CA | 6.33 | 128.67 | 120.44 |
| 9 | T | 542 | THR | CA-CB-CG2 | 6.33 | 121.27 | 110.50 |
| 17 | k | 64 | PRO | CA-C-O | -6.33 | 114.12 | 121.34 |
| 21 | t | 25 | LEU | N-CA-C | 6.33 | 118.18 | 111.28 |
| 15 | b | 264 | CYS | N-CA-C | -6.33 | 104.38 | 111.28 |
| 15 | b | 515 | THR | N-CA-C | -6.33 | 97.31 | 110.80 |
| 20 | g | 977 | ASN | N-CA-CB | 6.33 | 122.71 | 111.69 |
| 1 | 0 | 1242 | PHE | CA-CB-CG | -6.33 | 107.47 | 113.80 |
| 20 | n | 356 | CYS | N-CA-C | -6.33 | 97.32 | 110.80 |
| 7 | M | 3 | TRP | N-CA-CB | 6.33 | 121.18 | 110.49 |
| 7 | M | 1240 | HIS | CB-CG-CD2 | -6.33 | 122.97 | 131.20 |
| 8 | N | 440 | ILE | O-C-N | -6.33 | 113.89 | 121.10 |
| 8 | N | 1593 | HIS | ND1-CE1-NE2 | 6.33 | 114.73 | 108.40 |
| 8 | P | 365 | LEU | CA-C-N | 6.33 | 128.76 | 120.28 |
| 8 | P | 365 | LEU | C-N-CA | 6.33 | 128.76 | 120.28 |
| 9 | Q | 565 | GLY | CA-C-N | 6.33 | 127.75 | 119.84 |
| 9 | Q | 565 | GLY | C-N-CA | 6.33 | 127.75 | 119.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | f | 30 | GLN | N-CA-C | -6.33 | 105.43 | 113.02 |
| 14 | a | 1010 | PHE | CA-CB-CG | -6.33 | 107.47 | 113.80 |
| 2 | 1 | 1299 | LYS | N-CA-CB | 6.33 | 120.60 | 110.16 |
| 9 | S | 437 | TRP | CB-CG-CD1 | -6.33 | 117.41 | 126.90 |
| 10 | W | 311 | ASP | N-CA-C | -6.33 | 104.31 | 111.14 |
| 14 | h | 567 | LEU | CA-C-O | -6.33 | 114.11 | 121.07 |
| 15 | i | 601 | ALA | N-CA-C | -6.33 | 103.06 | 113.50 |
| 20 | n | 100 | ASN | CA-C-O | 6.33 | 128.45 | 121.56 |
| 5 | K | 530 | ASP | O-C-N | -6.32 | 115.26 | 122.09 |
| 7 | M | 921 | PRO | N-CD-CG | 6.32 | 112.69 | 103.20 |
| 7 | M | 1571 | GLN | O-C-N | -6.32 | 115.40 | 122.86 |
| 9 | Q | 442 | LEU | CA-C-N | 6.32 | 133.35 | 121.97 |
| 9 | Q | 442 | LEU | C-N-CA | 6.32 | 133.35 | 121.97 |
| 1 | Y | 374 | LYS | CG-CD-CE | 6.32 | 125.84 | 111.30 |
| 1 | Y | 530 | ILE | N-CA-CB | 6.32 | 118.61 | 111.21 |
| 12 | u | 687 | LEU | N-CA-CB | 6.32 | 119.18 | 110.01 |
| 14 | a | 650 | HIS | CA-C-N | 6.32 | 128.65 | 120.56 |
| 14 | a | 650 | HIS | C-N-CA | 6.32 | 128.65 | 120.56 |
| 2 | 1 | 1217 | GLU | CA-C-O | 6.32 | 127.12 | 120.42 |
| 5 | E | 393 | ASP | N-CA-CB | 6.32 | 121.17 | 110.49 |
| 1 | 0 | 1287 | SER | N-CA-C | 6.32 | 119.84 | 111.75 |
| 6 | L | 301 | HIS | CG-CD2-NE2 | 6.32 | 113.52 | 107.20 |
| 7 | M | 1661 | GLN | CA-C-O | 6.32 | 126.67 | 119.27 |
| 8 | N | 705 | TYR | CA-CB-CG | 6.32 | 125.28 | 113.90 |
| 8 | P | 1255 | ILE | CA-CB-CG1 | 6.32 | 121.14 | 110.40 |
| 9 | T | 44 | VAL | N-CA-CB | 6.32 | 121.66 | 111.23 |
| 15 | i | 510 | HIS | CE1-NE2-CD2 | -6.32 | 102.68 | 109.00 |
| 19 | f | 454 | ASP | CA-CB-CG | 6.32 | 118.92 | 112.60 |
| 7 | O | 884 | GLU | N-CA-C | 6.32 | 118.25 | 111.36 |
| 16 | j | 507 | ILE | CA-C-N | 6.32 | 128.66 | 120.44 |
| 16 | j | 507 | ILE | C-N-CA | 6.32 | 128.66 | 120.44 |
| 8 | N | 475 | TYR | N-CA-CB | 6.32 | 119.36 | 109.69 |
| 9 | S | 229 | ASN | CA-CB-CG | 6.32 | 118.92 | 112.60 |
| 9 | S | 231 | ASN | CA-CB-CG | 6.32 | 118.92 | 112.60 |
| 11 | X | 290 | HIS | CE1-NE2-CD2 | -6.32 | 102.68 | 109.00 |
| 14 | h | 559 | GLU | N-CA-CB | 6.32 | 121.17 | 110.49 |
| 19 | m | 224 | ASP | N-CA-C | -6.32 | 97.51 | 108.69 |
| 14 | a | 383 | ASN | CA-C-O | 6.32 | 127.04 | 119.59 |
| 5 | H | 412 | ILE | N-CA-CB | 6.32 | 117.94 | 110.55 |
| 7 | M | 1366 | ARG | NE-CZ-NH2 | 6.32 | 124.88 | 119.20 |
| 9 | S | 743 | ASP | N-CA-C | 6.32 | 120.11 | 111.39 |
| 20 | n | 748 | ILE | CA-CB-CG1 | 6.32 | 121.14 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | n | 1148 | ILE | N-CA-CB | 6.32 | 119.98 | 110.13 |
| 19 | f | 652 | LEU | N-CA-C | -6.32 | 105.47 | 113.43 |
| 20 | g | 303 | HIS | CA-CB-CG | 6.31 | 120.11 | 113.80 |
| 20 | g | 857 | LEU | N-CA-C | -6.31 | 106.54 | 114.56 |
| 2 | 1 | 538 | LEU | O-C-N | -6.31 | 115.95 | 123.27 |
| 8 | N | 182 | PHE | CA-CB-CG | -6.31 | 107.49 | 113.80 |
| 8 | P | 191 | ILE | CA-C-O | -6.31 | 114.38 | 120.95 |
| 8 | P | 904 | LEU | CA-C-O | -6.31 | 113.86 | 120.55 |
| 2 | Z | 437 | SER | CA-C-N | 6.31 | 128.96 | 120.50 |
| 2 | Z | 437 | SER | C-N-CA | 6.31 | 128.96 | 120.50 |
| 19 | m | 376 | SER | N-CA-C | -6.31 | 98.33 | 109.06 |
| 20 | g | 640 | ASP | N-CA-C | -6.31 | 97.35 | 110.80 |
| 7 | M | 1345 | PHE | CA-CB-CG | -6.31 | 107.49 | 113.80 |
| 7 | O | 198 | TYR | N-CA-CB | 6.31 | 120.69 | 110.40 |
| 18 | e | 71 | ILE | N-CA-C | -6.31 | 99.39 | 108.48 |
| 7 | M | 889 | ILE | O-C-N | 6.31 | 127.99 | 121.87 |
| 8 | P | 1074 | LEU | N-CA-CB | 6.31 | 119.41 | 109.82 |
| 9 | S | 767 | ILE | CA-C-N | 6.31 | 128.51 | 120.56 |
| 9 | S | 767 | ILE | C-N-CA | 6.31 | 128.51 | 120.56 |
| 9 | T | 475 | SER | N-CA-C | -6.31 | 98.33 | 108.55 |
| 9 | T | 626 | GLN | N-CA-C | 6.31 | 118.16 | 111.28 |
| 12 | u | 386 | PHE | N-CA-C | -6.31 | 104.14 | 113.61 |
| 15 | i | 403 | HIS | CE1-NE2-CD2 | -6.31 | 102.69 | 109.00 |
| 17 | k | 41 | GLU | N-CA-C | -6.31 | 105.55 | 113.18 |
| 7 | M | 976 | ALA | CA-C-N | 6.31 | 128.73 | 120.28 |
| 7 | M | 976 | ALA | C-N-CA | 6.31 | 128.73 | 120.28 |
| 8 | N | 697 | SER | N-CA-CB | 6.31 | 121.01 | 110.92 |
| 12 | u | 95 | TRP | N-CA-C | -6.31 | 104.74 | 112.88 |
| 12 | u | 270 | VAL | CA-C-N | 6.31 | 131.08 | 122.19 |
| 12 | u | 270 | VAL | C-N-CA | 6.31 | 131.08 | 122.19 |
| 14 | h | 1013 | ALA | N-CA-CB | 6.31 | 121.15 | 110.49 |
| 15 | b | 142 | ALA | O-C-N | 6.31 | 125.50 | 120.83 |
| 14 | a | 74 | SER | N-CA-C | -6.31 | 105.07 | 112.89 |
| 14 | a | 751 | ARG | NE-CZ-NH1 | 6.31 | 127.81 | 121.50 |
| 7 | M | 877 | ASP | CA-CB-CG | -6.31 | 106.29 | 112.60 |
| 7 | O | 489 | TYR | CA-CB-CG | -6.31 | 102.55 | 113.90 |
| 12 | u | 711 | LYS | CA-C-N | 6.31 | 131.25 | 120.72 |
| 12 | u | 711 | LYS | C-N-CA | 6.31 | 131.25 | 120.72 |
| 4 | y | 685 | MET | N-CA-C | -6.31 | 104.41 | 111.28 |
| 15 | b | 249 | LEU | N-CA-C | -6.31 | 104.29 | 112.68 |
| 8 | N | 218 | ASN | N-CA-C | -6.30 | 103.93 | 113.89 |
| 8 | N | 1599 | SER | CA-C-N | 6.30 | 128.73 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 1599 | SER | C-N-CA | 6.30 | 128.73 | 120.28 |
| 2 | Z | 1172 | ASP | CA-C-N | 6.30 | 128.63 | 120.44 |
| 2 | Z | 1172 | ASP | C-N-CA | 6.30 | 128.63 | 120.44 |
| 14 | h | 663 | LEU | CA-C-N | 6.30 | 129.24 | 120.29 |
| 14 | h | 663 | LEU | C-N-CA | 6.30 | 129.24 | 120.29 |
| 20 | n | 479 | VAL | N-CA-C | -6.30 | 99.04 | 108.12 |
| 7 | O | 1453 | ARG | CA-C-O | -6.30 | 114.21 | 120.70 |
| 10 | U | 358 | LYS | N-CA-C | -6.30 | 100.61 | 109.69 |
| 20 | n | 987 | LEU | CA-C-N | 6.30 | 128.50 | 120.56 |
| 20 | n | 987 | LEU | C-N-CA | 6.30 | 128.50 | 120.56 |
| 20 | g | 639 | PRO | N-CD-CG | 6.30 | 112.66 | 103.20 |
| 4 | A | 758 | LEU | N-CA-C | 6.30 | 120.69 | 113.19 |
| 7 | M | 1334 | THR | CA-C-N | 6.30 | 128.50 | 120.56 |
| 7 | M | 1334 | THR | C-N-CA | 6.30 | 128.50 | 120.56 |
| 1 | Y | 128 | ASN | N-CA-C | -6.30 | 103.63 | 113.02 |
| 1 | Y | 1289 | ILE | CA-C-O | 6.30 | 125.25 | 119.20 |
| 2 | Z | 616 | THR | O-C-N | -6.30 | 114.37 | 121.43 |
| 18 | l | 7 | GLY | CA-C-N | 6.30 | 130.83 | 120.94 |
| 18 | l | 7 | GLY | C-N-CA | 6.30 | 130.83 | 120.94 |
| 15 | b | 285 | VAL | N-CA-CB | 6.30 | 119.11 | 110.54 |
| 20 | g | 493 | PHE | CA-CB-CG | 6.30 | 120.10 | 113.80 |
| 14 | a | 1018 | ILE | N-CA-C | -6.30 | 106.37 | 112.29 |
| 7 | O | 1155 | ASN | CA-CB-CG | 6.30 | 118.90 | 112.60 |
| 9 | Q | 246 | ASN | CA-CB-CG | -6.30 | 106.30 | 112.60 |
| 1 | Y | 637 | LEU | CA-C-O | -6.30 | 114.20 | 121.82 |
| 1 | Y | 1395 | CYS | CA-C-N | 6.30 | 128.72 | 120.28 |
| 1 | Y | 1395 | CYS | C-N-CA | 6.30 | 128.72 | 120.28 |
| 14 | h | 25 | ASP | N-CA-C | -6.30 | 96.84 | 107.99 |
| 6 | I | 370 | ASP | N-CA-CB | 6.30 | 121.13 | 110.49 |
| 9 | S | 612 | HIS | ND1-CE1-NE2 | 6.30 | 114.70 | 108.40 |
| 10 | U | 319 | LYS | CB-CA-C | -6.30 | 99.96 | 110.29 |
| 20 | n | 247 | LEU | N-CA-CB | 6.30 | 121.13 | 110.49 |
| 20 | n | 655 | PHE | N-CA-CB | 6.30 | 121.13 | 110.49 |
| 19 | f | 143 | LYS | O-C-N | 6.30 | 130.45 | 123.33 |
| 5 | B | 448 | GLU | N-CA-C | -6.30 | 105.54 | 112.72 |
| 9 | S | 162 | LEU | CA-C-N | 6.30 | 129.36 | 120.42 |
| 9 | S | 162 | LEU | C-N-CA | 6.30 | 129.36 | 120.42 |
| 9 | S | 496 | TYR | N-CA-C | 6.30 | 118.95 | 111.33 |
| 11 | V | 288 | PHE | CA-C-O | 6.30 | 126.33 | 119.15 |
| 1 | Y | 1318 | HIS | CE1-NE2-CD2 | -6.30 | 102.70 | 109.00 |
| 12 | v | 53 | LEU | O-C-N | 6.30 | 130.61 | 122.87 |
| 14 | h | 282 | LEU | N-CA-CB | 6.30 | 121.32 | 111.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | q | 23 | ASP | CA-CB-CG | 6.30 | 118.90 | 112.60 |
| 1 | 0 | 180 | ASN | OD1-CG-ND2 | 6.29 | 128.90 | 122.60 |
| 7 | M | 338 | MET | N-CA-C | -6.29 | 105.54 | 113.72 |
| 14 | h | 951 | GLN | N-CA-C | -6.29 | 104.52 | 111.82 |
| 20 | n | 784 | ASN | N-CA-CB | 6.29 | 119.32 | 109.94 |
| 1 | Y | 1332 | ASP | CA-CB-CG | 6.29 | 118.89 | 112.60 |
| 14 | h | 650 | HIS | CA-C-N | 6.29 | 128.62 | 120.56 |
| 14 | h | 650 | HIS | C-N-CA | 6.29 | 128.62 | 120.56 |
| 20 | n | 838 | GLU | CA-C-N | 6.29 | 130.01 | 121.20 |
| 20 | n | 838 | GLU | C-N-CA | 6.29 | 130.01 | 121.20 |
| 2 | 1 | 1217 | GLU | CA-C-N | 6.29 | 131.37 | 120.86 |
| 2 | 1 | 1217 | GLU | C-N-CA | 6.29 | 131.37 | 120.86 |
| 5 | B | 292 | VAL | N-CA-CB | 6.29 | 121.61 | 111.23 |
| 4 | J | 685 | MET | N-CA-C | 6.29 | 118.14 | 111.28 |
| 14 | a | 648 | GLY | CA-C-N | 6.29 | 128.95 | 120.65 |
| 14 | a | 648 | GLY | C-N-CA | 6.29 | 128.95 | 120.65 |
| 7 | M | 735 | ALA | N-CA-C | 6.29 | 119.12 | 111.82 |
| 7 | M | 1093 | SER | N-CA-C | 6.29 | 118.14 | 111.28 |
| 21 | p | 24 | ILE | O-C-N | 6.29 | 128.07 | 121.91 |
| 5 | K | 540 | LYS | N-CA-C | -6.29 | 98.13 | 108.76 |
| 8 | N | 71 | LEU | N-CA-CB | 6.29 | 121.12 | 110.49 |
| 8 | P | 1387 | LEU | CA-C-N | 6.29 | 128.61 | 120.44 |
| 8 | P | 1387 | LEU | C-N-CA | 6.29 | 128.61 | 120.44 |
| 16 | j | 772 | LEU | CA-C-O | -6.29 | 110.11 | 120.80 |
| 19 | m | 420 | LEU | CA-C-N | 6.29 | 128.71 | 120.28 |
| 19 | m | 420 | LEU | C-N-CA | 6.29 | 128.71 | 120.28 |
| 20 | n | 716 | ASN | CA-CB-CG | -6.29 | 106.31 | 112.60 |
| 19 | f | 320 | HIS | CA-CB-CG | 6.29 | 120.09 | 113.80 |
| 20 | g | 378 | PHE | CB-CG-CD1 | -6.29 | 110.01 | 120.70 |
| 20 | g | 752 | GLN | N-CA-CB | 6.29 | 120.06 | 110.44 |
| 2 | 1 | 886 | ASN | CA-C-N | 6.29 | 129.35 | 120.42 |
| 2 | 1 | 886 | ASN | C-N-CA | 6.29 | 129.35 | 120.42 |
| 20 | n | 684 | GLU | N-CA-C | -6.29 | 102.89 | 110.44 |
| 21 | p | 41 | ILE | N-CA-CB | 6.29 | 117.91 | 110.55 |
| 18 | e | 116 | PHE | N-CA-C | -6.29 | 102.06 | 110.55 |
| 6 | L | 312 | VAL | CB-CA-C | 6.29 | 120.02 | 111.97 |
| 7 | O | 211 | ASP | N-CA-CB | 6.29 | 119.46 | 110.16 |
| 9 | R | 287 | ASP | CA-CB-CG | -6.29 | 106.31 | 112.60 |
| 16 | c | 293 | GLN | N-CA-CB | 6.29 | 119.57 | 110.20 |
| 19 | f | 305 | ASN | CA-CB-CG | 6.29 | 118.89 | 112.60 |
| 20 | g | 74 | THR | O-C-N | 6.29 | 130.40 | 123.04 |
| 8 | N | 996 | THR | CA-C-O | 6.28 | 126.66 | 119.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 109 | ARG | NE-CZ-NH1 | -6.28 | 115.22 | 121.50 |
| 8 | P | 1615 | ARG | NH1-CZ-NH2 | 6.28 | 127.47 | 119.30 |
| 9 | Q | 234 | ILE | CA-C-N | 6.28 | 128.61 | 120.44 |
| 9 | Q | 234 | ILE | C-N-CA | 6.28 | 128.61 | 120.44 |
| 9 | Q | 546 | ARG | N-CA-C | -6.28 | 104.86 | 114.16 |
| 9 | Q | 547 | TYR | N-CA-C | -6.28 | 103.13 | 113.50 |
| 9 | S | 219 | VAL | CA-C-N | 6.28 | 129.21 | 120.29 |
| 9 | S | 219 | VAL | C-N-CA | 6.28 | 129.21 | 120.29 |
| 1 | Y | 1293 | LEU | CA-C-N | 6.28 | 129.12 | 122.14 |
| 1 | Y | 1293 | LEU | C-N-CA | 6.28 | 129.12 | 122.14 |
| 2 | Z | 1056 | HIS | CA-C-N | 6.28 | 128.99 | 120.44 |
| 2 | Z | 1056 | HIS | C-N-CA | 6.28 | 128.99 | 120.44 |
| 2 | Z | 1164 | PHE | N-CA-CB | 6.28 | 119.36 | 110.12 |
| 15 | i | 515 | THR | N-CA-CB | 6.28 | 119.30 | 109.69 |
| 15 | i | 717 | ASP | N-CA-C | -6.28 | 105.77 | 113.50 |
| 18 | l | 141 | GLU | CA-C-N | 6.28 | 127.42 | 120.45 |
| 18 | l | 141 | GLU | C-N-CA | 6.28 | 127.42 | 120.45 |
| 19 | m | 106 | GLU | N-CA-C | 6.28 | 118.13 | 111.28 |
| 19 | m | 649 | TYR | N-CA-C | -6.28 | 105.74 | 113.41 |
| 20 | n | 732 | GLU | CA-C-N | 6.28 | 133.73 | 121.41 |
| 20 | n | 732 | GLU | C-N-CA | 6.28 | 133.73 | 121.41 |
| 14 | a | 761 | ALA | N-CA-CB | 6.28 | 119.36 | 110.12 |
| 8 | P | 664 | LEU | N-CA-C | -6.28 | 105.62 | 113.28 |
| 2 | Z | 874 | ASN | N-CA-CB | 6.28 | 119.67 | 110.25 |
| 4 | z | 644 | TRP | CA-C-N | 6.28 | 128.61 | 120.44 |
| 4 | z | 644 | TRP | C-N-CA | 6.28 | 128.61 | 120.44 |
| 18 | l | 211 | HIS | ND1-CE1-NE2 | 6.28 | 114.68 | 108.40 |
| 1 | 0 | 414 | GLY | CA-C-N | 6.28 | 126.02 | 119.05 |
| 1 | 0 | 414 | GLY | C-N-CA | 6.28 | 126.02 | 119.05 |
| 4 | D | 768 | GLU | O-C-N | 6.28 | 128.54 | 122.07 |
| 5 | K | 294 | LYS | CA-C-N | 6.28 | 132.35 | 122.49 |
| 5 | K | 294 | LYS | C-N-CA | 6.28 | 132.35 | 122.49 |
| 1 | Y | 1111 | THR | CA-C-N | 6.28 | 130.80 | 120.94 |
| 1 | Y | 1111 | THR | C-N-CA | 6.28 | 130.80 | 120.94 |
| 12 | u | 326 | LEU | N-CA-CB | 6.28 | 119.54 | 110.06 |
| 16 | j | 351 | ASP | CA-CB-CG | -6.28 | 106.32 | 112.60 |
| 19 | m | 33 | ILE | CA-C-N | 6.28 | 129.09 | 120.67 |
| 19 | m | 33 | ILE | C-N-CA | 6.28 | 129.09 | 120.67 |
| 19 | m | 537 | PHE | O-C-N | -6.28 | 115.83 | 123.30 |
| 7 | M | 519 | ASP | N-CA-C | -6.28 | 105.78 | 113.50 |
| 7 | M | 1247 | ARG | NE-CZ-NH1 | 6.28 | 127.78 | 121.50 |
| 8 | N | 498 | GLU | CA-C-N | 6.28 | 133.17 | 122.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 498 | GLU | C-N-CA | 6.28 | 133.17 | 122.37 |
| 13 | w | 1216 | SER | N-CA-C | 6.28 | 117.79 | 111.07 |
| 19 | f | 194 | ASP | CA-CB-CG | 6.28 | 118.88 | 112.60 |
| 2 | 1 | 380 | ASP | CA-CB-CG | 6.28 | 118.88 | 112.60 |
| 8 | P | 343 | ASP | CA-CB-CG | 6.28 | 118.88 | 112.60 |
| 9 | S | 719 | ASN | N-CA-C | -6.28 | 104.32 | 112.23 |
| 9 | T | 408 | ARG | N-CA-C | 6.28 | 118.20 | 111.36 |
| 2 | Z | 584 | GLN | OE1-CD-NE2 | -6.28 | 116.32 | 122.60 |
| 12 | u | 223 | LEU | CB-CA-C | -6.28 | 100.77 | 110.81 |
| 15 | i | 671 | LEU | CA-C-N | 6.28 | 128.60 | 120.44 |
| 15 | i | 671 | LEU | C-N-CA | 6.28 | 128.60 | 120.44 |
| 19 | m | 298 | ILE | O-C-N | 6.28 | 128.06 | 121.91 |
| 19 | m | 442 | LEU | O-C-N | 6.28 | 129.72 | 122.25 |
| 19 | m | 703 | LEU | N-CA-C | -6.28 | 105.94 | 113.97 |
| 19 | f | 97 | HIS | CG-CD2-NE2 | 6.28 | 113.48 | 107.20 |
| 2 | 1 | 839 | LYS | CA-C-O | 6.28 | 126.61 | 119.27 |
| 2 | 1 | 884 | ILE | CB-CA-C | 6.28 | 120.00 | 111.97 |
| 5 | K | 358 | LEU | CA-C-N | 6.28 | 129.32 | 120.28 |
| 5 | K | 358 | LEU | C-N-CA | 6.28 | 129.32 | 120.28 |
| 5 | K | 512 | ILE | CA-C-O | -6.28 | 114.42 | 120.95 |
| 7 | M | 246 | VAL | N-CA-CB | -6.28 | 103.69 | 112.35 |
| 7 | M | 1654 | ASN | CA-C-N | 6.28 | 128.60 | 120.44 |
| 7 | M | 1654 | ASN | C-N-CA | 6.28 | 128.60 | 120.44 |
| 8 | N | 473 | LEU | N-CA-C | -6.28 | 103.73 | 112.45 |
| 8 | N | 1086 | ILE | CB-CA-C | -6.28 | 104.03 | 111.94 |
| 7 | O | 77 | LEU | N-CA-CB | 6.28 | 119.35 | 110.12 |
| 1 | Y | 1262 | ILE | N-CA-C | -6.28 | 106.68 | 112.96 |
| 13 | w | 1141 | PRO | N-CA-CB | 6.28 | 109.90 | 103.00 |
| 15 | i | 267 | ARG | NH1-CZ-NH2 | -6.28 | 111.14 | 119.30 |
| 16 | j | 450 | CYS | N-CA-CB | 6.28 | 119.45 | 110.16 |
| 20 | n | 305 | THR | CA-C-N | 6.28 | 129.62 | 120.71 |
| 20 | n | 305 | THR | C-N-CA | 6.28 | 129.62 | 120.71 |
| 14 | a | 370 | ASP | CA-C-N | 6.28 | 129.32 | 120.28 |
| 14 | a | 370 | ASP | C-N-CA | 6.28 | 129.32 | 120.28 |
| 7 | M | 980 | ASP | N-CA-C | -6.27 | 104.36 | 111.07 |
| 8 | N | 471 | ASN | N-CA-CB | 6.27 | 121.09 | 110.49 |
| 2 | 1 | 1199 | VAL | CA-C-O | 6.27 | 128.19 | 121.04 |
| 7 | M | 1569 | TYR | CB-CA-C | -6.27 | 100.56 | 110.85 |
| 18 | l | 154 | MET | O-C-N | -6.27 | 115.87 | 123.27 |
| 14 | h | 628 | ARG | CA-C-N | 6.27 | 128.46 | 120.56 |
| 14 | h | 628 | ARG | C-N-CA | 6.27 | 128.46 | 120.56 |
| 1 | 0 | 208 | LYS | CA-C-N | 6.27 | 133.51 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 208 | LYS | C-N-CA | 6.27 | 133.51 | 121.54 |
| 1 | 0 | 1166 | VAL | CA-C-O | -6.27 | 114.52 | 121.23 |
| 1 | 0 | 1402 | LEU | CA-C-N | 6.27 | 127.68 | 119.84 |
| 1 | 0 | 1402 | LEU | C-N-CA | 6.27 | 127.68 | 119.84 |
| 4 | J | 815 | GLU | CA-C-O | -6.27 | 111.67 | 119.38 |
| 1 | Y | 850 | ASN | CA-C-N | 6.27 | 128.68 | 120.28 |
| 1 | Y | 850 | ASN | C-N-CA | 6.27 | 128.68 | 120.28 |
| 12 | u | 400 | SER | N-CA-CB | 6.27 | 121.65 | 111.74 |
| 12 | u | 610 | SER | N-CA-C | 6.27 | 120.53 | 113.01 |
| 19 | f | 300 | ASN | CA-C-O | 6.27 | 127.16 | 120.70 |
| 2 | 1 | 183 | TRP | N-CA-CB | -6.27 | 100.43 | 110.46 |
| 1 | Y | 1341 | ASP | N-CA-CB | 6.27 | 119.06 | 109.91 |
| 2 | Z | 579 | TYR | N-CA-C | -6.27 | 105.27 | 113.17 |
| 12 | u | 179 | VAL | N-CA-C | -6.27 | 99.34 | 108.11 |
| 12 | u | 353 | ARG | N-CA-C | -6.27 | 98.19 | 108.41 |
| 20 | g | 632 | LYS | N-CA-CB | 6.27 | 121.64 | 110.80 |
| 14 | a | 652 | SER | N-CA-CB | 6.27 | 119.33 | 110.12 |
| 1 | Y | 1071 | ALA | CA-C-O | -6.27 | 114.24 | 120.82 |
| 2 | Z | 573 | LEU | CA-C-O | 6.27 | 127.87 | 119.47 |
| 19 | m | 216 | GLN | N-CA-CB | 6.27 | 120.04 | 110.70 |
| 19 | m | 287 | HIS | N-CA-C | 6.27 | 119.09 | 111.82 |
| 7 | O | 1529 | ALA | N-CA-CB | 6.26 | 119.09 | 110.01 |
| 8 | P | 1454 | GLU | CA-C-O | -6.26 | 112.26 | 118.34 |
| 11 | X | 377 | PHE | N-CA-CB | 6.26 | 121.08 | 110.49 |
| 1 | Y | 630 | THR | CA-C-O | 6.26 | 126.68 | 119.35 |
| 15 | i | 500 | LYS | N-CA-C | 6.26 | 119.09 | 111.82 |
| 16 | j | 510 | LEU | O-C-N | 6.26 | 128.76 | 122.12 |
| 19 | m | 638 | LEU | CA-C-N | 6.26 | 129.72 | 120.95 |
| 19 | m | 638 | LEU | C-N-CA | 6.26 | 129.72 | 120.95 |
| 20 | g | 940 | ASP | N-CA-C | -6.26 | 104.27 | 112.41 |
| 9 | R | 355 | GLU | CA-C-O | 6.26 | 126.03 | 119.14 |
| 9 | S | 80 | PHE | N-CA-CB | 6.26 | 121.08 | 110.49 |
| 9 | T | 76 | SER | CA-C-N | 6.26 | 132.08 | 120.87 |
| 9 | T | 76 | SER | C-N-CA | 6.26 | 132.08 | 120.87 |
| 4 | y | 773 | SER | N-CA-CB | 6.26 | 119.09 | 110.01 |
| 21 | r | 53 | TYR | N-CA-CB | 6.26 | 120.13 | 110.80 |
| 6 | F | 334 | SER | CA-C-N | 6.26 | 128.58 | 120.44 |
| 6 | F | 334 | SER | C-N-CA | 6.26 | 128.58 | 120.44 |
| 9 | Q | 684 | ASN | CA-CB-CG | -6.26 | 106.34 | 112.60 |
| 9 | R | 115 | THR | CA-C-O | -6.26 | 114.00 | 120.89 |
| 1 | Y | 1284 | ARG | CA-C-N | 6.26 | 133.24 | 121.97 |
| 1 | Y | 1284 | ARG | C-N-CA | 6.26 | 133.24 | 121.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 959 | GLU | N-CA-C | -6.26 | 99.63 | 108.96 |
| 21 | q | 43 | GLY | CA-C-N | 6.26 | 129.18 | 120.29 |
| 21 | q | 43 | GLY | C-N-CA | 6.26 | 129.18 | 120.29 |
| 15 | b | 577 | GLU | CA-C-N | 6.26 | 132.19 | 122.49 |
| 15 | b | 577 | GLU | C-N-CA | 6.26 | 132.19 | 122.49 |
| 7 | M | 110 | ARG | CA-C-N | 6.26 | 131.02 | 120.88 |
| 7 | M | 110 | ARG | C-N-CA | 6.26 | 131.02 | 120.88 |
| 19 | m | 697 | GLU | N-CA-C | -6.26 | 103.17 | 113.50 |
| 17 | d | 118 | VAL | N-CA-C | -6.26 | 99.45 | 108.53 |
| 1 | Y | 1012 | ARG | N-CA-CB | 6.26 | 119.24 | 110.04 |
| 16 | j | 768 | ASN | CB-CA-C | -6.26 | 99.34 | 109.67 |
| 15 | b | 475 | SER | CA-C-N | 6.26 | 128.67 | 120.28 |
| 15 | b | 475 | SER | C-N-CA | 6.26 | 128.67 | 120.28 |
| 1 | 0 | 598 | PHE | CA-C-O | 6.26 | 127.44 | 120.43 |
| 2 | 1 | 266 | TYR | CA-C-O | -6.26 | 113.89 | 120.58 |
| 6 | C | 457 | ILE | CA-C-N | 6.26 | 129.17 | 120.29 |
| 6 | C | 457 | ILE | C-N-CA | 6.26 | 129.17 | 120.29 |
| 8 | N | 18 | VAL | N-CA-C | -6.26 | 104.65 | 110.53 |
| 8 | N | 294 | THR | CA-C-N | 6.26 | 128.66 | 120.28 |
| 8 | N | 294 | THR | C-N-CA | 6.26 | 128.66 | 120.28 |
| 8 | N | 1093 | ASN | CA-C-N | 6.26 | 132.03 | 122.77 |
| 8 | N | 1093 | ASN | C-N-CA | 6.26 | 132.03 | 122.77 |
| 9 | Q | 147 | ASP | CA-C-N | 6.26 | 130.61 | 120.60 |
| 9 | Q | 147 | ASP | C-N-CA | 6.26 | 130.61 | 120.60 |
| 9 | S | 51 | ARG | N-CA-C | -6.26 | 105.30 | 113.12 |
| 14 | h | 803 | HIS | CB-CG-CD2 | -6.26 | 123.07 | 131.20 |
| 14 | h | 957 | ASP | CA-CB-CG | 6.26 | 118.86 | 112.60 |
| 7 | O | 1286 | PHE | CA-C-O | 6.25 | 127.59 | 120.90 |
| 14 | h | 708 | ASN | CA-C-N | 6.25 | 129.03 | 120.46 |
| 14 | h | 708 | ASN | C-N-CA | 6.25 | 129.03 | 120.46 |
| 20 | g | 1009 | LEU | N-CA-C | -6.25 | 99.04 | 109.24 |
| 7 | M | 535 | PHE | CA-C-N | 6.25 | 131.69 | 121.87 |
| 7 | M | 535 | PHE | C-N-CA | 6.25 | 131.69 | 121.87 |
| 2 | Z | 416 | GLU | N-CA-C | -6.25 | 97.48 | 110.80 |
| 2 | Z | 800 | LEU | N-CA-CB | 6.25 | 119.85 | 110.22 |
| 12 | u | 311 | GLN | N-CA-CB | 6.25 | 121.06 | 110.49 |
| 13 | w | 1452 | PHE | CA-CB-CG | -6.25 | 107.55 | 113.80 |
| 4 | z | 692 | LYS | O-C-N | -6.25 | 115.63 | 122.07 |
| 14 | h | 378 | TRP | CB-CG-CD1 | 6.25 | 136.28 | 126.90 |
| 14 | h | 992 | ASP | CA-C-O | -6.25 | 113.75 | 120.75 |
| 17 | k | 122 | ASP | CA-C-N | 6.25 | 130.14 | 121.26 |
| 17 | k | 122 | ASP | C-N-CA | 6.25 | 130.14 | 121.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 196 | ASN | N-CA-C | -6.25 | 105.51 | 113.01 |
| 1 | 0 | 1313 | VAL | O-C-N | -6.25 | 113.97 | 121.10 |
| 7 | M | 903 | ASN | CA-C-N | 6.25 | 131.31 | 121.56 |
| 7 | M | 903 | ASN | C-N-CA | 6.25 | 131.31 | 121.56 |
| 8 | N | 1093 | ASN | CA-CB-CG | 6.25 | 118.85 | 112.60 |
| 9 | S | 268 | ILE | N-CA-CB | 6.25 | 118.28 | 110.47 |
| 1 | Y | 957 | ASP | CA-CB-CG | -6.25 | 106.35 | 112.60 |
| 13 | w | 1236 | ASP | N-CA-C | 6.25 | 117.76 | 111.07 |
| 16 | j | 139 | MET | N-CA-C | -6.25 | 106.34 | 112.97 |
| 19 | m | 698 | ASN | OD1-CG-ND2 | -6.25 | 116.35 | 122.60 |
| 19 | f | 319 | SER | N-CA-C | -6.25 | 102.47 | 110.53 |
| 8 | P | 440 | ILE | CA-C-N | 6.25 | 127.65 | 119.84 |
| 8 | P | 440 | ILE | C-N-CA | 6.25 | 127.65 | 119.84 |
| 9 | T | 745 | LEU | O-C-N | -6.25 | 116.01 | 121.32 |
| 1 | Y | 263 | VAL | CA-C-O | -6.25 | 115.64 | 119.51 |
| 21 | o | 41 | ILE | CA-C-N | 6.25 | 128.66 | 120.28 |
| 21 | o | 41 | ILE | C-N-CA | 6.25 | 128.66 | 120.28 |
| 19 | f | 684 | ILE | N-CA-C | -6.25 | 106.71 | 112.96 |
| 4 | D | 678 | GLN | CB-CA-C | 6.25 | 120.69 | 110.88 |
| 4 | G | 767 | VAL | N-CA-C | -6.25 | 103.28 | 111.09 |
| 6 | L | 397 | ALA | N-CA-C | 6.25 | 118.17 | 111.36 |
| 7 | O | 1511 | LEU | N-CA-CB | 6.25 | 119.64 | 109.95 |
| 14 | a | 817 | VAL | CA-C-N | 6.25 | 127.65 | 119.84 |
| 14 | a | 817 | VAL | C-N-CA | 6.25 | 127.65 | 119.84 |
| 2 | 1 | 1001 | ARG | N-CA-C | 6.25 | 117.75 | 111.07 |
| 7 | O | 194 | SER | N-CA-CB | 6.25 | 119.30 | 110.12 |
| 7 | O | 1052 | LEU | N-CA-C | -6.25 | 104.47 | 111.28 |
| 7 | O | 1581 | THR | CA-C-N | 6.25 | 128.56 | 120.44 |
| 7 | O | 1581 | THR | C-N-CA | 6.25 | 128.56 | 120.44 |
| 9 | Q | 777 | ILE | O-C-N | 6.25 | 127.93 | 121.87 |
| 1 | Y | 666 | PRO | N-CA-C | -6.25 | 107.49 | 114.92 |
| 1 | Y | 1486 | LYS | N-CA-C | 6.25 | 117.75 | 111.07 |
| 12 | v | 431 | TRP | CE2-CD2-CE3 | 6.25 | 125.05 | 118.80 |
| 14 | a | 656 | ASP | CA-CB-CG | 6.25 | 118.85 | 112.60 |
| 7 | M | 1426 | VAL | O-C-N | -6.25 | 115.81 | 121.87 |
| 7 | O | 1464 | ILE | CB-CA-C | -6.25 | 103.98 | 111.97 |
| 7 | O | 1481 | LYS | CA-C-N | 6.25 | 133.47 | 121.54 |
| 7 | O | 1481 | LYS | C-N-CA | 6.25 | 133.47 | 121.54 |
| 8 | P | 43 | PHE | CA-CB-CG | -6.25 | 107.56 | 113.80 |
| 7 | O | 572 | PHE | CA-CB-CG | -6.24 | 107.56 | 113.80 |
| 8 | P | 980 | LYS | N-CA-C | -6.24 | 97.64 | 108.69 |
| 9 | Q | 728 | PHE | N-CA-C | -6.24 | 107.50 | 114.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | T | 799 | LYS | N-CA-C | 6.24 | 118.89 | 111.71 |
| 11 | X | 393 | GLU | CB-CG-CD | -6.24 | 101.99 | 112.60 |
| 1 | Y | 1044 | ILE | CA-C-N | 6.24 | 133.46 | 121.54 |
| 1 | Y | 1044 | ILE | C-N-CA | 6.24 | 133.46 | 121.54 |
| 12 | v | 28 | SER | N-CA-C | -6.24 | 97.90 | 108.26 |
| 20 | n | 713 | ASP | N-CA-CB | 6.24 | 121.04 | 110.49 |
| 20 | g | 858 | ASN | O-C-N | -6.24 | 114.12 | 122.49 |
| 7 | M | 205 | ALA | N-CA-C | -6.24 | 104.94 | 113.30 |
| 5 | E | 392 | LEU | CA-C-N | 6.24 | 133.46 | 121.54 |
| 5 | E | 392 | LEU | C-N-CA | 6.24 | 133.46 | 121.54 |
| 9 | Q | 806 | LEU | N-CA-CB | 6.24 | 119.06 | 110.01 |
| 1 | Y | 162 | HIS | CA-C-N | 6.24 | 128.64 | 120.28 |
| 1 | Y | 162 | HIS | C-N-CA | 6.24 | 128.64 | 120.28 |
| 1 | 0 | 1101 | ARG | NH1-CZ-NH2 | 6.24 | 127.41 | 119.30 |
| 2 | 1 | 568 | LYS | N-CA-C | -6.24 | 104.63 | 112.93 |
| 8 | P | 1594 | ASP | CA-C-N | 6.24 | 129.26 | 120.28 |
| 8 | P | 1594 | ASP | C-N-CA | 6.24 | 129.26 | 120.28 |
| 9 | R | 281 | GLN | OE1-CD-NE2 | 6.24 | 128.84 | 122.60 |
| 9 | T | 631 | ALA | CA-C-N | 6.24 | 128.55 | 120.44 |
| 9 | T | 631 | ALA | C-N-CA | 6.24 | 128.55 | 120.44 |
| 1 | Y | 433 | ASN | CA-CB-CG | -6.24 | 106.36 | 112.60 |
| 1 | Y | 628 | PHE | CA-CB-CG | -6.24 | 107.56 | 113.80 |
| 4 | z | 645 | THR | O-C-N | -6.24 | 115.64 | 122.07 |
| 14 | a | 706 | ASN | CA-CB-CG | 6.24 | 118.84 | 112.60 |
| 5 | B | 367 | GLU | CA-C-N | 6.24 | 129.15 | 120.29 |
| 5 | B | 367 | GLU | C-N-CA | 6.24 | 129.15 | 120.29 |
| 8 | N | 1542 | ALA | N-CA-CB | 6.24 | 121.03 | 110.49 |
| 1 | Y | 1468 | TYR | N-CA-CB | 6.24 | 121.03 | 110.49 |
| 20 | n | 281 | ARG | NE-CZ-NH1 | 6.24 | 127.74 | 121.50 |
| 20 | n | 988 | VAL | CA-C-O | -6.24 | 114.56 | 121.17 |
| 6 | I | 462 | GLN | N-CA-CB | 6.24 | 119.94 | 110.28 |
| 7 | O | 1575 | PHE | CA-C-N | 6.24 | 133.45 | 121.54 |
| 7 | O | 1575 | PHE | C-N-CA | 6.24 | 133.45 | 121.54 |
| 8 | P | 1030 | SER | N-CA-C | -6.24 | 97.52 | 110.80 |
| 9 | Q | 629 | ARG | NE-CZ-NH1 | -6.24 | 115.26 | 121.50 |
| 1 | Y | 459 | ALA | CA-C-O | -6.24 | 114.94 | 121.55 |
| 14 | h | 983 | GLN | CA-C-O | 6.24 | 126.26 | 119.15 |
| 14 | h | 1001 | LEU | CB-CA-C | -6.24 | 99.63 | 110.17 |
| 20 | n | 920 | CYS | N-CA-C | 6.24 | 118.88 | 111.33 |
| 21 | o | 31 | ALA | CA-C-N | 6.24 | 129.26 | 120.28 |
| 21 | o | 31 | ALA | C-N-CA | 6.24 | 129.26 | 120.28 |
| 15 | b | 170 | ASN | CA-CB-CG | -6.24 | 106.36 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 130 | ASP | CA-CB-CG | 6.24 | 118.84 | 112.60 |
| 8 | N | 916 | TYR | CA-C-O | -6.23 | 114.57 | 119.99 |
| 4 | D | 790 | ASN | CA-C-N | 6.23 | 129.00 | 120.46 |
| 4 | D | 790 | ASN | C-N-CA | 6.23 | 129.00 | 120.46 |
| 8 | N | 1313 | ARG | N-CA-C | 6.23 | 117.74 | 111.07 |
| 9 | R | 437 | TRP | CA-C-O | -6.23 | 113.06 | 120.10 |
| 10 | W | 267 | ILE | N-CA-C | -6.23 | 104.26 | 110.62 |
| 1 | Y | 1232 | ARG | NE-CZ-NH2 | -6.23 | 113.59 | 119.20 |
| 14 | h | 425 | GLN | N-CA-C | -6.23 | 105.71 | 113.38 |
| 1 | 0 | 1382 | GLU | N-CA-CB | 6.23 | 121.02 | 110.49 |
| 5 | B | 510 | VAL | CA-CB-CG2 | -6.23 | 99.81 | 110.40 |
| 5 | H | 439 | GLN | CA-C-N | 6.23 | 128.63 | 120.28 |
| 5 | H | 439 | GLN | C-N-CA | 6.23 | 128.63 | 120.28 |
| 9 | S | 686 | VAL | N-CA-C | -6.23 | 106.25 | 112.17 |
| 12 | v | 196 | CYS | CB-CA-C | -6.23 | 98.97 | 109.50 |
| 13 | x | 1391 | ALA | CA-C-N | 6.23 | 128.63 | 120.28 |
| 13 | x | 1391 | ALA | C-N-CA | 6.23 | 128.63 | 120.28 |
| 21 | q | 7 | SER | CA-C-N | 6.23 | 129.34 | 120.49 |
| 21 | q | 7 | SER | C-N-CA | 6.23 | 129.34 | 120.49 |
| 21 | s | 48 | GLN | CA-C-N | 6.23 | 129.14 | 120.29 |
| 21 | s | 48 | GLN | C-N-CA | 6.23 | 129.14 | 120.29 |
| 18 | e | 144 | ASP | O-C-N | -6.23 | 115.79 | 123.33 |
| 20 | g | 85 | GLU | N-CA-CB | 6.23 | 119.66 | 110.56 |
| 14 | a | 115 | GLN | N-CA-CB | 6.23 | 121.02 | 110.49 |
| 6 | L | 372 | PHE | O-C-N | 6.23 | 129.25 | 122.15 |
| 7 | M | 1202 | ASN | CA-CB-CG | -6.23 | 106.37 | 112.60 |
| 11 | X | 355 | TRP | N-CA-C | -6.23 | 98.58 | 108.73 |
| 12 | v | 161 | GLU | CB-CG-CD | -6.23 | 102.01 | 112.60 |
| 5 | B | 516 | GLN | CA-C-O | -6.23 | 114.28 | 120.70 |
| 8 | N | 1081 | ILE | O-C-N | -6.23 | 115.61 | 121.90 |
| 9 | S | 53 | VAL | CA-C-N | 6.23 | 128.62 | 120.28 |
| 9 | S | 53 | VAL | C-N-CA | 6.23 | 128.62 | 120.28 |
| 9 | S | 222 | PHE | CA-CB-CG | 6.23 | 120.03 | 113.80 |
| 4 | y | 725 | VAL | O-C-N | 6.23 | 127.91 | 121.87 |
| 15 | i | 641 | ASP | N-CA-CB | 6.23 | 121.01 | 110.49 |
| 20 | n | 351 | ILE | CA-CB-CG1 | 6.23 | 120.99 | 110.40 |
| 15 | b | 186 | ARG | CA-C-N | 6.23 | 128.87 | 120.65 |
| 15 | b | 186 | ARG | C-N-CA | 6.23 | 128.87 | 120.65 |
| 8 | N | 57 | THR | CA-CB-OG1 | 6.23 | 118.94 | 109.60 |
| 1 | Y | 1340 | TRP | CA-C-N | 6.23 | 128.87 | 120.65 |
| 1 | Y | 1340 | TRP | C-N-CA | 6.23 | 128.87 | 120.65 |
| 20 | g | 571 | VAL | CA-C-N | 6.23 | 128.53 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 571 | VAL | C-N-CA | 6.23 | 128.53 | 120.44 |
| 20 | g | 648 | GLN | OE1-CD-NE2 | -6.23 | 116.37 | 122.60 |
| 7 | M | 278 | ILE | CA-C-N | 6.22 | 128.94 | 120.54 |
| 7 | M | 278 | ILE | C-N-CA | 6.22 | 128.94 | 120.54 |
| 8 | P | 297 | THR | N-CA-C | 6.22 | 118.06 | 111.28 |
| 8 | P | 1426 | SER | CA-C-N | 6.22 | 133.43 | 121.54 |
| 8 | P | 1426 | SER | C-N-CA | 6.22 | 133.43 | 121.54 |
| 12 | u | 213 | PRO | N-CA-C | 6.22 | 120.99 | 111.34 |
| 4 | z | 762 | LEU | O-C-N | -6.22 | 115.52 | 122.12 |
| 14 | h | 629 | ILE | N-CA-CB | 6.22 | 117.83 | 110.55 |
| 19 | f | 480 | THR | N-CA-C | -6.22 | 104.32 | 112.41 |
| 1 | 0 | 1406 | HIS | N-CA-C | -6.22 | 105.00 | 112.59 |
| 7 | M | 481 | PHE | CA-C-N | 6.22 | 129.24 | 120.28 |
| 7 | M | 481 | PHE | C-N-CA | 6.22 | 129.24 | 120.28 |
| 7 | M | 1354 | VAL | N-CA-C | 6.22 | 116.97 | 110.62 |
| 8 | P | 221 | VAL | N-CA-C | -6.22 | 106.44 | 112.29 |
| 9 | S | 486 | GLY | O-C-N | 6.22 | 129.70 | 122.30 |
| 9 | S | 787 | HIS | N-CA-C | -6.22 | 104.58 | 111.36 |
| 2 | Z | 996 | VAL | CB-CA-C | -6.22 | 103.74 | 112.14 |
| 14 | a | 272 | LYS | O-C-N | -6.22 | 116.00 | 123.03 |
| 2 | 1 | 154 | VAL | CB-CA-C | 6.22 | 116.86 | 110.70 |
| 7 | M | 34 | ASN | N-CA-CB | 6.22 | 120.55 | 110.41 |
| 8 | P | 1482 | ASP | N-CA-C | -6.22 | 97.55 | 110.80 |
| 20 | n | 748 | ILE | CA-C-N | 6.22 | 132.75 | 122.73 |
| 20 | n | 748 | ILE | C-N-CA | 6.22 | 132.75 | 122.73 |
| 15 | b | 597 | LYS | N-CA-C | -6.22 | 105.69 | 113.28 |
| 2 | 1 | 287 | GLN | CA-C-N | 6.22 | 129.80 | 119.35 |
| 2 | 1 | 287 | GLN | C-N-CA | 6.22 | 129.80 | 119.35 |
| 7 | M | 83 | LEU | N-CA-C | -6.22 | 97.55 | 110.80 |
| 7 | M | 136 | LYS | CA-C-N | 6.22 | 133.42 | 121.54 |
| 7 | M | 136 | LYS | C-N-CA | 6.22 | 133.42 | 121.54 |
| 7 | M | 658 | SER | CB-CA-C | -6.22 | 101.03 | 110.92 |
| 20 | n | 156 | ASN | N-CA-CB | 6.22 | 121.00 | 110.49 |
| 14 | a | 906 | GLN | OE1-CD-NE2 | 6.22 | 128.82 | 122.60 |
| 9 | Q | 801 | GLN | CA-C-N | 6.22 | 128.52 | 120.44 |
| 9 | Q | 801 | GLN | C-N-CA | 6.22 | 128.52 | 120.44 |
| 16 | j | 286 | ASN | N-CA-CB | -6.22 | 101.22 | 110.61 |
| 20 | n | 408 | ASN | N-CA-CB | 6.22 | 122.25 | 111.00 |
| 20 | n | 686 | GLU | CA-C-O | 6.22 | 126.87 | 119.60 |
| 20 | g | 119 | TYR | CG-CD2-CE2 | -6.22 | 111.87 | 121.20 |
| 20 | g | 384 | ASN | N-CA-CB | 6.22 | 120.42 | 110.16 |
| 8 | P | 1406 | VAL | N-CA-CB | 6.22 | 117.15 | 110.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 100 | ASP | CA-CB-CG | 6.22 | 118.82 | 112.60 |
| 2 | Z | 1008 | ILE | CA-C-O | -6.22 | 114.15 | 121.05 |
| 12 | u | 154 | PHE | N-CA-C | -6.22 | 98.86 | 109.24 |
| 20 | n | 760 | ILE | O-C-N | -6.22 | 114.80 | 122.57 |
| 14 | a | 778 | GLN | CA-C-N | 6.22 | 129.76 | 120.31 |
| 14 | a | 778 | GLN | C-N-CA | 6.22 | 129.76 | 120.31 |
| 7 | M | 354 | ARG | N-CA-C | 6.21 | 118.73 | 110.53 |
| 7 | M | 1247 | ARG | NH1-CZ-NH2 | -6.21 | 111.22 | 119.30 |
| 7 | O | 95 | GLY | CA-C-O | -6.21 | 116.12 | 121.78 |
| 2 | Z | 440 | ARG | NE-CZ-NH1 | 6.21 | 127.72 | 121.50 |
| 12 | v | 274 | LYS | CA-CB-CG | -6.21 | 101.67 | 114.10 |
| 16 | j | 317 | HIS | CG-CD2-NE2 | 6.21 | 113.42 | 107.20 |
| 21 | r | 18 | ASP | N-CA-CB | 6.21 | 119.26 | 110.12 |
| 20 | g | 716 | ASN | CA-CB-CG | -6.21 | 106.39 | 112.60 |
| 2 | 1 | 1206 | PHE | CA-CB-CG | 6.21 | 120.01 | 113.80 |
| 5 | K | 391 | GLU | N-CA-C | -6.21 | 105.38 | 114.39 |
| 8 | N | 1606 | LEU | N-CA-C | 6.21 | 117.72 | 111.07 |
| 7 | O | 611 | SER | N-CA-C | 6.21 | 118.86 | 111.71 |
| 20 | g | 452 | ASP | CA-C-N | 6.21 | 133.15 | 121.97 |
| 20 | g | 452 | ASP | C-N-CA | 6.21 | 133.15 | 121.97 |
| 1 | 0 | 1482 | ASP | CA-C-N | 6.21 | 125.83 | 119.56 |
| 1 | 0 | 1482 | ASP | C-N-CA | 6.21 | 125.83 | 119.56 |
| 8 | N | 67 | ASP | CA-CB-CG | 6.21 | 118.81 | 112.60 |
| 9 | R | 680 | ASN | N-CA-C | -6.21 | 104.59 | 111.36 |
| 12 | u | 313 | GLU | N-CA-C | -6.21 | 99.24 | 108.99 |
| 6 | L | 381 | GLU | N-CA-C | -6.21 | 105.67 | 113.18 |
| 7 | M | 120 | ILE | N-CA-C | -6.21 | 104.28 | 110.30 |
| 7 | M | 926 | LEU | CA-C-N | 6.21 | 127.01 | 119.99 |
| 7 | M | 926 | LEU | C-N-CA | 6.21 | 127.01 | 119.99 |
| 7 | M | 1312 | ILE | CA-CB-CG2 | -6.21 | 99.94 | 110.50 |
| 7 | O | 352 | ILE | CA-C-O | -6.21 | 111.63 | 119.95 |
| 8 | P | 1552 | ASN | CA-C-N | 6.21 | 128.60 | 120.28 |
| 8 | P | 1552 | ASN | C-N-CA | 6.21 | 128.60 | 120.28 |
| 16 | j | 558 | ASN | N-CA-CB | -6.21 | 101.47 | 110.47 |
| 8 | N | 1025 | ASN | OD1-CG-ND2 | 6.21 | 128.81 | 122.60 |
| 7 | O | 1583 | ASP | N-CA-CB | 6.21 | 119.01 | 110.01 |
| 8 | P | 64 | SER | CA-C-N | 6.21 | 132.49 | 121.75 |
| 8 | P | 64 | SER | C-N-CA | 6.21 | 132.49 | 121.75 |
| 9 | R | 65 | ASP | CA-C-N | 6.21 | 128.89 | 120.38 |
| 9 | R | 65 | ASP | C-N-CA | 6.21 | 128.89 | 120.38 |
| 21 | p | 22 | GLU | N-CA-C | 6.21 | 118.05 | 111.28 |
| 1 | 0 | 1205 | SER | N-CA-C | -6.21 | 105.46 | 113.16 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 343 | ASP | CA-C-N | 6.21 | 128.92 | 120.54 |
| 8 | N | 343 | ASP | C-N-CA | 6.21 | 128.92 | 120.54 |
| 8 | N | 718 | PHE | N-CA-CB | 6.21 | 118.97 | 109.91 |
| 9 | T | 745 | LEU | CA-C-N | 6.21 | 127.60 | 119.84 |
| 9 | T | 745 | LEU | C-N-CA | 6.21 | 127.60 | 119.84 |
| 2 | Z | 258 | PHE | CA-C-O | 6.21 | 129.07 | 121.87 |
| 7 | M | 1483 | THR | CA-CB-OG1 | 6.21 | 118.91 | 109.60 |
| 8 | N | 68 | HIS | N-CA-C | -6.21 | 106.03 | 113.97 |
| 7 | O | 1623 | VAL | CA-C-O | 6.21 | 126.44 | 119.92 |
| 1 | Y | 605 | VAL | N-CA-CB | 6.21 | 117.94 | 110.31 |
| 12 | v | 346 | ASN | CB-CA-C | -6.21 | 100.11 | 110.29 |
| 20 | g | 1008 | MET | N-CA-C | -6.21 | 105.47 | 113.16 |
| 1 | 0 | 524 | THR | N-CA-C | -6.20 | 99.91 | 109.52 |
| 7 | M | 310 | MET | N-CA-C | 6.20 | 117.71 | 111.07 |
| 1 | Y | 680 | SER | O-C-N | -6.20 | 115.54 | 122.12 |
| 14 | h | 503 | GLY | O-C-N | -6.20 | 117.76 | 123.78 |
| 20 | n | 837 | ASN | CA-CB-CG | -6.20 | 106.40 | 112.60 |
| 9 | S | 704 | ARG | CA-C-N | 6.20 | 128.50 | 120.44 |
| 9 | S | 704 | ARG | C-N-CA | 6.20 | 128.50 | 120.44 |
| 9 | T | 288 | ASN | CA-CB-CG | 6.20 | 118.80 | 112.60 |
| 11 | X | 295 | MET | N-CA-C | -6.20 | 103.17 | 112.54 |
| 15 | i | 592 | ASN | N-CA-C | -6.20 | 99.61 | 109.59 |
| 2 | 1 | 383 | HIS | CE1-NE2-CD2 | -6.20 | 102.80 | 109.00 |
| 7 | M | 1454 | VAL | CA-CB-CG2 | -6.20 | 99.86 | 110.40 |
| 12 | u | 35 | ILE | O-C-N | -6.20 | 116.50 | 123.20 |
| 14 | a | 18 | PRO | CA-C-N | 6.20 | 132.18 | 122.26 |
| 14 | a | 18 | PRO | C-N-CA | 6.20 | 132.18 | 122.26 |
| 1 | 0 | 1341 | ASP | O-C-N | 6.20 | 128.71 | 122.08 |
| 1 | 0 | 1434 | ILE | CB-CA-C | -6.20 | 102.55 | 112.16 |
| 8 | N | 1348 | VAL | O-C-N | -6.20 | 113.57 | 122.12 |
| 7 | O | 1290 | ILE | N-CA-CB | 6.20 | 117.80 | 110.55 |
| 7 | O | 1347 | ILE | CA-C-N | 6.20 | 128.87 | 120.38 |
| 7 | O | 1347 | ILE | C-N-CA | 6.20 | 128.87 | 120.38 |
| 14 | a | 113 | VAL | N-CA-C | -6.20 | 105.31 | 111.88 |
| 2 | 1 | 974 | ILE | O-C-N | 6.20 | 127.88 | 121.87 |
| 4 | G | 762 | LEU | N-CA-C | 6.20 | 117.70 | 111.07 |
| 7 | M | 1251 | ARG | N-CA-C | 6.20 | 118.03 | 111.28 |
| 7 | M | 1258 | HIS | CB-CG-ND1 | 6.20 | 132.00 | 122.70 |
| 8 | P | 656 | GLN | CA-C-N | 6.20 | 130.36 | 121.50 |
| 8 | P | 656 | GLN | C-N-CA | 6.20 | 130.36 | 121.50 |
| 9 | Q | 45 | SER | CA-C-N | 6.20 | 133.12 | 121.97 |
| 9 | Q | 45 | SER | C-N-CA | 6.20 | 133.12 | 121.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | S | 217 | ARG | N-CA-C | 6.20 | 117.83 | 111.14 |
| 12 | u | 423 | ILE | CA-C-O | -6.20 | 114.31 | 119.76 |
| 15 | i | 242 | THR | CA-C-N | 6.20 | 129.09 | 120.29 |
| 15 | i | 242 | THR | C-N-CA | 6.20 | 129.09 | 120.29 |
| 1 | 0 | 1295 | LYS | CA-C-N | 6.20 | 133.38 | 121.54 |
| 1 | 0 | 1295 | LYS | C-N-CA | 6.20 | 133.38 | 121.54 |
| 5 | H | 404 | ARG | NE-CZ-NH2 | -6.20 | 113.62 | 119.20 |
| 7 | M | 819 | VAL | CA-C-O | 6.20 | 125.77 | 119.20 |
| 8 | P | 563 | SER | CA-C-N | 6.20 | 129.09 | 120.29 |
| 8 | P | 563 | SER | C-N-CA | 6.20 | 129.09 | 120.29 |
| 15 | i | 727 | LEU | N-CA-CB | 6.20 | 119.12 | 110.26 |
| 16 | j | 764 | LEU | O-C-N | 6.20 | 128.78 | 122.09 |
| 20 | g | 315 | ALA | N-CA-C | -6.20 | 105.85 | 113.41 |
| 8 | N | 1131 | LYS | N-CA-C | -6.19 | 105.00 | 113.30 |
| 8 | P | 730 | ILE | CA-C-N | 6.19 | 129.51 | 120.71 |
| 8 | P | 730 | ILE | C-N-CA | 6.19 | 129.51 | 120.71 |
| 14 | h | 156 | TYR | CA-C-O | 6.19 | 127.93 | 120.99 |
| 20 | n | 659 | PRO | CA-C-O | -6.19 | 114.28 | 121.34 |
| 2 | 1 | 1112 | ALA | N-CA-CB | 6.19 | 119.22 | 110.12 |
| 5 | E | 382 | LYS | N-CA-C | 6.19 | 117.70 | 111.07 |
| 6 | I | 461 | HIS | O-C-N | -6.19 | 114.65 | 122.27 |
| 7 | O | 1053 | ILE | N-CA-C | 6.19 | 116.36 | 110.42 |
| 9 | Q | 801 | GLN | N-CA-C | -6.19 | 104.07 | 111.69 |
| 9 | R | 417 | ARG | NE-CZ-NH2 | -6.19 | 113.63 | 119.20 |
| 9 | R | 430 | LEU | N-CA-CB | 6.19 | 119.16 | 110.98 |
| 2 | Z | 618 | ASP | CA-CB-CG | -6.19 | 106.41 | 112.60 |
| 14 | h | 845 | ILE | N-CA-C | -6.19 | 107.46 | 113.53 |
| 15 | i | 140 | HIS | CE1-NE2-CD2 | -6.19 | 102.81 | 109.00 |
| 18 | l | 13 | HIS | CE1-NE2-CD2 | -6.19 | 102.81 | 109.00 |
| 8 | N | 761 | PHE | N-CA-CB | 6.19 | 117.47 | 110.35 |
| 8 | P | 1201 | ILE | CA-CB-CG2 | 6.19 | 121.02 | 110.50 |
| 9 | R | 584 | LYS | CA-C-N | -6.19 | 114.46 | 123.00 |
| 9 | R | 584 | LYS | C-N-CA | -6.19 | 114.46 | 123.00 |
| 12 | v | 130 | VAL | O-C-N | -6.19 | 116.74 | 123.18 |
| 2 | 1 | 92 | GLN | N-CA-C | 6.19 | 120.96 | 113.41 |
| 14 | h | 172 | GLN | N-CA-CB | 6.19 | 120.95 | 110.49 |
| 18 | l | 146 | ARG | NE-CZ-NH1 | 6.19 | 127.69 | 121.50 |
| 15 | b | 185 | LEU | CA-C-N | 6.19 | 128.57 | 120.28 |
| 15 | b | 185 | LEU | C-N-CA | 6.19 | 128.57 | 120.28 |
| 5 | E | 507 | ASN | CA-CB-CG | -6.19 | 106.41 | 112.60 |
| 5 | H | 390 | HIS | CA-C-N | 6.19 | 129.19 | 120.28 |
| 5 | H | 390 | HIS | C-N-CA | 6.19 | 129.19 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | H | 440 | PHE | N-CA-CB | 6.19 | 119.22 | 110.12 |
| 6 | L | 348 | GLN | OE1-CD-NE2 | -6.19 | 116.41 | 122.60 |
| 8 | P | 1049 | ASP | N-CA-CB | 6.19 | 119.08 | 110.17 |
| 9 | R | 294 | MET | N-CA-CB | 6.19 | 120.95 | 110.49 |
| 20 | n | 263 | THR | N-CA-C | -6.19 | 101.36 | 110.52 |
| 17 | d | 113 | GLY | CA-C-N | 6.19 | 127.58 | 119.84 |
| 17 | d | 113 | GLY | C-N-CA | 6.19 | 127.58 | 119.84 |
| 19 | f | 213 | CYS | N-CA-CB | 6.19 | 119.87 | 110.28 |
| 16 | c | 523 | ASN | CA-C-N | 6.19 | 129.19 | 120.28 |
| 16 | c | 523 | ASN | C-N-CA | 6.19 | 129.19 | 120.28 |
| 19 | f | 427 | GLU | N-CA-CB | 6.19 | 120.51 | 111.54 |
| 14 | a | 693 | PHE | CA-CB-CG | -6.19 | 107.61 | 113.80 |
| 1 | 0 | 1095 | LYS | CA-C-N | 6.18 | 129.41 | 120.38 |
| 1 | 0 | 1095 | LYS | C-N-CA | 6.18 | 129.41 | 120.38 |
| 5 | B | 472 | ASN | CA-CB-CG | -6.18 | 106.42 | 112.60 |
| 8 | N | 162 | HIS | CE1-NE2-CD2 | -6.18 | 102.82 | 109.00 |
| 8 | N | 333 | ARG | N-CA-C | -6.18 | 106.37 | 114.04 |
| 9 | S | 68 | LYS | N-CA-CB | 6.18 | 119.21 | 110.12 |
| 4 | A | 791 | ILE | CA-CB-CG1 | 6.18 | 120.91 | 110.40 |
| 6 | C | 439 | ILE | N-CA-C | -6.18 | 106.71 | 112.83 |
| 6 | F | 333 | ILE | O-C-N | 6.18 | 127.87 | 121.87 |
| 4 | G | 810 | ASN | CA-C-N | 6.18 | 129.07 | 120.29 |
| 4 | G | 810 | ASN | C-N-CA | 6.18 | 129.07 | 120.29 |
| 8 | N | 163 | ASP | N-CA-C | -6.18 | 104.22 | 112.94 |
| 7 | O | 713 | PHE | CA-CB-CG | 6.18 | 119.98 | 113.80 |
| 8 | P | 992 | SER | CA-C-N | 6.18 | 129.89 | 121.05 |
| 8 | P | 992 | SER | C-N-CA | 6.18 | 129.89 | 121.05 |
| 20 | n | 760 | ILE | CA-C-O | 6.18 | 128.51 | 120.78 |
| 21 | o | 75 | HIS | CB-CG-CD2 | -6.18 | 123.16 | 131.20 |
| 16 | c | 182 | LYS | CA-C-O | 6.18 | 126.98 | 119.31 |
| 14 | a | 122 | ILE | CB-CA-C | -6.18 | 104.55 | 111.23 |
| 5 | E | 339 | MET | N-CA-CB | 6.18 | 119.31 | 110.16 |
| 9 | R | 792 | SER | CA-C-N | 6.18 | 132.61 | 121.92 |
| 9 | R | 792 | SER | C-N-CA | 6.18 | 132.61 | 121.92 |
| 20 | n | 582 | GLU | N-CA-C | -6.18 | 105.70 | 113.18 |
| 2 | 1 | 1343 | MET | N-CA-C | 6.18 | 118.09 | 111.36 |
| 5 | H | 403 | SER | N-CA-CB | 6.18 | 118.97 | 110.01 |
| 7 | M | 528 | LEU | N-CA-C | 6.18 | 117.71 | 110.97 |
| 8 | P | 785 | ILE | CA-CB-CG1 | 6.18 | 120.91 | 110.40 |
| 9 | Q | 49 | LEU | N-CA-CB | 6.18 | 120.93 | 110.49 |
| 9 | Q | 754 | ARG | NE-CZ-NH1 | -6.18 | 115.32 | 121.50 |
| 9 | T | 829 | TYR | CA-C-O | -6.18 | 113.87 | 120.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 906 | LEU | CA-C-O | 6.18 | 125.58 | 118.97 |
| 9 | R | 282 | PHE | O-C-N | 6.18 | 130.71 | 122.43 |
| 13 | w | 1110 | GLN | N-CA-CB | 6.18 | 120.54 | 110.90 |
| 16 | c | 499 | ASP | CA-CB-CG | 6.18 | 118.78 | 112.60 |
| 8 | N | 957 | THR | CA-C-N | 6.18 | 131.93 | 122.23 |
| 8 | N | 957 | THR | C-N-CA | 6.18 | 131.93 | 122.23 |
| 8 | P | 1193 | ASN | CA-CB-CG | -6.18 | 106.42 | 112.60 |
| 9 | R | 94 | GLN | CA-C-N | 6.18 | 129.70 | 120.31 |
| 9 | R | 94 | GLN | C-N-CA | 6.18 | 129.70 | 120.31 |
| 1 | Y | 164 | PHE | CA-C-N | 6.18 | 128.56 | 120.28 |
| 1 | Y | 164 | PHE | C-N-CA | 6.18 | 128.56 | 120.28 |
| 2 | 1 | 1380 | GLN | OE1-CD-NE2 | 6.17 | 128.78 | 122.60 |
| 4 | D | 744 | ALA | N-CA-C | -6.17 | 104.11 | 112.26 |
| 7 | M | 1404 | ASP | CA-CB-CG | 6.17 | 118.77 | 112.60 |
| 8 | N | 764 | LYS | N-CA-C | -6.17 | 105.25 | 114.64 |
| 9 | R | 827 | GLU | N-CA-C | 6.17 | 118.01 | 111.28 |
| 11 | V | 293 | HIS | O-C-N | 6.17 | 130.50 | 122.97 |
| 2 | Z | 1352 | GLN | N-CA-C | -6.17 | 105.33 | 112.92 |
| 14 | h | 329 | TRP | N-CA-C | 6.17 | 119.18 | 110.23 |
| 16 | j | 556 | VAL | CA-C-N | 6.17 | 128.55 | 120.28 |
| 16 | j | 556 | VAL | C-N-CA | 6.17 | 128.55 | 120.28 |
| 20 | n | 147 | ASP | CA-CB-CG | 6.17 | 118.78 | 112.60 |
| 19 | f | 171 | VAL | N-CA-C | -6.17 | 103.92 | 112.50 |
| 2 | 1 | 882 | ASP | CA-CB-CG | 6.17 | 118.77 | 112.60 |
| 9 | S | 370 | TYR | CB-CG-CD1 | -6.17 | 111.54 | 120.80 |
| 9 | T | 796 | SER | N-CA-C | -6.17 | 99.30 | 108.99 |
| 4 | A | 679 | LEU | CA-C-N | 6.17 | 128.46 | 120.44 |
| 4 | A | 679 | LEU | C-N-CA | 6.17 | 128.46 | 120.44 |
| 13 | w | 1391 | ALA | CA-C-N | 6.17 | 129.05 | 120.29 |
| 13 | w | 1391 | ALA | C-N-CA | 6.17 | 129.05 | 120.29 |
| 20 | g | 838 | GLU | CA-C-O | 6.17 | 126.19 | 119.15 |
| 20 | g | 478 | PHE | CA-CB-CG | -6.17 | 107.63 | 113.80 |
| 2 | 1 | 634 | SER | CB-CA-C | -6.17 | 101.08 | 109.28 |
| 2 | 1 | 1039 | LEU | CB-CA-C | -6.17 | 98.38 | 110.10 |
| 4 | G | 808 | ASP | CA-C-O | -6.17 | 112.88 | 119.97 |
| 6 | L | 402 | ASP | N-CA-C | -6.17 | 104.64 | 111.36 |
| 7 | O | 1002 | LEU | CA-C-N | 6.17 | 128.46 | 120.44 |
| 7 | O | 1002 | LEU | C-N-CA | 6.17 | 128.46 | 120.44 |
| 7 | O | 1244 | ASN | CA-CB-CG | 6.17 | 118.77 | 112.60 |
| 8 | P | 569 | LEU | N-CA-C | -6.17 | 104.36 | 113.61 |
| 9 | S | 577 | ARG | NE-CZ-NH1 | 6.17 | 127.67 | 121.50 |
| 9 | T | 87 | ILE | CA-C-O | -6.17 | 114.64 | 121.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | v | 188 | SER | N-CA-C | -6.17 | 101.64 | 110.59 |
| 4 | z | 642 | THR | CA-C-N | 6.17 | 128.55 | 120.28 |
| 4 | z | 642 | THR | C-N-CA | 6.17 | 128.55 | 120.28 |
| 20 | n | 761 | ASN | N-CA-C | -6.17 | 101.07 | 110.14 |
| 16 | c | 489 | HIS | ND1-CE1-NE2 | 6.17 | 114.57 | 108.40 |
| 17 | d | 85 | GLU | CB-CA-C | -6.17 | 102.39 | 111.77 |
| 18 | e | 192 | ILE | CA-CB-CG1 | 6.17 | 120.89 | 110.40 |
| 20 | g | 946 | LYS | CA-CB-CG | 6.17 | 126.44 | 114.10 |
| 9 | R | 582 | GLU | CB-CG-CD | -6.17 | 102.12 | 112.60 |
| 2 | Z | 751 | GLN | N-CA-C | -6.17 | 104.83 | 112.72 |
| 12 | u | 139 | ASP | CA-CB-CG | 6.17 | 118.77 | 112.60 |
| 14 | h | 777 | PHE | N-CA-CB | 6.17 | 118.95 | 110.01 |
| 18 | e | 157 | LEU | CA-C-N | 6.17 | 128.83 | 120.44 |
| 18 | e | 157 | LEU | C-N-CA | 6.17 | 128.83 | 120.44 |
| 1 | 0 | 1289 | ILE | N-CA-C | -6.17 | 104.62 | 113.07 |
| 1 | 0 | 1458 | SER | N-CA-C | -6.17 | 103.45 | 113.19 |
| 2 | 1 | 409 | ILE | N-CA-CB | 6.17 | 118.04 | 112.06 |
| 12 | v | 259 | LEU | CA-C-O | -6.17 | 114.35 | 120.82 |
| 20 | n | 288 | ASN | CA-C-O | 6.17 | 126.00 | 119.03 |
| 19 | f | 689 | ALA | N-CA-C | -6.17 | 105.04 | 113.30 |
| 2 | 1 | 981 | GLN | N-CA-CB | 6.16 | 119.18 | 110.12 |
| 7 | M | 9 | GLN | N-CA-C | 6.16 | 120.97 | 112.90 |
| 7 | M | 1374 | LYS | N-CA-C | 6.16 | 120.41 | 113.01 |
| 7 | M | 1392 | ILE | CB-CA-C | -6.16 | 103.72 | 112.22 |
| 8 | P | 684 | LYS | N-CA-C | -6.16 | 105.41 | 113.17 |
| 9 | R | 489 | GLY | CA-C-N | 6.16 | 128.54 | 120.28 |
| 9 | R | 489 | GLY | C-N-CA | 6.16 | 128.54 | 120.28 |
| 9 | T | 315 | LYS | O-C-N | 6.16 | 128.46 | 121.93 |
| 1 | Y | 1426 | MET | CG-SD-CE | -6.16 | 87.34 | 100.90 |
| 12 | v | 308 | ASP | N-CA-CB | 6.16 | 120.91 | 110.49 |
| 16 | j | 441 | ARG | CA-C-O | 6.16 | 122.21 | 118.33 |
| 7 | M | 119 | PHE | CA-C-N | 6.16 | 128.40 | 120.70 |
| 7 | M | 119 | PHE | C-N-CA | 6.16 | 128.40 | 120.70 |
| 7 | O | 306 | VAL | CA-C-N | 6.16 | 133.31 | 121.54 |
| 7 | O | 306 | VAL | C-N-CA | 6.16 | 133.31 | 121.54 |
| 9 | S | 148 | TRP | CA-C-N | 6.16 | 128.82 | 120.44 |
| 9 | S | 148 | TRP | C-N-CA | 6.16 | 128.82 | 120.44 |
| 14 | h | 632 | GLN | CB-CG-CD | 6.16 | 123.08 | 112.60 |
| 14 | h | 913 | ILE | CA-CB-CG2 | -6.16 | 100.03 | 110.50 |
| 5 | E | 351 | GLN | OE1-CD-NE2 | -6.16 | 116.44 | 122.60 |
| 7 | O | 1438 | VAL | O-C-N | 6.16 | 127.95 | 121.91 |
| 9 | T | 273 | VAL | N-CA-C | -6.16 | 104.50 | 110.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | b | 607 | ILE | O-C-N | -6.16 | 114.08 | 121.10 |
| 14 | a | 627 | TYR | N-CA-C | -6.16 | 104.49 | 111.14 |
| 14 | a | 958 | TRP | CB-CA-C | 6.16 | 120.47 | 109.38 |
| 6 | L | 293 | HIS | CB-CG-CD2 | -6.16 | 123.19 | 131.20 |
| 7 | M | 103 | LYS | O-C-N | 6.16 | 128.41 | 122.07 |
| 7 | O | 1172 | GLY | CA-C-N | 6.16 | 130.62 | 122.30 |
| 7 | O | 1172 | GLY | C-N-CA | 6.16 | 130.62 | 122.30 |
| 8 | P | 1253 | GLU | CA-C-O | -6.16 | 114.35 | 120.82 |
| 9 | T | 460 | GLU | N-CA-C | -6.16 | 105.77 | 113.28 |
| 10 | W | 282 | VAL | CA-C-N | 6.16 | 131.47 | 123.10 |
| 10 | W | 282 | VAL | C-N-CA | 6.16 | 131.47 | 123.10 |
| 1 | Y | 1267 | GLU | N-CA-C | 6.16 | 117.66 | 111.07 |
| 12 | u | 71 | VAL | O-C-N | 6.16 | 129.85 | 123.20 |
| 12 | u | 151 | ILE | CA-CB-CG2 | -6.16 | 100.03 | 110.50 |
| 17 | k | 99 | SER | CA-C-N | 6.16 | 132.22 | 122.36 |
| 17 | k | 99 | SER | C-N-CA | 6.16 | 132.22 | 122.36 |
| 15 | b | 308 | ASN | N-CA-C | -6.16 | 106.74 | 114.56 |
| 19 | f | 144 | TRP | N-CA-CB | 6.16 | 120.90 | 110.49 |
| 20 | g | 181 | ILE | N-CA-C | -6.16 | 106.75 | 111.62 |
| 9 | Q | 148 | TRP | CA-C-N | 6.16 | 128.81 | 120.44 |
| 9 | Q | 148 | TRP | C-N-CA | 6.16 | 128.81 | 120.44 |
| 2 | Z | 508 | PHE | O-C-N | 6.16 | 130.72 | 122.96 |
| 15 | b | 209 | LEU | CA-C-N | 6.16 | 129.67 | 120.31 |
| 15 | b | 209 | LEU | C-N-CA | 6.16 | 129.67 | 120.31 |
| 1 | 0 | 176 | PHE | N-CA-CB | 6.16 | 120.51 | 110.05 |
| 7 | O | 83 | LEU | N-CA-C | -6.16 | 97.69 | 110.80 |
| 9 | Q | 624 | THR | N-CA-C | 6.16 | 117.79 | 111.14 |
| 9 | S | 575 | ALA | N-CA-C | 6.16 | 117.99 | 111.28 |
| 2 | Z | 799 | ILE | O-C-N | -6.16 | 115.49 | 121.83 |
| 14 | h | 804 | GLY | O-C-N | 6.16 | 128.17 | 122.57 |
| 15 | b | 730 | ASN | CB-CA-C | -6.16 | 100.38 | 110.85 |
| 20 | g | 115 | LYS | CA-C-N | 6.16 | 130.87 | 122.19 |
| 20 | g | 115 | LYS | C-N-CA | 6.16 | 130.87 | 122.19 |
| 14 | a | 318 | ASN | CB-CG-ND2 | 6.16 | 125.63 | 116.40 |
| 1 | 0 | 1356 | LYS | CA-C-N | 6.15 | 131.16 | 121.56 |
| 1 | 0 | 1356 | LYS | C-N-CA | 6.15 | 131.16 | 121.56 |
| 7 | M | 1296 | LEU | CB-CA-C | -6.15 | 101.22 | 110.88 |
| 8 | N | 1391 | LEU | CA-C-N | 6.15 | 128.44 | 120.44 |
| 8 | N | 1391 | LEU | C-N-CA | 6.15 | 128.44 | 120.44 |
| 7 | O | 535 | PHE | CA-C-N | 6.15 | 131.53 | 121.87 |
| 7 | O | 535 | PHE | C-N-CA | 6.15 | 131.53 | 121.87 |
| 9 | R | 152 | LYS | N-CA-CB | 6.15 | 118.99 | 110.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 977 | ALA | N-CA-C | -6.15 | 105.70 | 112.72 |
| 2 | 1 | 308 | ASN | N-CA-C | 6.15 | 119.74 | 107.62 |
| 7 | M | 1586 | LEU | CA-C-N | 6.15 | 128.52 | 120.28 |
| 7 | M | 1586 | LEU | C-N-CA | 6.15 | 128.52 | 120.28 |
| 7 | O | 154 | GLN | CA-C-N | 6.15 | 128.77 | 120.65 |
| 7 | O | 154 | GLN | C-N-CA | 6.15 | 128.77 | 120.65 |
| 7 | O | 783 | ILE | CA-CB-CG1 | 6.15 | 120.86 | 110.40 |
| 7 | O | 1139 | ILE | CA-C-O | 6.15 | 125.72 | 119.20 |
| 8 | P | 1177 | SER | CA-C-O | 6.15 | 127.05 | 119.97 |
| 9 | R | 42 | ILE | N-CA-CB | 6.15 | 121.38 | 111.23 |
| 9 | R | 347 | LYS | N-CA-C | 6.15 | 118.06 | 111.36 |
| 10 | W | 258 | TYR | N-CA-C | -6.15 | 102.59 | 108.13 |
| 14 | h | 7 | ILE | N-CA-C | -6.15 | 99.29 | 108.46 |
| 14 | h | 422 | ARG | N-CA-C | -6.15 | 103.07 | 111.56 |
| 15 | i | 344 | ARG | CD-NE-CZ | -6.15 | 115.79 | 124.40 |
| 19 | f | 416 | TYR | CA-C-N | 6.15 | 129.16 | 120.42 |
| 19 | f | 416 | TYR | C-N-CA | 6.15 | 129.16 | 120.42 |
| 20 | g | 861 | ILE | N-CA-C | -6.15 | 106.99 | 112.90 |
| 1 | 0 | 1344 | PHE | CA-C-N | 6.15 | 129.02 | 120.29 |
| 1 | 0 | 1344 | PHE | C-N-CA | 6.15 | 129.02 | 120.29 |
| 4 | A | 660 | LYS | CB-CA-C | 6.15 | 121.00 | 110.79 |
| 7 | M | 1065 | LYS | N-CA-CB | 6.15 | 121.42 | 112.13 |
| 7 | O | 48 | ARG | NE-CZ-NH1 | 6.15 | 127.65 | 121.50 |
| 9 | Q | 241 | ILE | N-CA-C | -6.15 | 105.06 | 111.58 |
| 9 | T | 371 | PHE | CA-CB-CG | -6.15 | 107.65 | 113.80 |
| 1 | Y | 661 | ASP | CA-CB-CG | 6.15 | 118.75 | 112.60 |
| 1 | Y | 1485 | GLU | CA-C-N | 6.15 | 128.44 | 120.44 |
| 1 | Y | 1485 | GLU | C-N-CA | 6.15 | 128.44 | 120.44 |
| 12 | u | 693 | ILE | N-CA-CB | 6.15 | 118.91 | 110.54 |
| 12 | v | 176 | ASP | CA-CB-CG | 6.15 | 118.75 | 112.60 |
| 21 | o | 91 | THR | N-CA-C | -6.15 | 97.70 | 110.80 |
| 17 | k | 103 | ASN | N-CA-CB | -6.15 | 102.39 | 110.88 |
| 20 | n | 927 | ALA | CB-CA-C | -6.15 | 98.86 | 110.67 |
| 2 | 1 | 237 | PHE | CA-CB-CG | 6.15 | 119.95 | 113.80 |
| 5 | B | 378 | HIS | O-C-N | 6.15 | 128.40 | 122.07 |
| 7 | M | 1096 | LEU | CA-C-N | 6.15 | 129.34 | 120.79 |
| 7 | M | 1096 | LEU | C-N-CA | 6.15 | 129.34 | 120.79 |
| 7 | O | 1208 | GLU | CA-C-N | 6.15 | 126.11 | 119.78 |
| 7 | O | 1208 | GLU | C-N-CA | 6.15 | 126.11 | 119.78 |
| 2 | Z | 620 | VAL | CA-C-N | 6.15 | 130.99 | 120.72 |
| 2 | Z | 620 | VAL | C-N-CA | 6.15 | 130.99 | 120.72 |
| 15 | i | 388 | ASN | N-CA-CB | 6.15 | 120.88 | 110.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 586 | ASP | CA-CB-CG | 6.15 | 118.75 | 112.60 |
| 16 | j | 439 | ARG | NE-CZ-NH2 | -6.15 | 113.67 | 119.20 |
| 19 | f | 263 | ILE | CA-C-N | 6.15 | 129.65 | 120.31 |
| 19 | f | 263 | ILE | C-N-CA | 6.15 | 129.65 | 120.31 |
| 14 | a | 513 | LEU | CA-C-O | -6.15 | 111.87 | 119.18 |
| 1 | 0 | 1465 | ILE | CA-C-N | 6.14 | 130.38 | 120.55 |
| 1 | 0 | 1465 | ILE | C-N-CA | 6.14 | 130.38 | 120.55 |
| 4 | G | 727 | SER | CA-CB-OG | -6.14 | 98.81 | 111.10 |
| 7 | O | 236 | ALA | N-CA-C | 6.14 | 117.98 | 111.28 |
| 9 | R | 372 | LYS | O-C-N | -6.14 | 115.61 | 122.12 |
| 1 | Y | 509 | PHE | CA-C-N | 6.14 | 131.85 | 122.08 |
| 1 | Y | 509 | PHE | C-N-CA | 6.14 | 131.85 | 122.08 |
| 13 | x | 1218 | PHE | CA-C-N | 6.14 | 128.43 | 120.44 |
| 13 | x | 1218 | PHE | C-N-CA | 6.14 | 128.43 | 120.44 |
| 14 | h | 264 | ASP | CA-C-N | 6.14 | 133.28 | 121.54 |
| 14 | h | 264 | ASP | C-N-CA | 6.14 | 133.28 | 121.54 |
| 19 | m | 146 | ASN | CA-CB-CG | 6.14 | 118.74 | 112.60 |
| 20 | n | 397 | PRO | N-CA-C | 6.14 | 120.88 | 111.11 |
| 21 | p | 21 | LYS | O-C-N | 6.14 | 128.48 | 122.09 |
| 14 | a | 378 | TRP | N-CA-CB | 6.14 | 119.11 | 109.83 |
| 1 | 0 | 142 | LEU | N-CA-C | -6.14 | 99.96 | 109.24 |
| 2 | 1 | 1264 | SER | CA-C-N | 6.14 | 131.12 | 120.86 |
| 2 | 1 | 1264 | SER | C-N-CA | 6.14 | 131.12 | 120.86 |
| 6 | C | 293 | HIS | ND1-CE1-NE2 | 6.14 | 114.54 | 108.40 |
| 8 | N | 148 | VAL | O-C-N | -6.14 | 113.64 | 122.12 |
| 7 | O | 420 | THR | N-CA-C | -6.14 | 97.82 | 108.69 |
| 9 | S | 87 | ILE | CA-C-N | 6.14 | 128.43 | 120.44 |
| 9 | S | 87 | ILE | C-N-CA | 6.14 | 128.43 | 120.44 |
| 1 | Y | 1198 | ASN | N-CA-CB | 6.14 | 120.87 | 110.49 |
| 15 | b | 666 | LEU | N-CA-C | 6.14 | 117.64 | 111.07 |
| 1 | 0 | 110 | HIS | CE1-NE2-CD2 | -6.14 | 102.86 | 109.00 |
| 9 | T | 475 | SER | CA-C-N | 6.14 | 133.27 | 121.54 |
| 9 | T | 475 | SER | C-N-CA | 6.14 | 133.27 | 121.54 |
| 15 | b | 592 | ASN | CA-C-O | 6.14 | 125.89 | 119.14 |
| 7 | M | 502 | ASP | CA-CB-CG | 6.14 | 118.74 | 112.60 |
| 7 | M | 1400 | ALA | N-CA-C | 6.14 | 118.05 | 111.36 |
| 8 | N | 1517 | GLU | CA-C-O | 6.14 | 127.06 | 120.55 |
| 8 | P | 1070 | LYS | CA-C-N | 6.14 | 130.97 | 120.72 |
| 8 | P | 1070 | LYS | C-N-CA | 6.14 | 130.97 | 120.72 |
| 1 | Y | 268 | ILE | N-CA-C | -6.14 | 101.64 | 109.80 |
| 18 | e | 309 | SER | N-CA-C | 6.14 | 118.42 | 107.80 |
| 19 | f | 587 | TYR | CA-C-O | -6.14 | 114.37 | 120.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 1231 | GLU | O-C-N | 6.14 | 128.61 | 122.10 |
| 21 | p | 71 | HIS | CG-CD2-NE2 | 6.14 | 113.34 | 107.20 |
| 17 | d | 15 | ALA | CA-C-O | 6.14 | 126.29 | 120.09 |
| 1 | 0 | 1261 | ARG | NE-CZ-NH2 | 6.14 | 124.72 | 119.20 |
| 5 | E | 381 | GLU | N-CA-C | 6.14 | 117.97 | 111.28 |
| 6 | L | 464 | THR | CA-C-O | -6.14 | 112.91 | 119.97 |
| 9 | Q | 321 | LYS | N-CA-C | -6.14 | 105.10 | 112.59 |
| 2 | Z | 447 | LYS | N-CA-C | -6.14 | 100.08 | 109.41 |
| 12 | u | 636 | ASN | O-C-N | 6.14 | 128.41 | 122.03 |
| 12 | v | 126 | SER | O-C-N | 6.14 | 130.42 | 122.87 |
| 14 | h | 233 | TYR | CB-CG-CD1 | 6.14 | 130.00 | 120.80 |
| 18 | l | 89 | ASP | CA-C-N | 6.14 | 130.57 | 120.94 |
| 18 | l | 89 | ASP | C-N-CA | 6.14 | 130.57 | 120.94 |
| 20 | n | 858 | ASN | CA-C-N | 6.14 | 133.72 | 122.92 |
| 20 | n | 858 | ASN | C-N-CA | 6.14 | 133.72 | 122.92 |
| 20 | g | 905 | ASN | CA-CB-CG | -6.14 | 106.46 | 112.60 |
| 14 | a | 146 | ASN | N-CA-CB | 6.14 | 120.91 | 111.46 |
| 14 | a | 220 | TYR | N-CA-CB | 6.14 | 119.01 | 110.17 |
| 14 | a | 437 | ASN | CB-CA-C | -6.14 | 98.97 | 109.65 |
| 14 | a | 527 | SER | CA-C-O | -6.14 | 111.83 | 119.38 |
| 4 | J | 693 | ILE | N-CA-C | -6.13 | 106.76 | 112.83 |
| 7 | M | 776 | VAL | N-CA-C | 6.13 | 116.92 | 110.72 |
| 7 | O | 772 | ASN | N-CA-C | -6.13 | 106.43 | 114.04 |
| 12 | v | 328 | PHE | O-C-N | -6.13 | 115.91 | 123.33 |
| 16 | j | 289 | ASN | N-CA-CB | 6.13 | 121.57 | 111.08 |
| 7 | M | 40 | ASP | CA-C-O | 6.13 | 126.53 | 119.35 |
| 8 | N | 1439 | LEU | O-C-N | 6.13 | 128.62 | 122.12 |
| 8 | P | 192 | LEU | CA-C-N | 6.13 | 128.82 | 120.54 |
| 8 | P | 192 | LEU | C-N-CA | 6.13 | 128.82 | 120.54 |
| 9 | R | 670 | LEU | CA-C-O | -6.13 | 112.35 | 119.59 |
| 9 | T | 340 | LEU | CA-C-N | 6.13 | 128.41 | 120.44 |
| 9 | T | 340 | LEU | C-N-CA | 6.13 | 128.41 | 120.44 |
| 9 | T | 461 | ASP | N-CA-C | -6.13 | 104.50 | 112.23 |
| 2 | Z | 166 | PHE | CA-C-N | 6.13 | 128.41 | 120.44 |
| 2 | Z | 166 | PHE | C-N-CA | 6.13 | 128.41 | 120.44 |
| 20 | n | 819 | GLN | CB-CG-CD | -6.13 | 102.17 | 112.60 |
| 6 | F | 375 | LYS | CA-C-N | 6.13 | 129.00 | 120.29 |
| 6 | F | 375 | LYS | C-N-CA | 6.13 | 129.00 | 120.29 |
| 7 | O | 625 | GLU | O-C-N | 6.13 | 129.39 | 122.22 |
| 7 | O | 1214 | SER | CA-C-O | -6.13 | 111.74 | 120.51 |
| 9 | S | 67 | THR | N-CA-CB | 6.13 | 120.85 | 110.49 |
| 1 | Y | 854 | ILE | CA-CB-CG2 | -6.13 | 100.08 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 650 | HIS | ND1-CE1-NE2 | 6.13 | 114.53 | 108.40 |
| 20 | n | 575 | PHE | CA-CB-CG | 6.13 | 119.93 | 113.80 |
| 20 | n | 785 | HIS | CE1-NE2-CD2 | -6.13 | 102.87 | 109.00 |
| 20 | g | 103 | LYS | N-CA-C | -6.13 | 106.44 | 114.04 |
| 7 | M | 1411 | HIS | O-C-N | -6.13 | 115.62 | 122.12 |
| 8 | N | 1411 | SER | CA-C-N | 6.13 | 129.00 | 120.29 |
| 8 | N | 1411 | SER | C-N-CA | 6.13 | 129.00 | 120.29 |
| 1 | Y | 940 | VAL | CA-C-O | -6.13 | 114.35 | 120.85 |
| 14 | h | 776 | ILE | CA-C-N | 6.13 | 128.41 | 120.44 |
| 14 | h | 776 | ILE | C-N-CA | 6.13 | 128.41 | 120.44 |
| 15 | b | 561 | ARG | N-CA-C | -6.13 | 105.56 | 113.16 |
| 7 | M | 1604 | ILE | O-C-N | 6.13 | 127.81 | 121.87 |
| 8 | N | 501 | SER | N-CA-C | -6.13 | 100.02 | 109.52 |
| 8 | P | 455 | PHE | CB-CA-C | -6.13 | 100.97 | 110.78 |
| 9 | T | 163 | ILE | CB-CA-C | -6.13 | 102.33 | 112.26 |
| 13 | x | 1227 | VAL | CA-C-N | 6.13 | 129.62 | 120.31 |
| 13 | x | 1227 | VAL | C-N-CA | 6.13 | 129.62 | 120.31 |
| 4 | D | 710 | PHE | CA-C-O | -6.13 | 114.06 | 120.55 |
| 5 | E | 302 | ASN | CB-CA-C | -6.13 | 108.25 | 117.07 |
| 5 | K | 330 | VAL | N-CA-C | -6.13 | 98.88 | 108.81 |
| 7 | O | 1108 | ARG | N-CA-C | 6.13 | 118.75 | 111.71 |
| 11 | V | 355 | TRP | CA-C-O | 6.13 | 127.12 | 120.32 |
| 13 | x | 1215 | GLU | N-CA-C | 6.13 | 117.62 | 111.07 |
| 19 | f | 456 | GLN | OE1-CD-NE2 | -6.13 | 116.47 | 122.60 |
| 20 | g | 333 | ILE | N-CA-C | -6.13 | 105.39 | 111.88 |
| 7 | O | 1627 | LYS | CA-C-N | 6.12 | 126.74 | 119.94 |
| 7 | O | 1627 | LYS | C-N-CA | 6.12 | 126.74 | 119.94 |
| 8 | P | 325 | TRP | CA-C-N | 6.12 | 129.46 | 120.82 |
| 8 | P | 325 | TRP | C-N-CA | 6.12 | 129.46 | 120.82 |
| 8 | P | 455 | PHE | CA-CB-CG | -6.12 | 107.67 | 113.80 |
| 1 | Y | 144 | ALA | N-CA-CB | 6.12 | 120.84 | 110.49 |
| 1 | Y | 1158 | HIS | N-CA-C | -6.12 | 104.69 | 111.36 |
| 12 | u | 213 | PRO | CA-C-N | 6.12 | 128.81 | 120.54 |
| 12 | u | 213 | PRO | C-N-CA | 6.12 | 128.81 | 120.54 |
| 12 | v | 162 | LYS | CA-C-O | -6.12 | 113.98 | 120.23 |
| 15 | i | 136 | PHE | O-C-N | -6.12 | 114.45 | 122.59 |
| 16 | j | 441 | ARG | N-CA-CB | 6.12 | 120.84 | 110.49 |
| 2 | 1 | 1349 | ASP | CA-CB-CG | 6.12 | 118.72 | 112.60 |
| 6 | I | 278 | GLU | O-C-N | 6.12 | 128.70 | 122.09 |
| 7 | O | 545 | HIS | N-CA-CB | 6.12 | 119.65 | 110.22 |
| 7 | O | 1310 | VAL | CA-CB-CG1 | -6.12 | 99.99 | 110.40 |
| 8 | P | 366 | SER | CA-C-N | 6.12 | 128.77 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 366 | SER | C-N-CA | 6.12 | 128.77 | 120.44 |
| 9 | S | 711 | LYS | CA-C-N | 6.12 | 128.48 | 120.28 |
| 9 | S | 711 | LYS | C-N-CA | 6.12 | 128.48 | 120.28 |
| 9 | T | 61 | LYS | N-CA-C | -6.12 | 104.64 | 113.21 |
| 9 | T | 414 | LEU | CA-C-O | 6.12 | 126.01 | 119.34 |
| 17 | k | 58 | ARG | NE-CZ-NH1 | 6.12 | 127.62 | 121.50 |
| 21 | p | 51 | VAL | N-CA-C | 6.12 | 116.28 | 110.53 |
| 2 | 1 | 773 | PHE | CA-CB-CG | -6.12 | 107.68 | 113.80 |
| 14 | h | 583 | LEU | CA-C-O | 6.12 | 127.01 | 119.79 |
| 15 | i | 55 | ASP | N-CA-C | -6.12 | 97.86 | 108.69 |
| 2 | 1 | 804 | SER | CA-C-N | 6.12 | 130.33 | 120.30 |
| 2 | 1 | 804 | SER | C-N-CA | 6.12 | 130.33 | 120.30 |
| 6 | C | 325 | TYR | CA-C-N | 6.12 | 128.48 | 120.28 |
| 6 | C | 325 | TYR | C-N-CA | 6.12 | 128.48 | 120.28 |
| 7 | M | 38 | ASN | CA-CB-CG | 6.12 | 118.72 | 112.60 |
| 7 | O | 62 | SER | N-CA-CB | 6.12 | 120.83 | 110.49 |
| 7 | O | 1008 | SER | N-CA-C | 6.12 | 117.75 | 111.14 |
| 9 | S | 570 | GLU | CA-C-N | 6.12 | 129.09 | 120.28 |
| 9 | S | 570 | GLU | C-N-CA | 6.12 | 129.09 | 120.28 |
| 15 | i | 683 | MET | CA-C-O | 6.12 | 127.83 | 121.10 |
| 18 | e | 103 | THR | N-CA-C | -6.12 | 96.84 | 107.49 |
| 7 | O | 632 | SER | O-C-N | 6.12 | 128.60 | 122.12 |
| 19 | m | 97 | HIS | CA-C-O | -6.12 | 113.64 | 120.25 |
| 20 | n | 825 | ASP | CB-CA-C | -6.12 | 101.17 | 111.02 |
| 20 | g | 549 | MET | O-C-N | 6.12 | 129.59 | 122.19 |
| 7 | M | 911 | SER | N-CA-CB | 6.12 | 119.11 | 110.12 |
| 8 | N | 802 | LEU | CA-C-N | 6.12 | 129.09 | 120.28 |
| 8 | N | 802 | LEU | C-N-CA | 6.12 | 129.09 | 120.28 |
| 7 | O | 150 | PHE | O-C-N | 6.12 | 128.60 | 122.12 |
| 7 | O | 736 | PHE | CA-CB-CG | -6.12 | 107.68 | 113.80 |
| 9 | R | 739 | MET | CA-C-O | 6.12 | 127.00 | 119.97 |
| 12 | v | 703 | GLN | N-CA-CB | 6.12 | 119.21 | 110.16 |
| 19 | m | 121 | ILE | O-C-N | -6.12 | 115.94 | 121.87 |
| 7 | O | 359 | GLN | CA-C-O | 6.11 | 125.77 | 119.05 |
| 9 | R | 687 | LEU | CA-C-N | 6.11 | 128.47 | 120.28 |
| 9 | R | 687 | LEU | C-N-CA | 6.11 | 128.47 | 120.28 |
| 19 | m | 436 | LEU | O-C-N | 6.11 | 130.43 | 122.97 |
| 20 | n | 1098 | THR | N-CA-C | -6.11 | 105.86 | 113.38 |
| 15 | b | 215 | SER | N-CA-C | -6.11 | 104.17 | 111.69 |
| 14 | a | 159 | THR | N-CA-CB | 6.11 | 119.18 | 110.13 |
| 1 | 0 | 1307 | LEU | N-CA-C | -6.11 | 98.65 | 108.55 |
| 8 | N | 48 | LYS | CA-C-N | 6.11 | 132.46 | 121.15 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 48 | LYS | C-N-CA | 6.11 | 132.46 | 121.15 |
| 8 | P | 507 | PRO | CA-C-O | -6.11 | 111.70 | 120.56 |
| 14 | h | 269 | HIS | CG-CD2-NE2 | 6.11 | 113.31 | 107.20 |
| 2 | 1 | 994 | ARG | NE-CZ-NH2 | -6.11 | 113.70 | 119.20 |
| 5 | K | 376 | LEU | N-CA-CB | 6.11 | 119.75 | 110.28 |
| 7 | O | 41 | LYS | N-CA-C | -6.11 | 103.25 | 111.87 |
| 1 | Y | 663 | ILE | N-CA-C | -6.11 | 107.17 | 113.10 |
| 1 | Y | 1396 | ASN | CA-CB-CG | 6.11 | 118.71 | 112.60 |
| 2 | Z | 1278 | ASP | CA-CB-CG | 6.11 | 118.71 | 112.60 |
| 12 | v | 128 | LYS | N-CA-C | -6.11 | 105.63 | 114.12 |
| 13 | w | 1280 | GLN | O-C-N | 6.11 | 128.60 | 122.12 |
| 4 | y | 796 | ILE | CB-CA-C | -6.11 | 103.89 | 112.14 |
| 13 | x | 1456 | LEU | CB-CA-C | 6.11 | 121.71 | 110.10 |
| 15 | i | 79 | MET | CG-SD-CE | -6.11 | 87.46 | 100.90 |
| 1 | Y | 1059 | TYR | N-CA-CB | 6.11 | 120.81 | 110.49 |
| 2 | Z | 1188 | ARG | NE-CZ-NH2 | -6.11 | 113.70 | 119.20 |
| 12 | u | 680 | TRP | CA-C-N | 6.11 | 128.38 | 120.44 |
| 12 | u | 680 | TRP | C-N-CA | 6.11 | 128.38 | 120.44 |
| 14 | h | 246 | TRP | N-CA-C | -6.11 | 100.47 | 109.81 |
| 19 | m | 393 | ALA | CB-CA-C | -6.11 | 100.65 | 110.79 |
| 21 | r | 63 | LYS | O-C-N | 6.11 | 129.86 | 122.35 |
| 15 | b | 111 | LEU | CA-C-N | 6.11 | 128.47 | 120.28 |
| 15 | b | 111 | LEU | C-N-CA | 6.11 | 128.47 | 120.28 |
| 1 | 0 | 140 | ASN | N-CA-CB | 6.11 | 120.81 | 110.49 |
| 1 | 0 | 1022 | ASP | CA-C-O | 6.11 | 129.24 | 120.51 |
| 6 | L | 377 | ILE | CA-C-N | 6.11 | 128.46 | 120.28 |
| 6 | L | 377 | ILE | C-N-CA | 6.11 | 128.46 | 120.28 |
| 8 | N | 1439 | LEU | CA-C-N | 6.11 | 126.72 | 120.00 |
| 8 | N | 1439 | LEU | C-N-CA | 6.11 | 126.72 | 120.00 |
| 8 | N | 1538 | ASP | N-CA-C | -6.11 | 105.12 | 113.30 |
| 19 | m | 146 | ASN | CA-C-O | 6.11 | 125.86 | 119.51 |
| 16 | c | 458 | ARG | CA-C-N | 6.11 | 129.59 | 120.31 |
| 16 | c | 458 | ARG | C-N-CA | 6.11 | 129.59 | 120.31 |
| 14 | a | 99 | ASN | CA-CB-CG | 6.11 | 118.70 | 112.60 |
| 2 | 1 | 238 | ASN | OD1-CG-ND2 | 6.10 | 128.70 | 122.60 |
| 8 | N | 1016 | LEU | O-C-N | 6.10 | 128.59 | 122.12 |
| 7 | O | 545 | HIS | CE1-NE2-CD2 | -6.10 | 102.90 | 109.00 |
| 9 | T | 511 | ALA | CA-C-N | 6.10 | 128.46 | 120.28 |
| 9 | T | 511 | ALA | C-N-CA | 6.10 | 128.46 | 120.28 |
| 4 | y | 809 | ASP | CA-C-N | 6.10 | 128.46 | 120.28 |
| 4 | y | 809 | ASP | C-N-CA | 6.10 | 128.46 | 120.28 |
| 4 | G | 671 | LYS | CA-C-N | 6.10 | 127.77 | 120.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | G | 671 | LYS | C-N-CA | 6.10 | 127.77 | 120.14 |
| 8 | N | 897 | LYS | N-CA-C | -6.10 | 97.80 | 110.80 |
| 8 | P | 1492 | HIS | CE1-NE2-CD2 | -6.10 | 102.90 | 109.00 |
| 14 | h | 780 | HIS | N-CA-CB | 6.10 | 121.79 | 110.99 |
| 15 | i | 168 | ARG | CA-C-N | 6.10 | 130.79 | 120.29 |
| 15 | i | 168 | ARG | C-N-CA | 6.10 | 130.79 | 120.29 |
| 16 | j | 234 | TRP | N-CA-CB | 6.10 | 119.19 | 110.16 |
| 21 | t | 50 | ASP | CB-CA-C | -6.10 | 100.66 | 110.79 |
| 14 | a | 86 | ASP | N-CA-CB | 6.10 | 122.04 | 112.46 |
| 1 | 0 | 1012 | ARG | CB-CG-CD | 6.10 | 125.33 | 111.30 |
| 9 | R | 246 | ASN | CA-C-O | 6.10 | 126.95 | 120.36 |
| 16 | c | 351 | ASP | CA-C-O | 6.10 | 126.95 | 120.36 |
| 1 | 0 | 1109 | PHE | CA-CB-CG | -6.10 | 107.70 | 113.80 |
| 2 | 1 | 641 | CYS | N-CA-C | -6.10 | 104.55 | 112.23 |
| 5 | E | 380 | LEU | N-CA-CB | 6.10 | 119.08 | 110.12 |
| 5 | K | 445 | GLN | OE1-CD-NE2 | -6.10 | 116.50 | 122.60 |
| 7 | O | 1279 | CYS | N-CA-CB | 6.10 | 118.85 | 110.01 |
| 9 | T | 563 | ASN | CA-CB-CG | -6.10 | 106.50 | 112.60 |
| 13 | x | 1396 | LEU | CA-C-N | 6.10 | 128.37 | 120.44 |
| 13 | x | 1396 | LEU | C-N-CA | 6.10 | 128.37 | 120.44 |
| 20 | n | 942 | ASN | CA-CB-CG | 6.10 | 118.70 | 112.60 |
| 1 | 0 | 184 | ILE | N-CA-CB | 6.10 | 121.46 | 111.58 |
| 2 | 1 | 679 | SER | CA-CB-OG | -6.10 | 98.90 | 111.10 |
| 5 | K | 421 | THR | CA-CB-OG1 | 6.10 | 118.75 | 109.60 |
| 6 | L | 314 | TYR | N-CA-CB | 6.10 | 119.21 | 110.06 |
| 7 | O | 14 | SER | CA-C-N | 6.10 | 130.10 | 120.47 |
| 7 | O | 14 | SER | C-N-CA | 6.10 | 130.10 | 120.47 |
| 7 | O | 1296 | LEU | O-C-N | 6.10 | 128.58 | 122.12 |
| 7 | O | 1334 | THR | CA-C-O | -6.10 | 112.69 | 120.31 |
| 1 | Y | 181 | ARG | N-CA-CB | 6.10 | 121.44 | 110.83 |
| 12 | v | 698 | ASN | CA-C-O | -6.10 | 114.42 | 120.82 |
| 13 | x | 1350 | PHE | N-CA-C | 6.10 | 117.59 | 111.07 |
| 15 | b | 194 | GLY | CA-C-O | -6.10 | 111.51 | 119.44 |
| 5 | B | 394 | THR | N-CA-C | -6.10 | 105.07 | 113.18 |
| 7 | M | 197 | LEU | N-CA-C | 6.10 | 117.59 | 111.07 |
| 8 | P | 389 | PHE | CA-C-N | 6.10 | 131.97 | 119.72 |
| 8 | P | 389 | PHE | C-N-CA | 6.10 | 131.97 | 119.72 |
| 9 | S | 619 | PHE | CA-C-N | 6.10 | 132.39 | 121.66 |
| 9 | S | 619 | PHE | C-N-CA | 6.10 | 132.39 | 121.66 |
| 4 | z | 818 | ILE | N-CA-CB | 6.10 | 118.83 | 110.54 |
| 15 | i | 72 | GLY | CA-C-N | 6.10 | 127.46 | 119.84 |
| 15 | i | 72 | GLY | C-N-CA | 6.10 | 127.46 | 119.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 708 | TRP | CB-CG-CD1 | -6.10 | 117.76 | 126.90 |
| 6 | F | 352 | VAL | N-CA-CB | 6.09 | 117.68 | 110.55 |
| 6 | I | 305 | ILE | N-CA-C | -6.09 | 104.56 | 110.72 |
| 4 | J | 678 | GLN | OE1-CD-NE2 | 6.09 | 128.69 | 122.60 |
| 4 | J | 794 | ILE | CB-CA-C | -6.09 | 102.22 | 112.16 |
| 7 | M | 1153 | TYR | CA-C-N | 6.09 | 128.94 | 120.29 |
| 7 | M | 1153 | TYR | C-N-CA | 6.09 | 128.94 | 120.29 |
| 9 | S | 461 | ASP | CA-CB-CG | 6.09 | 118.69 | 112.60 |
| 9 | T | 319 | SER | N-CA-CB | 6.09 | 120.79 | 110.49 |
| 1 | Y | 977 | LYS | N-CA-C | -6.09 | 100.69 | 110.14 |
| 2 | Z | 714 | LEU | CB-CA-C | 6.09 | 121.21 | 110.85 |
| 2 | 1 | 1053 | ARG | CD-NE-CZ | -6.09 | 115.87 | 124.40 |
| 5 | E | 298 | SER | CA-C-O | 6.09 | 128.99 | 120.52 |
| 7 | O | 172 | ASN | N-CA-CB | 6.09 | 119.00 | 110.04 |
| 8 | P | 465 | VAL | CA-CB-CG1 | -6.09 | 100.04 | 110.40 |
| 2 | Z | 351 | ARG | CA-C-O | -6.09 | 111.80 | 120.51 |
| 1 | 0 | 1385 | PHE | CA-C-N | 6.09 | 126.10 | 119.89 |
| 1 | 0 | 1385 | PHE | C-N-CA | 6.09 | 126.10 | 119.89 |
| 1 | 0 | 1445 | ASN | CA-CB-CG | 6.09 | 118.69 | 112.60 |
| 5 | B | 377 | ASN | CA-C-N | 6.09 | 128.36 | 120.44 |
| 5 | B | 377 | ASN | C-N-CA | 6.09 | 128.36 | 120.44 |
| 5 | B | 469 | ARG | NH1-CZ-NH2 | -6.09 | 111.38 | 119.30 |
| 7 | M | 1452 | SER | N-CA-C | 6.09 | 118.42 | 111.11 |
| 7 | O | 688 | SER | N-CA-C | -6.09 | 98.68 | 108.55 |
| 8 | P | 398 | ARG | NE-CZ-NH1 | 6.09 | 127.59 | 121.50 |
| 8 | P | 996 | THR | N-CA-C | -6.09 | 104.92 | 112.72 |
| 9 | R | 237 | GLU | N-CA-C | 6.09 | 118.70 | 111.33 |
| 9 | R | 434 | ASP | CA-C-O | 6.09 | 126.98 | 120.10 |
| 9 | R | 736 | LEU | N-CA-C | -6.09 | 104.55 | 111.07 |
| 1 | Y | 889 | GLU | N-CA-C | -6.09 | 105.65 | 114.12 |
| 15 | i | 387 | THR | CA-CB-CG2 | 6.09 | 120.85 | 110.50 |
| 21 | o | 37 | LEU | CA-C-N | 6.09 | 128.76 | 120.54 |
| 21 | o | 37 | LEU | C-N-CA | 6.09 | 128.76 | 120.54 |
| 2 | 1 | 1336 | VAL | CA-C-N | 6.09 | 129.27 | 120.38 |
| 2 | 1 | 1336 | VAL | C-N-CA | 6.09 | 129.27 | 120.38 |
| 7 | O | 256 | HIS | CE1-NE2-CD2 | -6.09 | 102.91 | 109.00 |
| 9 | R | 759 | ASP | CA-C-N | 6.09 | 132.32 | 120.99 |
| 9 | R | 759 | ASP | C-N-CA | 6.09 | 132.32 | 120.99 |
| 9 | T | 591 | GLY | CA-C-N | 6.09 | 131.79 | 122.11 |
| 9 | T | 591 | GLY | C-N-CA | 6.09 | 131.79 | 122.11 |
| 2 | Z | 1240 | ARG | NE-CZ-NH1 | 6.09 | 127.59 | 121.50 |
| 20 | n | 410 | THR | CA-CB-OG1 | 6.09 | 118.73 | 109.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | f | 393 | ALA | N-CA-C | 6.09 | 117.92 | 111.28 |
| 10 | U | 266 | ILE | CB-CA-C | -6.09 | 103.92 | 112.14 |
| 20 | n | 330 | THR | CA-CB-CG2 | -6.09 | 100.15 | 110.50 |
| 7 | M | 885 | GLU | CA-C-N | 6.09 | 133.17 | 121.54 |
| 7 | M | 885 | GLU | C-N-CA | 6.09 | 133.17 | 121.54 |
| 8 | N | 63 | THR | N-CA-C | -6.09 | 105.89 | 113.38 |
| 8 | N | 1436 | GLU | CA-C-O | -6.09 | 115.66 | 121.08 |
| 7 | O | 632 | SER | CA-CB-OG | 6.09 | 123.27 | 111.10 |
| 1 | Y | 1419 | ALA | N-CA-CB | 6.09 | 120.78 | 110.49 |
| 2 | Z | 1191 | LEU | CA-C-O | -6.09 | 114.43 | 120.82 |
| 12 | u | 420 | ILE | CB-CA-C | 6.09 | 118.28 | 111.59 |
| 12 | u | 648 | GLN | N-CA-C | 6.09 | 117.58 | 111.07 |
| 18 | l | 23 | HIS | CE1-NE2-CD2 | -6.09 | 102.91 | 109.00 |
| 15 | b | 482 | TRP | O-C-N | -6.09 | 114.32 | 121.32 |
| 16 | c | 651 | CYS | CB-CA-C | 6.09 | 122.53 | 110.42 |
| 8 | P | 276 | ASN | N-CA-CB | 6.08 | 120.77 | 110.49 |
| 8 | P | 1429 | HIS | CB-CG-CD2 | -6.08 | 123.29 | 131.20 |
| 10 | U | 337 | GLY | CA-C-O | 6.08 | 127.29 | 119.68 |
| 14 | h | 855 | GLU | CA-C-N | 6.08 | 128.80 | 120.46 |
| 14 | h | 855 | GLU | C-N-CA | 6.08 | 128.80 | 120.46 |
| 20 | g | 370 | SER | N-CA-CB | 6.08 | 120.77 | 110.49 |
| 20 | g | 706 | LEU | N-CA-C | 6.08 | 121.80 | 113.16 |
| 20 | g | 745 | ILE | N-CA-C | -6.08 | 107.20 | 113.10 |
| 5 | B | 318 | GLU | CB-CA-C | -6.08 | 98.31 | 110.42 |
| 5 | K | 313 | TYR | CB-CG-CD1 | 6.08 | 129.92 | 120.80 |
| 8 | N | 1025 | ASN | N-CA-C | 6.08 | 118.82 | 110.24 |
| 7 | O | 864 | LEU | CA-C-O | -6.08 | 114.10 | 120.55 |
| 2 | Z | 1277 | ARG | N-CA-CB | 6.08 | 120.77 | 110.49 |
| 12 | v | 366 | LEU | O-C-N | -6.08 | 116.81 | 121.55 |
| 19 | m | 721 | THR | CA-C-N | 6.08 | 129.56 | 120.31 |
| 19 | m | 721 | THR | C-N-CA | 6.08 | 129.56 | 120.31 |
| 2 | 1 | 128 | GLU | CA-C-N | 6.08 | 132.92 | 121.97 |
| 2 | 1 | 128 | GLU | C-N-CA | 6.08 | 132.92 | 121.97 |
| 6 | L | 303 | GLU | CB-CG-CD | -6.08 | 102.26 | 112.60 |
| 7 | O | 1162 | GLY | CA-C-O | -6.08 | 114.84 | 120.80 |
| 8 | P | 748 | HIS | CE1-NE2-CD2 | -6.08 | 102.92 | 109.00 |
| 8 | P | 1063 | ASP | CA-CB-CG | 6.08 | 118.68 | 112.60 |
| 8 | P | 1071 | LYS | N-CA-C | 6.08 | 119.96 | 112.54 |
| 8 | P | 1526 | GLY | CA-C-N | 6.08 | 128.93 | 120.29 |
| 8 | P | 1526 | GLY | C-N-CA | 6.08 | 128.93 | 120.29 |
| 11 | V | 382 | ILE | N-CA-C | -6.08 | 99.36 | 108.12 |
| 1 | Y | 1102 | ILE | N-CA-C | -6.08 | 106.83 | 112.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | v | 190 | ASP | CA-CB-CG | -6.08 | 106.52 | 112.60 |
| 7 | O | 722 | ARG | CD-NE-CZ | -6.08 | 115.89 | 124.40 |
| 7 | O | 925 | HIS | CG-CD2-NE2 | 6.08 | 113.28 | 107.20 |
| 9 | T | 353 | LEU | CA-C-O | 6.08 | 126.86 | 120.42 |
| 20 | n | 850 | TYR | CB-CG-CD2 | -6.08 | 111.68 | 120.80 |
| 2 | 1 | 1107 | HIS | N-CA-C | -6.08 | 98.99 | 108.90 |
| 9 | Q | 307 | SER | N-CA-C | -6.08 | 105.89 | 113.55 |
| 9 | S | 139 | PHE | CA-C-N | 6.08 | 128.22 | 120.56 |
| 9 | S | 139 | PHE | C-N-CA | 6.08 | 128.22 | 120.56 |
| 9 | T | 576 | LEU | O-C-N | 6.08 | 128.33 | 122.07 |
| 1 | Y | 665 | ASN | O-C-N | -6.08 | 115.79 | 121.32 |
| 14 | h | 426 | ILE | N-CA-C | -6.08 | 99.45 | 108.45 |
| 19 | m | 589 | HIS | CE1-NE2-CD2 | -6.08 | 102.92 | 109.00 |
| 1 | 0 | 273 | ILE | O-C-N | -6.08 | 116.77 | 123.03 |
| 2 | Z | 1326 | SER | CA-C-O | -6.08 | 114.11 | 120.55 |
| 14 | h | 826 | TYR | CB-CG-CD1 | -6.08 | 111.68 | 120.80 |
| 18 | l | 226 | ARG | NE-CZ-NH2 | 6.08 | 124.67 | 119.20 |
| 6 | I | 468 | ALA | N-CA-C | -6.08 | 105.63 | 113.16 |
| 7 | O | 1573 | SER | N-CA-CB | 6.08 | 120.76 | 110.49 |
| 2 | Z | 417 | ASN | OD1-CG-ND2 | 6.08 | 128.68 | 122.60 |
| 18 | l | 67 | GLU | CB-CG-CD | -6.08 | 102.27 | 112.60 |
| 18 | l | 120 | HIS | CE1-NE2-CD2 | -6.08 | 102.92 | 109.00 |
| 1 | 0 | 620 | LYS | CA-C-O | -6.07 | 113.85 | 120.17 |
| 1 | 0 | 1026 | TYR | N-CA-C | -6.07 | 105.05 | 112.88 |
| 6 | I | 452 | ASP | CA-CB-CG | 6.07 | 118.67 | 112.60 |
| 8 | N | 923 | LEU | CA-C-O | 6.07 | 128.53 | 121.49 |
| 20 | n | 64 | ASN | CA-CB-CG | 6.07 | 118.67 | 112.60 |
| 20 | n | 586 | ASP | N-CA-C | -6.07 | 105.71 | 112.57 |
| 18 | e | 37 | LYS | O-C-N | -6.07 | 116.11 | 123.16 |
| 19 | f | 358 | VAL | N-CA-CB | 6.07 | 117.66 | 110.55 |
| 2 | 1 | 214 | PHE | N-CA-C | 6.07 | 118.69 | 111.71 |
| 8 | P | 945 | ASP | CA-CB-CG | 6.07 | 118.67 | 112.60 |
| 8 | P | 1077 | ARG | CA-C-N | 6.07 | 129.04 | 120.42 |
| 8 | P | 1077 | ARG | C-N-CA | 6.07 | 129.04 | 120.42 |
| 9 | R | 697 | PHE | N-CA-CB | 6.07 | 120.75 | 110.49 |
| 12 | v | 331 | LEU | N-CA-C | -6.07 | 100.07 | 109.24 |
| 13 | w | 1442 | ALA | CA-C-O | -6.07 | 114.11 | 120.55 |
| 14 | h | 844 | CYS | N-CA-CB | 6.07 | 119.48 | 110.49 |
| 19 | f | 235 | GLN | N-CA-C | 6.07 | 118.13 | 110.24 |
| 4 | J | 754 | ASN | O-C-N | 6.07 | 128.56 | 122.12 |
| 6 | L | 331 | LYS | CG-CD-CE | 6.07 | 125.26 | 111.30 |
| 7 | M | 282 | PHE | CA-C-N | 6.07 | 128.91 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 282 | PHE | C-N-CA | 6.07 | 128.91 | 120.29 |
| 7 | M | 620 | THR | N-CA-C | 6.07 | 123.73 | 110.80 |
| 8 | N | 1504 | LEU | O-C-N | 6.07 | 128.32 | 122.07 |
| 8 | P | 153 | ASP | CA-CB-CG | 6.07 | 118.67 | 112.60 |
| 2 | Z | 962 | LYS | CA-C-N | 6.07 | 128.41 | 120.28 |
| 2 | Z | 962 | LYS | C-N-CA | 6.07 | 128.41 | 120.28 |
| 18 | l | 241 | ARG | N-CA-CB | 6.07 | 120.30 | 110.77 |
| 15 | b | 220 | ASP | CA-CB-CG | 6.07 | 118.67 | 112.60 |
| 14 | a | 782 | TYR | CA-CB-CG | -6.07 | 102.97 | 113.90 |
| 10 | U | 271 | ALA | N-CA-C | -6.07 | 105.05 | 112.88 |
| 17 | k | 148 | VAL | CA-CB-CG1 | -6.07 | 100.08 | 110.40 |
| 2 | 1 | 1301 | SER | CA-C-O | -6.07 | 111.83 | 120.51 |
| 7 | M | 980 | ASP | N-CA-CB | 6.07 | 118.81 | 110.01 |
| 8 | N | 210 | ASN | N-CA-CB | 6.07 | 119.14 | 110.16 |
| 8 | N | 577 | MET | CA-CB-CG | 6.07 | 126.24 | 114.10 |
| 9 | Q | 27 | GLU | O-C-N | 6.07 | 129.73 | 122.27 |
| 9 | R | 459 | LEU | O-C-N | 6.07 | 129.74 | 122.94 |
| 14 | h | 158 | PHE | CA-CB-CG | -6.07 | 107.73 | 113.80 |
| 14 | h | 650 | HIS | CB-CG-CD2 | 6.07 | 139.09 | 131.20 |
| 19 | f | 596 | GLU | N-CA-C | -6.07 | 105.53 | 113.17 |
| 19 | f | 707 | SER | N-CA-C | -6.07 | 105.19 | 112.59 |
| 14 | a | 692 | PHE | CB-CA-C | 6.07 | 119.73 | 109.84 |
| 5 | B | 515 | ASN | OD1-CG-ND2 | 6.07 | 128.66 | 122.60 |
| 8 | N | 369 | LEU | N-CA-C | -6.07 | 99.77 | 109.96 |
| 8 | N | 686 | GLY | CA-C-N | 6.07 | 129.45 | 120.90 |
| 8 | N | 686 | GLY | C-N-CA | 6.07 | 129.45 | 120.90 |
| 8 | N | 1559 | LYS | CA-C-O | 6.07 | 127.39 | 120.90 |
| 10 | W | 327 | ALA | N-CA-C | -6.07 | 105.83 | 113.72 |
| 10 | W | 352 | GLN | N-CA-C | -6.07 | 105.92 | 113.38 |
| 2 | Z | 1278 | ASP | CA-C-O | 6.07 | 125.19 | 118.52 |
| 12 | u | 704 | VAL | CA-C-N | 6.07 | 128.32 | 120.44 |
| 12 | u | 704 | VAL | C-N-CA | 6.07 | 128.32 | 120.44 |
| 4 | z | 640 | LEU | CA-C-N | 6.07 | 128.77 | 120.46 |
| 4 | z | 640 | LEU | C-N-CA | 6.07 | 128.77 | 120.46 |
| 20 | n | 210 | LEU | CA-C-O | -6.07 | 114.78 | 121.33 |
| 4 | G | 694 | ASP | CA-CB-CG | 6.06 | 118.66 | 112.60 |
| 2 | Z | 770 | ARG | N-CA-C | 6.06 | 123.21 | 109.81 |
| 20 | g | 976 | LYS | CA-CB-CG | 6.06 | 126.23 | 114.10 |
| 2 | 1 | 1327 | ARG | N-CA-CB | 6.06 | 119.03 | 110.12 |
| 6 | I | 272 | GLN | CA-C-N | 6.06 | 128.77 | 120.46 |
| 6 | I | 272 | GLN | C-N-CA | 6.06 | 128.77 | 120.46 |
| 7 | M | 1355 | SER | CA-C-N | 6.06 | 128.32 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 1355 | SER | C-N-CA | 6.06 | 128.32 | 120.44 |
| 8 | P | 298 | VAL | CA-C-N | 6.06 | 128.40 | 120.28 |
| 8 | P | 298 | VAL | C-N-CA | 6.06 | 128.40 | 120.28 |
| 14 | h | 514 | ASN | CA-CB-CG | 6.06 | 118.66 | 112.60 |
| 18 | e | 105 | ASN | CB-CG-ND2 | -6.06 | 107.31 | 116.40 |
| 1 | 0 | 850 | ASN | CA-C-O | -6.06 | 114.00 | 120.42 |
| 9 | T | 114 | ARG | N-CA-C | -6.06 | 99.75 | 108.60 |
| 20 | n | 638 | SER | CA-C-O | -6.06 | 114.19 | 121.22 |
| 2 | 1 | 712 | SER | CA-C-O | -6.06 | 114.13 | 120.55 |
| 5 | B | 540 | LYS | N-CA-C | -6.06 | 97.42 | 108.02 |
| 5 | H | 474 | SER | CA-C-N | 6.06 | 130.39 | 120.63 |
| 5 | H | 474 | SER | C-N-CA | 6.06 | 130.39 | 120.63 |
| 5 | H | 537 | TYR | CA-C-N | 6.06 | 128.32 | 120.44 |
| 5 | H | 537 | TYR | C-N-CA | 6.06 | 128.32 | 120.44 |
| 4 | J | 776 | PHE | N-CA-CB | 6.06 | 120.73 | 110.49 |
| 9 | R | 97 | GLU | O-C-N | 6.06 | 126.41 | 120.71 |
| 9 | T | 100 | PRO | N-CA-CB | 6.06 | 108.96 | 103.08 |
| 11 | V | 356 | VAL | CA-C-N | 6.06 | 130.34 | 121.31 |
| 11 | V | 356 | VAL | C-N-CA | 6.06 | 130.34 | 121.31 |
| 19 | m | 273 | ASN | N-CA-C | -6.06 | 104.52 | 113.61 |
| 18 | e | 9 | ASP | CA-CB-CG | 6.06 | 118.66 | 112.60 |
| 20 | g | 231 | ILE | N-CA-C | -6.06 | 98.25 | 106.85 |
| 20 | g | 708 | TRP | CB-CG-CD2 | 6.06 | 135.28 | 126.80 |
| 6 | I | 337 | LYS | N-CA-C | 6.06 | 118.85 | 111.82 |
| 7 | M | 1668 | LYS | CA-C-N | 6.06 | 128.31 | 120.44 |
| 7 | M | 1668 | LYS | C-N-CA | 6.06 | 128.31 | 120.44 |
| 7 | O | 38 | ASN | OD1-CG-ND2 | -6.06 | 116.54 | 122.60 |
| 7 | O | 682 | ASP | CA-CB-CG | 6.06 | 118.66 | 112.60 |
| 1 | Y | 674 | GLY | N-CA-C | -6.06 | 103.85 | 112.81 |
| 1 | Y | 1182 | ILE | N-CA-C | -6.06 | 103.45 | 110.05 |
| 12 | v | 341 | ASN | CA-CB-CG | -6.06 | 106.54 | 112.60 |
| 15 | b | 113 | GLU | CA-C-N | 6.06 | 129.02 | 120.42 |
| 15 | b | 113 | GLU | C-N-CA | 6.06 | 129.02 | 120.42 |
| 16 | c | 382 | LEU | N-CA-C | -6.06 | 104.60 | 112.23 |
| 1 | 0 | 1329 | ASP | N-CA-C | 6.06 | 119.89 | 111.90 |
| 20 | g | 145 | THR | CA-C-N | -6.06 | 109.97 | 121.54 |
| 20 | g | 145 | THR | C-N-CA | -6.06 | 109.97 | 121.54 |
| 20 | g | 230 | PHE | N-CA-C | -6.06 | 97.84 | 108.20 |
| 14 | a | 164 | HIS | CA-CB-CG | 6.06 | 119.86 | 113.80 |
| 1 | 0 | 381 | VAL | CB-CA-C | 6.05 | 119.02 | 111.15 |
| 2 | 1 | 594 | TYR | N-CA-CB | 6.05 | 121.00 | 110.65 |
| 7 | M | 340 | LEU | N-CA-C | -6.05 | 102.38 | 110.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 1005 | PHE | CA-C-O | -6.05 | 114.46 | 120.82 |
| 7 | M | 1006 | LEU | CA-C-N | 6.05 | 128.39 | 120.28 |
| 7 | M | 1006 | LEU | C-N-CA | 6.05 | 128.39 | 120.28 |
| 7 | M | 1023 | LEU | CA-C-N | 6.05 | 129.22 | 120.38 |
| 7 | M | 1023 | LEU | C-N-CA | 6.05 | 129.22 | 120.38 |
| 12 | v | 75 | THR | CB-CA-C | 6.05 | 122.47 | 110.42 |
| 20 | n | 267 | VAL | N-CA-C | -6.05 | 106.91 | 112.96 |
| 20 | n | 746 | VAL | CA-CB-CG1 | 6.05 | 120.69 | 110.40 |
| 14 | a | 295 | ASN | N-CA-CB | 6.05 | 120.72 | 110.49 |
| 14 | a | 971 | ASN | O-C-N | 6.05 | 129.83 | 122.75 |
| 4 | A | 646 | ASN | CA-CB-CG | 6.05 | 118.65 | 112.60 |
| 5 | E | 449 | ASP | CA-CB-CG | 6.05 | 118.65 | 112.60 |
| 7 | M | 1650 | GLU | CA-C-N | 6.05 | 128.71 | 120.54 |
| 7 | M | 1650 | GLU | C-N-CA | 6.05 | 128.71 | 120.54 |
| 19 | f | 623 | PHE | N-CA-C | -6.05 | 104.60 | 111.14 |
| 1 | 0 | 714 | LYS | N-CA-C | -6.05 | 96.44 | 109.81 |
| 7 | O | 310 | MET | CA-C-N | 6.05 | 128.39 | 120.28 |
| 7 | O | 310 | MET | C-N-CA | 6.05 | 128.39 | 120.28 |
| 8 | P | 1018 | GLU | CA-C-N | 6.05 | 128.99 | 120.28 |
| 8 | P | 1018 | GLU | C-N-CA | 6.05 | 128.99 | 120.28 |
| 9 | R | 252 | GLN | O-C-N | -6.05 | 115.70 | 122.12 |
| 1 | Y | 1350 | GLU | N-CA-C | -6.05 | 97.91 | 110.80 |
| 12 | u | 297 | TYR | N-CA-CB | 6.05 | 120.28 | 110.42 |
| 20 | n | 398 | LYS | N-CA-C | -6.05 | 97.98 | 108.69 |
| 15 | b | 661 | HIS | CE1-NE2-CD2 | -6.05 | 102.95 | 109.00 |
| 16 | c | 301 | ASN | N-CA-CB | 6.05 | 120.72 | 110.49 |
| 20 | g | 643 | PRO | CA-C-N | 6.05 | 128.18 | 120.56 |
| 20 | g | 643 | PRO | C-N-CA | 6.05 | 128.18 | 120.56 |
| 7 | O | 899 | PHE | N-CA-CB | 6.05 | 120.72 | 110.49 |
| 9 | Q | 88 | LYS | CA-C-N | 6.05 | 128.30 | 120.44 |
| 9 | Q | 88 | LYS | C-N-CA | 6.05 | 128.30 | 120.44 |
| 2 | Z | 302 | ILE | CA-C-N | 6.05 | 129.46 | 120.87 |
| 2 | Z | 302 | ILE | C-N-CA | 6.05 | 129.46 | 120.87 |
| 2 | Z | 567 | ILE | CA-CB-CG1 | 6.05 | 120.69 | 110.40 |
| 2 | Z | 588 | ASN | N-CA-C | -6.05 | 100.14 | 109.76 |
| 13 | w | 1392 | ARG | CA-C-O | -6.05 | 114.01 | 120.42 |
| 13 | x | 1288 | ILE | CA-C-N | 6.05 | 128.30 | 120.44 |
| 13 | x | 1288 | ILE | C-N-CA | 6.05 | 128.30 | 120.44 |
| 15 | b | 643 | GLY | N-CA-C | -6.05 | 98.84 | 113.18 |
| 20 | g | 392 | ASP | CA-CB-CG | 6.05 | 118.65 | 112.60 |
| 1 | 0 | 715 | PRO | CA-C-O | -6.05 | 114.39 | 121.95 |
| 6 | C | 461 | HIS | CE1-NE2-CD2 | -6.05 | 102.95 | 109.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | H | 452 | GLY | CA-C-N | 6.05 | 130.68 | 120.88 |
| 5 | H | 452 | GLY | C-N-CA | 6.05 | 130.68 | 120.88 |
| 8 | P | 423 | LYS | N-CA-C | -6.05 | 105.86 | 113.72 |
| 9 | R | 324 | ASN | CA-CB-CG | 6.05 | 118.65 | 112.60 |
| 11 | X | 371 | GLN | N-CA-C | -6.05 | 104.01 | 113.02 |
| 2 | 1 | 994 | ARG | CA-C-N | 6.05 | 128.99 | 120.28 |
| 2 | 1 | 994 | ARG | C-N-CA | 6.05 | 128.99 | 120.28 |
| 4 | G | 707 | LEU | CA-C-N | 6.05 | 128.38 | 120.28 |
| 4 | G | 707 | LEU | C-N-CA | 6.05 | 128.38 | 120.28 |
| 4 | J | 789 | GLU | N-CA-C | -6.05 | 106.51 | 114.31 |
| 8 | P | 1171 | ARG | N-CA-C | -6.05 | 98.87 | 108.73 |
| 9 | T | 490 | LEU | CA-C-O | -6.05 | 114.14 | 120.55 |
| 14 | h | 887 | ASP | N-CA-C | -6.05 | 103.34 | 111.87 |
| 15 | i | 452 | GLU | N-CA-C | -6.05 | 106.54 | 114.04 |
| 15 | b | 281 | SER | N-CA-C | -6.05 | 106.51 | 114.31 |
| 1 | 0 | 614 | LEU | N-CA-CB | 6.04 | 118.91 | 110.26 |
| 9 | T | 89 | ASP | CA-C-O | 6.04 | 126.92 | 119.97 |
| 4 | J | 804 | LEU | O-C-N | 6.04 | 128.53 | 122.12 |
| 5 | K | 359 | ASN | CA-CB-CG | -6.04 | 106.56 | 112.60 |
| 7 | M | 96 | ASP | CA-C-O | -6.04 | 114.91 | 121.44 |
| 7 | O | 1258 | HIS | CE1-NE2-CD2 | -6.04 | 102.96 | 109.00 |
| 8 | P | 1389 | LEU | N-CA-CB | 6.04 | 119.61 | 110.30 |
| 9 | Q | 477 | TYR | N-CA-C | -6.04 | 105.86 | 113.72 |
| 9 | R | 61 | LYS | N-CA-C | -6.04 | 99.50 | 108.99 |
| 9 | R | 622 | THR | N-CA-C | 6.04 | 117.87 | 111.28 |
| 9 | S | 434 | ASP | O-C-N | 6.04 | 129.04 | 122.15 |
| 15 | b | 140 | HIS | N-CA-C | -6.04 | 105.77 | 113.02 |
| 15 | b | 344 | ARG | NE-CZ-NH2 | -6.04 | 113.76 | 119.20 |
| 15 | b | 702 | ALA | CA-C-O | -6.04 | 114.65 | 122.14 |
| 20 | g | 611 | ASN | N-CA-C | -6.04 | 104.69 | 111.28 |
| 5 | K | 516 | GLN | N-CA-C | 6.04 | 117.53 | 111.07 |
| 8 | P | 431 | LYS | CA-C-O | -6.04 | 112.85 | 120.28 |
| 8 | P | 1125 | GLU | CA-C-O | 6.04 | 125.79 | 119.51 |
| 14 | h | 803 | HIS | CA-C-N | 6.04 | 132.08 | 120.66 |
| 14 | h | 803 | HIS | C-N-CA | 6.04 | 132.08 | 120.66 |
| 15 | i | 613 | ASP | N-CA-CB | 6.04 | 120.70 | 110.49 |
| 14 | h | 459 | GLU | CA-C-N | 6.04 | 129.41 | 120.95 |
| 14 | h | 459 | GLU | C-N-CA | 6.04 | 129.41 | 120.95 |
| 18 | e | 303 | HIS | CG-CD2-NE2 | 6.04 | 113.24 | 107.20 |
| 7 | O | 875 | VAL | N-CA-C | 6.04 | 116.78 | 110.62 |
| 7 | O | 1147 | PHE | CA-C-N | 6.04 | 128.29 | 120.44 |
| 7 | O | 1147 | PHE | C-N-CA | 6.04 | 128.29 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1023 | VAL | N-CA-C | 6.04 | 118.60 | 111.05 |
| 1 | Y | 979 | ALA | N-CA-CB | 6.04 | 120.70 | 110.49 |
| 2 | Z | 1253 | VAL | CB-CA-C | 6.04 | 119.49 | 110.98 |
| 14 | h | 324 | SER | N-CA-C | -6.04 | 105.75 | 112.57 |
| 19 | m | 396 | LEU | CA-C-N | 6.04 | 128.37 | 120.28 |
| 19 | m | 396 | LEU | C-N-CA | 6.04 | 128.37 | 120.28 |
| 20 | g | 1073 | ASN | CB-CG-ND2 | -6.04 | 107.34 | 116.40 |
| 14 | a | 749 | TYR | CA-C-N | 6.04 | 133.07 | 121.54 |
| 14 | a | 749 | TYR | C-N-CA | 6.04 | 133.07 | 121.54 |
| 7 | O | 1253 | ARG | NE-CZ-NH1 | 6.04 | 127.54 | 121.50 |
| 19 | f | 713 | GLU | CA-C-O | 6.04 | 126.95 | 120.55 |
| 8 | P | 1627 | LEU | CA-C-O | 6.04 | 126.41 | 119.35 |
| 9 | Q | 619 | PHE | CA-C-N | 6.04 | 130.94 | 120.68 |
| 9 | Q | 619 | PHE | C-N-CA | 6.04 | 130.94 | 120.68 |
| 10 | U | 341 | GLY | O-C-N | -6.04 | 118.25 | 123.80 |
| 2 | Z | 1238 | TRP | CA-C-O | 6.04 | 126.95 | 120.55 |
| 15 | b | 329 | ARG | NE-CZ-NH1 | -6.04 | 115.46 | 121.50 |
| 19 | f | 525 | ASP | N-CA-C | -6.04 | 105.64 | 114.39 |
| 20 | g | 66 | ARG | O-C-N | 6.04 | 129.32 | 122.20 |
| 14 | a | 772 | GLN | N-CA-C | -6.04 | 104.78 | 111.36 |
| 14 | a | 943 | LYS | O-C-N | 6.04 | 128.29 | 122.07 |
| 8 | P | 589 | GLU | N-CA-C | -6.03 | 105.10 | 112.88 |
| 1 | Y | 1369 | ASN | OD1-CG-ND2 | -6.03 | 116.57 | 122.60 |
| 1 | Y | 1484 | ILE | N-CA-CB | 6.03 | 121.19 | 111.23 |
| 2 | Z | 242 | HIS | CE1-NE2-CD2 | -6.03 | 102.97 | 109.00 |
| 19 | m | 655 | ILE | N-CA-C | -6.03 | 105.18 | 111.58 |
| 20 | g | 110 | ILE | N-CA-C | -6.03 | 99.00 | 108.95 |
| 20 | g | 547 | PRO | CA-C-O | -6.03 | 111.81 | 120.56 |
| 14 | a | 780 | HIS | ND1-CE1-NE2 | 6.03 | 114.43 | 108.40 |
| 12 | v | 204 | ASP | CA-CB-CG | 6.03 | 118.63 | 112.60 |
| 14 | h | 165 | PHE | CA-C-N | 6.03 | 131.68 | 122.93 |
| 14 | h | 165 | PHE | C-N-CA | 6.03 | 131.68 | 122.93 |
| 17 | k | 95 | HIS | CG-CD2-NE2 | 6.03 | 113.23 | 107.20 |
| 19 | m | 639 | THR | N-CA-CB | 6.03 | 118.84 | 109.85 |
| 14 | a | 938 | ARG | NE-CZ-NH1 | 6.03 | 127.53 | 121.50 |
| 5 | K | 329 | HIS | N-CA-CB | 6.03 | 120.68 | 110.49 |
| 8 | N | 1423 | ASN | CA-C-N | 6.03 | 128.28 | 120.44 |
| 8 | N | 1423 | ASN | C-N-CA | 6.03 | 128.28 | 120.44 |
| 9 | T | 320 | TRP | CB-CG-CD1 | -6.03 | 117.86 | 126.90 |
| 11 | V | 399 | LYS | N-CA-CB | 6.03 | 120.68 | 110.49 |
| 17 | d | 52 | HIS | CB-CG-CD2 | -6.03 | 123.36 | 131.20 |
| 17 | d | 190 | ASP | N-CA-C | -6.03 | 105.88 | 113.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | f | 303 | LEU | N-CA-C | -6.03 | 106.25 | 113.97 |
| 20 | g | 1099 | TYR | N-CA-C | -6.03 | 104.56 | 113.61 |
| 1 | 0 | 248 | ASP | N-CA-C | -6.03 | 100.14 | 109.24 |
| 8 | P | 389 | PHE | CA-CB-CG | -6.03 | 107.77 | 113.80 |
| 9 | R | 744 | LEU | N-CA-CB | 6.03 | 119.08 | 110.16 |
| 2 | Z | 127 | ASP | CA-C-O | -6.03 | 114.39 | 120.96 |
| 12 | u | 348 | LEU | N-CA-CB | 6.03 | 119.93 | 110.71 |
| 2 | 1 | 1325 | LEU | N-CA-CB | 6.03 | 119.62 | 110.28 |
| 1 | Y | 141 | GLY | CA-C-O | -6.03 | 115.96 | 122.47 |
| 4 | A | 650 | GLU | N-CA-C | -6.03 | 104.79 | 111.36 |
| 7 | M | 150 | PHE | CA-C-N | 6.03 | 128.71 | 120.46 |
| 7 | M | 150 | PHE | C-N-CA | 6.03 | 128.71 | 120.46 |
| 7 | O | 1541 | ASN | OD1-CG-ND2 | 6.03 | 128.62 | 122.60 |
| 8 | P | 1169 | ALA | CA-C-N | -6.03 | 113.03 | 122.49 |
| 8 | P | 1169 | ALA | C-N-CA | -6.03 | 113.03 | 122.49 |
| 9 | T | 625 | GLU | N-CA-C | 6.03 | 117.54 | 110.97 |
| 1 | Y | 433 | ASN | N-CA-C | -6.03 | 105.69 | 113.16 |
| 2 | Z | 645 | LEU | N-CA-CB | 6.03 | 118.93 | 110.07 |
| 19 | m | 205 | ASN | CA-C-N | 6.03 | 130.84 | 122.28 |
| 19 | m | 205 | ASN | C-N-CA | 6.03 | 130.84 | 122.28 |
| 20 | n | 554 | GLY | CA-C-N | -6.03 | 113.20 | 122.60 |
| 20 | n | 554 | GLY | C-N-CA | -6.03 | 113.20 | 122.60 |
| 16 | c | 509 | ARG | CA-C-N | 6.03 | 128.35 | 120.28 |
| 16 | c | 509 | ARG | C-N-CA | 6.03 | 128.35 | 120.28 |
| 7 | O | 1445 | VAL | CA-C-N | 6.02 | 130.22 | 121.18 |
| 7 | O | 1445 | VAL | C-N-CA | 6.02 | 130.22 | 121.18 |
| 8 | P | 918 | PHE | CA-C-N | 6.02 | 131.93 | 122.17 |
| 8 | P | 918 | PHE | C-N-CA | 6.02 | 131.93 | 122.17 |
| 12 | u | 208 | PHE | CA-C-O | -6.02 | 113.69 | 120.32 |
| 12 | v | 131 | LEU | N-CA-CB | 6.02 | 120.09 | 111.05 |
| 14 | a | 2 | ALA | CA-C-O | -6.02 | 114.41 | 121.16 |
| 2 | 1 | 391 | LEU | N-CA-C | -6.02 | 104.80 | 111.36 |
| 2 | 1 | 1319 | LEU | CB-CA-C | -6.02 | 100.79 | 110.79 |
| 5 | E | 473 | ILE | N-CA-C | -6.02 | 104.13 | 112.50 |
| 8 | N | 1462 | ASN | CA-CB-CG | 6.02 | 118.62 | 112.60 |
| 9 | Q | 583 | THR | N-CA-C | -6.02 | 101.86 | 110.59 |
| 1 | Y | 1444 | PHE | CA-CB-CG | 6.02 | 119.82 | 113.80 |
| 2 | Z | 1066 | ASN | CA-CB-CG | 6.02 | 118.62 | 112.60 |
| 4 | y | 696 | SER | CB-CA-C | -6.02 | 100.79 | 110.79 |
| 4 | y | 808 | ASP | CA-C-O | -6.02 | 114.50 | 120.70 |
| 14 | h | 284 | ASN | OD1-CG-ND2 | -6.02 | 116.58 | 122.60 |
| 15 | i | 668 | ALA | CA-C-O | 6.02 | 126.91 | 120.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | a | 822 | SER | N-CA-C | -6.02 | 104.45 | 112.94 |
| 14 | a | 832 | PHE | CA-CB-CG | 6.02 | 119.82 | 113.80 |
| 4 | G | 713 | ASN | CA-C-N | -6.02 | 113.16 | 122.49 |
| 4 | G | 713 | ASN | C-N-CA | -6.02 | 113.16 | 122.49 |
| 8 | P | 214 | LEU | N-CA-CB | 6.02 | 119.50 | 110.53 |
| 2 | Z | 656 | HIS | CE1-NE2-CD2 | -6.02 | 102.98 | 109.00 |
| 2 | Z | 809 | LEU | N-CA-C | -6.02 | 106.09 | 113.50 |
| 4 | z | 807 | LEU | O-C-N | 6.02 | 129.01 | 122.15 |
| 15 | i | 153 | ASN | CA-CB-CG | 6.02 | 118.62 | 112.60 |
| 18 | e | 325 | ASP | CA-CB-CG | 6.02 | 118.62 | 112.60 |
| 2 | 1 | 536 | HIS | CG-CD2-NE2 | 6.02 | 113.22 | 107.20 |
| 6 | C | 462 | GLN | OE1-CD-NE2 | 6.02 | 128.62 | 122.60 |
| 6 | I | 373 | PHE | CA-C-O | 6.02 | 126.89 | 119.97 |
| 7 | M | 1161 | LEU | CA-C-O | -6.02 | 113.30 | 120.10 |
| 8 | N | 84 | ASP | O-C-N | -6.02 | 114.94 | 122.35 |
| 8 | N | 376 | THR | N-CA-C | -6.02 | 105.23 | 113.30 |
| 12 | u | 440 | MET | CA-C-O | 6.02 | 126.86 | 120.36 |
| 4 | D | 755 | LEU | CA-C-N | 6.02 | 128.84 | 120.29 |
| 4 | D | 755 | LEU | C-N-CA | 6.02 | 128.84 | 120.29 |
| 7 | M | 171 | TYR | CB-CA-C | 6.02 | 118.82 | 110.16 |
| 12 | v | 261 | GLU | CA-C-N | 6.02 | 128.84 | 120.29 |
| 12 | v | 261 | GLU | C-N-CA | 6.02 | 128.84 | 120.29 |
| 13 | x | 1288 | ILE | CA-C-O | -6.02 | 114.69 | 120.95 |
| 15 | i | 492 | SER | N-CA-CB | 6.02 | 120.66 | 110.49 |
| 21 | s | 25 | LEU | CA-C-N | 6.02 | 128.26 | 120.44 |
| 21 | s | 25 | LEU | C-N-CA | 6.02 | 128.26 | 120.44 |
| 20 | g | 138 | CYS | CA-C-O | 6.02 | 126.90 | 120.46 |
| 14 | a | 647 | PHE | N-CA-C | -6.02 | 106.19 | 112.93 |
| 7 | O | 1018 | THR | CA-C-N | 6.02 | 130.91 | 120.86 |
| 7 | O | 1018 | THR | C-N-CA | 6.02 | 130.91 | 120.86 |
| 1 | Y | 1186 | LEU | N-CA-C | -6.02 | 105.02 | 112.90 |
| 12 | v | 584 | GLN | N-CA-C | -6.02 | 105.60 | 113.12 |
| 18 | l | 336 | SER | N-CA-CB | 6.02 | 120.66 | 110.49 |
| 2 | 1 | 115 | ASP | O-C-N | -6.01 | 115.10 | 123.34 |
| 5 | B | 441 | GLN | OE1-CD-NE2 | 6.01 | 128.62 | 122.60 |
| 7 | O | 936 | ILE | CA-C-N | 6.01 | 130.22 | 120.60 |
| 7 | O | 936 | ILE | C-N-CA | 6.01 | 130.22 | 120.60 |
| 9 | R | 354 | VAL | CA-C-O | 6.01 | 124.67 | 118.96 |
| 13 | x | 1397 | LYS | N-CA-CB | 6.01 | 118.73 | 110.01 |
| 15 | i | 338 | VAL | CB-CA-C | 6.01 | 119.90 | 112.02 |
| 18 | e | 137 | TYR | N-CA-CB | 6.01 | 119.98 | 110.84 |
| 1 | 0 | 850 | ASN | O-C-N | 6.01 | 129.00 | 122.15 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | K | 522 | TYR | CA-CB-CG | -6.01 | 103.08 | 113.90 |
| 7 | M | 523 | ARG | CA-C-O | -6.01 | 114.47 | 120.90 |
| 8 | N | 1207 | TRP | N-CA-CB | 6.01 | 118.96 | 110.12 |
| 9 | Q | 640 | SER | N-CA-CB | 6.01 | 118.73 | 110.01 |
| 9 | T | 593 | ILE | N-CA-C | -6.01 | 99.50 | 108.46 |
| 2 | Z | 341 | THR | CB-CA-C | 6.01 | 118.86 | 109.84 |
| 4 | y | 814 | LEU | CA-C-O | -6.01 | 114.05 | 120.42 |
| 14 | a | 70 | TYR | N-CA-CB | 6.01 | 119.68 | 110.60 |
| 1 | 0 | 712 | ASP | CA-CB-CG | 6.01 | 118.61 | 112.60 |
| 5 | B | 338 | ALA | CA-C-N | 6.01 | 128.94 | 120.28 |
| 5 | B | 338 | ALA | C-N-CA | 6.01 | 128.94 | 120.28 |
| 7 | M | 237 | PHE | CA-CB-CG | 6.01 | 119.81 | 113.80 |
| 8 | N | 844 | TYR | CB-CA-C | -6.01 | 101.44 | 110.88 |
| 8 | P | 1514 | VAL | CA-C-O | 6.01 | 126.44 | 119.89 |
| 13 | x | 1108 | ASP | N-CA-C | 6.01 | 119.08 | 110.24 |
| 17 | k | 208 | ARG | CD-NE-CZ | -6.01 | 115.98 | 124.40 |
| 19 | m | 533 | LEU | N-CA-C | -6.01 | 106.28 | 113.97 |
| 20 | n | 916 | SER | CA-C-N | 6.01 | 128.83 | 120.29 |
| 20 | n | 916 | SER | C-N-CA | 6.01 | 128.83 | 120.29 |
| 17 | d | 144 | HIS | CB-CG-CD2 | -6.01 | 123.39 | 131.20 |
| 18 | e | 106 | ASP | CA-C-N | 6.01 | 130.02 | 121.42 |
| 18 | e | 106 | ASP | C-N-CA | 6.01 | 130.02 | 121.42 |
| 2 | 1 | 1366 | ILE | N-CA-C | -6.01 | 106.88 | 113.43 |
| 8 | P | 1644 | ILE | CA-CB-CG2 | -6.01 | 100.28 | 110.50 |
| 10 | U | 282 | VAL | CA-C-N | 6.01 | 130.40 | 122.95 |
| 10 | U | 282 | VAL | C-N-CA | 6.01 | 130.40 | 122.95 |
| 11 | V | 280 | ILE | O-C-N | 6.01 | 129.57 | 123.20 |
| 1 | Y | 1145 | SER | O-C-N | 6.01 | 129.00 | 122.15 |
| 2 | Z | 388 | MET | N-CA-C | 6.01 | 117.91 | 111.36 |
| 13 | x | 1296 | THR | N-CA-CB | 6.01 | 118.72 | 110.01 |
| 14 | h | 150 | PHE | N-CA-C | -6.01 | 98.60 | 108.76 |
| 14 | h | 224 | ILE | N-CA-C | -6.01 | 108.00 | 113.71 |
| 16 | j | 173 | LYS | O-C-N | -6.01 | 116.15 | 123.30 |
| 16 | j | 339 | GLN | N-CA-CB | 6.01 | 118.95 | 110.12 |
| 17 | k | 14 | ASP | N-CA-CB | 6.01 | 121.91 | 111.39 |
| 19 | f | 62 | VAL | O-C-N | -6.01 | 115.64 | 121.83 |
| 19 | f | 290 | LEU | CA-C-N | 6.01 | 128.33 | 120.28 |
| 19 | f | 290 | LEU | C-N-CA | 6.01 | 128.33 | 120.28 |
| 14 | a | 501 | THR | CA-C-O | 6.01 | 126.27 | 119.18 |
| 1 | 0 | 1270 | GLY | CA-C-N | 6.01 | 128.69 | 120.46 |
| 1 | 0 | 1270 | GLY | C-N-CA | 6.01 | 128.69 | 120.46 |
| 5 | E | 304 | THR | N-CA-CB | 6.01 | 119.37 | 109.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 720 | HIS | CE1-NE2-CD2 | -6.01 | 102.99 | 109.00 |
| 2 | Z | 349 | GLN | N-CA-C | 6.01 | 118.79 | 111.82 |
| 4 | J | 760 | SER | O-C-N | 6.01 | 129.00 | 122.15 |
| 4 | J | 768 | GLU | CA-C-N | 6.01 | 128.69 | 120.46 |
| 4 | J | 768 | GLU | C-N-CA | 6.01 | 128.69 | 120.46 |
| 7 | M | 1534 | GLY | O-C-N | -6.01 | 117.48 | 122.77 |
| 8 | N | 256 | THR | N-CA-C | 6.01 | 127.82 | 111.00 |
| 8 | N | 872 | ASN | N-CA-C | 6.01 | 119.71 | 112.38 |
| 9 | S | 354 | VAL | N-CA-CB | -6.01 | 104.35 | 112.16 |
| 10 | U | 325 | SER | N-CA-C | 6.01 | 117.83 | 111.28 |
| 12 | u | 540 | VAL | N-CA-C | 6.01 | 116.75 | 110.62 |
| 13 | x | 1401 | LEU | CA-C-N | 6.01 | 128.82 | 120.29 |
| 13 | x | 1401 | LEU | C-N-CA | 6.01 | 128.82 | 120.29 |
| 16 | j | 660 | VAL | N-CA-C | 6.01 | 117.95 | 111.58 |
| 16 | c | 201 | ALA | N-CA-C | -6.01 | 99.45 | 109.24 |
| 16 | c | 585 | ASN | CA-CB-CG | -6.01 | 106.59 | 112.60 |
| 17 | d | 135 | THR | CA-C-N | 6.01 | 129.24 | 120.71 |
| 17 | d | 135 | THR | C-N-CA | 6.01 | 129.24 | 120.71 |
| 18 | e | 23 | HIS | CA-C-N | 6.01 | 131.09 | 123.10 |
| 18 | e | 23 | HIS | C-N-CA | 6.01 | 131.09 | 123.10 |
| 20 | g | 259 | LYS | CA-C-N | 6.01 | 129.99 | 122.48 |
| 20 | g | 259 | LYS | C-N-CA | 6.01 | 129.99 | 122.48 |
| 2 | 1 | 167 | LEU | N-CA-C | -6.00 | 105.71 | 113.16 |
| 6 | L | 394 | ILE | CA-C-N | 6.00 | 128.82 | 120.29 |
| 6 | L | 394 | ILE | C-N-CA | 6.00 | 128.82 | 120.29 |
| 7 | O | 1513 | TYR | N-CA-C | -6.00 | 105.87 | 112.72 |
| 8 | P | 184 | ASP | CA-C-N | 6.00 | 128.33 | 120.28 |
| 8 | P | 184 | ASP | C-N-CA | 6.00 | 128.33 | 120.28 |
| 8 | P | 822 | ASN | CA-CB-CG | -6.00 | 106.59 | 112.60 |
| 8 | N | 900 | ILE | N-CA-C | 6.00 | 118.56 | 111.05 |
| 12 | v | 560 | LEU | N-CA-CB | 6.00 | 118.71 | 110.01 |
| 14 | h | 918 | PHE | CA-CB-CG | -6.00 | 107.80 | 113.80 |
| 19 | f | 204 | ASP | N-CA-CB | 6.00 | 120.64 | 110.49 |
| 14 | a | 561 | GLN | N-CA-C | -6.00 | 106.29 | 113.97 |
| 7 | M | 1032 | ILE | CA-CB-CG1 | 6.00 | 120.60 | 110.40 |
| 9 | R | 737 | SER | N-CA-C | 6.00 | 117.82 | 111.28 |
| 12 | v | 328 | PHE | CA-C-O | 6.00 | 127.80 | 120.60 |
| 7 | M | 477 | ASP | N-CA-C | -6.00 | 106.50 | 113.88 |
| 9 | T | 218 | ILE | CA-C-N | 6.00 | 128.68 | 120.46 |
| 9 | T | 218 | ILE | C-N-CA | 6.00 | 128.68 | 120.46 |
| 1 | Y | 901 | GLN | N-CA-C | 6.00 | 118.78 | 111.82 |
| 19 | m | 194 | ASP | CA-CB-CG | 6.00 | 118.60 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | L | 271 | PRO | CA-C-N | 6.00 | 128.32 | 120.28 |
| 6 | L | 271 | PRO | C-N-CA | 6.00 | 128.32 | 120.28 |
| 6 | L | 282 | GLN | CA-C-O | 6.00 | 126.76 | 119.38 |
| 8 | N | 86 | ASP | CA-C-N | 6.00 | 125.55 | 119.19 |
| 8 | N | 86 | ASP | C-N-CA | 6.00 | 125.55 | 119.19 |
| 7 | O | 963 | ASN | CA-C-N | 6.00 | 133.00 | 121.54 |
| 7 | O | 963 | ASN | C-N-CA | 6.00 | 133.00 | 121.54 |
| 9 | Q | 51 | ARG | N-CA-C | -6.00 | 105.62 | 113.12 |
| 9 | Q | 434 | ASP | CA-CB-CG | -6.00 | 106.60 | 112.60 |
| 9 | R | 639 | ASP | CA-C-N | 6.00 | 128.81 | 120.29 |
| 9 | R | 639 | ASP | C-N-CA | 6.00 | 128.81 | 120.29 |
| 2 | Z | 373 | LEU | N-CA-CB | 6.00 | 118.81 | 110.17 |
| 12 | u | 576 | ASP | CA-C-N | 6.00 | 128.32 | 120.28 |
| 12 | u | 576 | ASP | C-N-CA | 6.00 | 128.32 | 120.28 |
| 4 | y | 676 | ILE | CA-C-N | 6.00 | 129.43 | 120.31 |
| 4 | y | 676 | ILE | C-N-CA | 6.00 | 129.43 | 120.31 |
| 15 | i | 111 | LEU | CA-C-N | 6.00 | 128.81 | 120.29 |
| 15 | i | 111 | LEU | C-N-CA | 6.00 | 128.81 | 120.29 |
| 15 | i | 427 | LYS | N-CA-CB | 6.00 | 119.16 | 110.88 |
| 15 | b | 213 | ASN | CA-CB-CG | -6.00 | 106.60 | 112.60 |
| 2 | 1 | 1005 | TYR | CA-C-N | 6.00 | 128.81 | 120.29 |
| 2 | 1 | 1005 | TYR | C-N-CA | 6.00 | 128.81 | 120.29 |
| 8 | N | 256 | THR | CA-CB-OG1 | -6.00 | 100.61 | 109.60 |
| 8 | N | 760 | ASN | CA-C-N | 6.00 | 131.00 | 122.24 |
| 8 | N | 760 | ASN | C-N-CA | 6.00 | 131.00 | 122.24 |
| 8 | P | 1519 | CYS | N-CA-C | 6.00 | 117.49 | 111.07 |
| 9 | T | 435 | TRP | CB-CG-CD2 | 6.00 | 135.19 | 126.80 |
| 12 | v | 544 | THR | CA-C-N | 6.00 | 128.31 | 120.28 |
| 12 | v | 544 | THR | C-N-CA | 6.00 | 128.31 | 120.28 |
| 14 | h | 410 | ASN | CB-CG-ND2 | 6.00 | 125.40 | 116.40 |
| 14 | h | 681 | LYS | N-CA-C | 6.00 | 118.78 | 111.82 |
| 15 | b | 452 | GLU | N-CA-C | -6.00 | 106.00 | 113.38 |
| 20 | g | 586 | ASP | N-CA-C | -6.00 | 105.88 | 112.72 |
| 2 | 1 | 120 | GLY | CA-C-O | -6.00 | 114.88 | 122.01 |
| 2 | Z | 1281 | VAL | N-CA-CB | 6.00 | 121.12 | 111.23 |
| 16 | c | 438 | VAL | CA-C-O | 6.00 | 126.98 | 120.57 |
| 19 | f | 51 | LEU | CA-C-O | 6.00 | 127.03 | 119.78 |
| 1 | 0 | 247 | LEU | N-CA-CB | 5.99 | 119.98 | 110.57 |
| 2 | 1 | 371 | ASN | O-C-N | -5.99 | 114.62 | 122.59 |
| 5 | E | 411 | ARG | CA-C-O | 5.99 | 126.77 | 120.42 |
| 7 | M | 1438 | VAL | CA-C-N | 5.99 | 128.63 | 120.54 |
| 7 | M | 1438 | VAL | C-N-CA | 5.99 | 128.63 | 120.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | R | 286 | THR | N-CA-CB | 5.99 | 118.66 | 109.91 |
| 9 | T | 97 | GLU | CA-C-N | 5.99 | 125.70 | 119.05 |
| 9 | T | 97 | GLU | C-N-CA | 5.99 | 125.70 | 119.05 |
| 1 | Y | 392 | SER | O-C-N | 5.99 | 129.69 | 122.68 |
| 12 | v | 370 | LEU | CA-C-O | -5.99 | 114.37 | 121.32 |
| 14 | h | 412 | LYS | N-CA-C | 5.99 | 118.60 | 111.71 |
| 16 | j | 339 | GLN | OE1-CD-NE2 | -5.99 | 116.61 | 122.60 |
| 16 | j | 644 | PHE | N-CA-C | -5.99 | 105.83 | 113.02 |
| 21 | p | 75 | HIS | ND1-CE1-NE2 | 5.99 | 114.39 | 108.40 |
| 14 | a | 934 | GLU | CA-C-N | 5.99 | 129.63 | 120.82 |
| 14 | a | 934 | GLU | C-N-CA | 5.99 | 129.63 | 120.82 |
| 6 | L | 397 | ALA | CB-CA-C | -5.99 | 100.66 | 110.85 |
| 8 | P | 676 | LEU | CA-C-N | 5.99 | 132.99 | 121.54 |
| 8 | P | 676 | LEU | C-N-CA | 5.99 | 132.99 | 121.54 |
| 17 | d | 179 | ASP | CB-CA-C | 5.99 | 120.30 | 110.17 |
| 2 | 1 | 1126 | LYS | CA-C-N | 5.99 | 130.19 | 120.60 |
| 2 | 1 | 1126 | LYS | C-N-CA | 5.99 | 130.19 | 120.60 |
| 9 | Q | 622 | THR | N-CA-C | 5.99 | 117.48 | 111.07 |
| 9 | S | 811 | ARG | NE-CZ-NH2 | -5.99 | 113.81 | 119.20 |
| 1 | Y | 1045 | GLU | CA-C-N | 5.99 | 132.43 | 122.54 |
| 1 | Y | 1045 | GLU | C-N-CA | 5.99 | 132.43 | 122.54 |
| 20 | n | 351 | ILE | O-C-N | 5.99 | 129.68 | 123.03 |
| 16 | c | 601 | GLU | CA-C-O | -5.99 | 113.33 | 120.10 |
| 1 | 0 | 676 | ALA | N-CA-C | -5.99 | 103.92 | 112.13 |
| 6 | F | 436 | LEU | N-CA-C | -5.99 | 105.88 | 113.43 |
| 5 | H | 435 | LYS | N-CA-C | -5.99 | 106.02 | 113.38 |
| 6 | I | 325 | TYR | O-C-N | 5.99 | 128.47 | 122.12 |
| 8 | N | 143 | SER | N-CA-CB | 5.99 | 120.61 | 110.49 |
| 8 | P | 420 | THR | CA-C-N | 5.99 | 129.26 | 120.82 |
| 8 | P | 420 | THR | C-N-CA | 5.99 | 129.26 | 120.82 |
| 1 | Y | 282 | ILE | CA-CB-CG2 | -5.99 | 100.32 | 110.50 |
| 12 | u | 312 | ASN | OD1-CG-ND2 | 5.99 | 128.59 | 122.60 |
| 12 | u | 550 | HIS | CA-C-N | 5.99 | 128.30 | 120.28 |
| 12 | u | 550 | HIS | C-N-CA | 5.99 | 128.30 | 120.28 |
| 12 | v | 209 | TYR | CA-C-O | -5.99 | 111.96 | 120.16 |
| 12 | v | 356 | LEU | N-CA-CB | 5.99 | 119.45 | 110.65 |
| 12 | v | 441 | SER | N-CA-C | -5.99 | 100.68 | 109.18 |
| 4 | z | 795 | LYS | N-CA-CB | 5.99 | 118.69 | 110.01 |
| 15 | i | 568 | VAL | N-CA-CB | 5.99 | 121.11 | 111.23 |
| 18 | e | 303 | HIS | CB-CG-CD2 | -5.99 | 123.42 | 131.20 |
| 14 | a | 237 | LEU | N-CA-C | -5.99 | 99.94 | 109.76 |
| 7 | M | 1276 | ASP | O-C-N | -5.99 | 115.77 | 122.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 284 | ASN | N-CA-C | -5.99 | 98.05 | 110.80 |
| 2 | 1 | 922 | LYS | N-CA-C | -5.99 | 98.05 | 110.80 |
| 5 | H | 299 | TRP | N-CA-C | -5.99 | 104.83 | 113.21 |
| 6 | I | 394 | ILE | O-C-N | -5.99 | 116.06 | 121.87 |
| 7 | M | 1256 | SER | N-CA-CB | 5.99 | 118.58 | 110.38 |
| 9 | Q | 507 | ALA | N-CA-C | 5.99 | 117.80 | 111.28 |
| 9 | R | 725 | GLU | CA-CB-CG | 5.99 | 126.07 | 114.10 |
| 9 | S | 672 | GLN | CA-C-O | -5.99 | 113.57 | 120.03 |
| 1 | Y | 1071 | ALA | CA-C-N | 5.99 | 131.36 | 122.86 |
| 1 | Y | 1071 | ALA | C-N-CA | 5.99 | 131.36 | 122.86 |
| 2 | Z | 1000 | LYS | CA-C-N | 5.99 | 128.58 | 120.44 |
| 2 | Z | 1000 | LYS | C-N-CA | 5.99 | 128.58 | 120.44 |
| 2 | Z | 1216 | TYR | CA-C-N | 5.99 | 130.71 | 120.71 |
| 2 | Z | 1216 | TYR | C-N-CA | 5.99 | 130.71 | 120.71 |
| 2 | Z | 1234 | ILE | CA-CB-CG1 | 5.99 | 120.58 | 110.40 |
| 19 | m | 426 | TYR | N-CA-C | -5.99 | 103.43 | 111.87 |
| 19 | m | 475 | ILE | CB-CA-C | -5.99 | 104.06 | 112.14 |
| 18 | e | 28 | SER | CA-C-O | -5.99 | 114.77 | 121.05 |
| 19 | f | 482 | ARG | N-CA-CB | 5.99 | 119.55 | 110.45 |
| 20 | g | 935 | GLU | N-CA-C | -5.99 | 103.62 | 113.50 |
| 7 | M | 444 | THR | CA-CB-OG1 | 5.98 | 118.58 | 109.60 |
| 4 | A | 817 | GLN | O-C-N | 5.98 | 129.37 | 122.25 |
| 4 | D | 658 | TYR | CA-C-N | 5.98 | 128.22 | 120.44 |
| 4 | D | 658 | TYR | C-N-CA | 5.98 | 128.22 | 120.44 |
| 9 | R | 564 | GLU | N-CA-C | -5.98 | 106.02 | 113.38 |
| 9 | R | 770 | ASN | N-CA-C | -5.98 | 105.94 | 113.72 |
| 2 | Z | 1260 | SER | CB-CA-C | -5.98 | 100.74 | 110.79 |
| 13 | w | 1350 | PHE | CB-CA-C | -5.98 | 100.86 | 110.79 |
| 14 | h | 632 | GLN | N-CA-C | 5.98 | 117.80 | 111.28 |
| 15 | i | 162 | VAL | CA-C-O | 5.98 | 126.99 | 119.39 |
| 16 | c | 445 | LEU | N-CA-C | -5.98 | 102.60 | 111.81 |
| 16 | c | 474 | THR | CA-C-N | 5.98 | 128.58 | 120.44 |
| 16 | c | 474 | THR | C-N-CA | 5.98 | 128.58 | 120.44 |
| 1 | 0 | 1290 | LYS | N-CA-C | -5.98 | 102.60 | 111.81 |
| 5 | E | 510 | VAL | O-C-N | -5.98 | 115.67 | 121.83 |
| 5 | H | 356 | GLU | CA-C-N | 5.98 | 126.62 | 119.98 |
| 5 | H | 356 | GLU | C-N-CA | 5.98 | 126.62 | 119.98 |
| 7 | M | 191 | ASP | N-CA-C | 5.98 | 117.47 | 111.07 |
| 8 | N | 1062 | ARG | CA-C-O | -5.98 | 114.87 | 121.33 |
| 8 | N | 1354 | GLU | N-CA-CB | 5.98 | 120.67 | 110.50 |
| 14 | h | 333 | ASP | CA-CB-CG | 5.98 | 118.58 | 112.60 |
| 17 | k | 266 | GLY | O-C-N | 5.98 | 127.99 | 122.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | n | 113 | THR | N-CA-CB | 5.98 | 119.62 | 109.87 |
| 20 | n | 1137 | ILE | N-CA-C | 5.98 | 116.72 | 110.62 |
| 20 | g | 401 | ILE | CA-C-O | -5.98 | 111.94 | 119.95 |
| 20 | g | 656 | VAL | CA-CB-CG1 | -5.98 | 100.23 | 110.40 |
| 2 | 1 | 1331 | ASN | CB-CA-C | -5.98 | 99.25 | 109.65 |
| 5 | H | 387 | GLN | CA-C-N | 5.98 | 128.29 | 120.28 |
| 5 | H | 387 | GLN | C-N-CA | 5.98 | 128.29 | 120.28 |
| 14 | a | 627 | TYR | CA-C-O | 5.98 | 126.86 | 120.70 |
| 1 | 0 | 832 | VAL | CA-C-O | 5.98 | 128.25 | 120.78 |
| 7 | O | 569 | ILE | CB-CA-C | 5.98 | 117.04 | 111.30 |
| 8 | P | 373 | PRO | N-CA-CB | 5.98 | 107.02 | 102.36 |
| 8 | P | 777 | ASP | CA-CB-CG | 5.98 | 118.58 | 112.60 |
| 1 | Y | 431 | ASN | CA-CB-CG | -5.98 | 106.62 | 112.60 |
| 1 | Y | 467 | PHE | CA-CB-CG | -5.98 | 107.82 | 113.80 |
| 2 | 1 | 963 | THR | CA-C-N | 5.98 | 128.21 | 120.56 |
| 2 | 1 | 963 | THR | C-N-CA | 5.98 | 128.21 | 120.56 |
| 7 | M | 102 | GLY | CA-C-N | 5.98 | 128.21 | 120.44 |
| 7 | M | 102 | GLY | C-N-CA | 5.98 | 128.21 | 120.44 |
| 9 | T | 481 | THR | CA-C-O | -5.98 | 114.08 | 120.42 |
| 9 | T | 658 | ASN | CA-C-N | 5.98 | 128.54 | 120.65 |
| 9 | T | 658 | ASN | C-N-CA | 5.98 | 128.54 | 120.65 |
| 14 | h | 89 | HIS | CA-C-N | 5.98 | 130.40 | 122.75 |
| 14 | h | 89 | HIS | C-N-CA | 5.98 | 130.40 | 122.75 |
| 14 | h | 133 | LEU | CA-C-N | 5.98 | 126.31 | 119.92 |
| 14 | h | 133 | LEU | C-N-CA | 5.98 | 126.31 | 119.92 |
| 1 | 0 | 1332 | ASP | N-CA-CB | 5.97 | 120.59 | 110.49 |
| 1 | 0 | 1410 | GLY | CA-C-N | 5.97 | 129.39 | 120.31 |
| 1 | 0 | 1410 | GLY | C-N-CA | 5.97 | 129.39 | 120.31 |
| 6 | I | 301 | HIS | ND1-CE1-NE2 | 5.97 | 114.38 | 108.40 |
| 5 | K | 436 | MET | N-CA-CB | 5.97 | 118.73 | 110.07 |
| 6 | L | 286 | LYS | CA-C-N | 5.97 | 128.28 | 120.28 |
| 6 | L | 286 | LYS | C-N-CA | 5.97 | 128.28 | 120.28 |
| 7 | M | 1561 | LEU | N-CA-C | 5.97 | 123.53 | 110.80 |
| 8 | N | 200 | LEU | N-CA-C | -5.97 | 105.85 | 113.02 |
| 7 | O | 212 | PHE | CA-CB-CG | -5.97 | 107.83 | 113.80 |
| 9 | S | 91 | GLN | N-CA-C | 5.97 | 117.46 | 111.07 |
| 10 | W | 350 | LEU | CB-CA-C | -5.97 | 100.58 | 109.90 |
| 1 | Y | 712 | ASP | CA-CB-CG | 5.97 | 118.58 | 112.60 |
| 20 | n | 111 | HIS | CB-CG-CD2 | -5.97 | 123.43 | 131.20 |
| 20 | n | 625 | GLN | CA-C-N | 5.97 | 128.29 | 120.28 |
| 20 | n | 625 | GLN | C-N-CA | 5.97 | 128.29 | 120.28 |
| 15 | b | 204 | PHE | CA-CB-CG | -5.97 | 107.83 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | f | 261 | ARG | CA-C-O | 5.97 | 125.36 | 118.97 |
| 20 | g | 295 | TRP | CB-CG-CD2 | 5.97 | 135.16 | 126.80 |
| 1 | 0 | 1149 | ALA | CB-CA-C | -5.97 | 101.69 | 110.95 |
| 7 | M | 1258 | HIS | CB-CG-CD2 | -5.97 | 123.44 | 131.20 |
| 8 | N | 256 | THR | CB-CA-C | -5.97 | 95.96 | 109.10 |
| 4 | y | 724 | ASP | O-C-N | 5.97 | 128.22 | 122.07 |
| 14 | h | 754 | GLU | N-CA-C | -5.97 | 105.08 | 112.72 |
| 15 | b | 524 | SER | CA-C-N | 5.97 | 128.90 | 120.42 |
| 15 | b | 524 | SER | C-N-CA | 5.97 | 128.90 | 120.42 |
| 7 | M | 1093 | SER | O-C-N | 5.97 | 128.45 | 122.12 |
| 11 | V | 299 | GLN | OE1-CD-NE2 | 5.97 | 128.57 | 122.60 |
| 12 | v | 261 | GLU | CA-C-O | -5.97 | 114.50 | 121.07 |
| 15 | b | 714 | ILE | N-CA-C | -5.97 | 106.94 | 112.43 |
| 8 | P | 366 | SER | N-CA-C | 5.97 | 117.79 | 111.28 |
| 8 | P | 590 | LEU | N-CA-C | -5.97 | 103.38 | 112.99 |
| 8 | P | 812 | SER | CA-C-N | 5.97 | 132.71 | 121.97 |
| 8 | P | 812 | SER | C-N-CA | 5.97 | 132.71 | 121.97 |
| 9 | R | 585 | GLU | O-C-N | 5.97 | 130.33 | 123.29 |
| 1 | Y | 1410 | GLY | CA-C-N | 5.97 | 128.88 | 120.28 |
| 1 | Y | 1410 | GLY | C-N-CA | 5.97 | 128.88 | 120.28 |
| 16 | j | 585 | ASN | CA-CB-CG | -5.97 | 106.63 | 112.60 |
| 20 | g | 499 | ASP | N-CA-C | -5.97 | 106.04 | 113.38 |
| 14 | a | 676 | ALA | CA-C-N | 5.97 | 128.88 | 120.28 |
| 14 | a | 676 | ALA | C-N-CA | 5.97 | 128.88 | 120.28 |
| 7 | M | 1109 | ILE | CA-C-O | 5.97 | 124.63 | 118.96 |
| 8 | P | 1021 | THR | N-CA-C | 5.97 | 118.55 | 111.33 |
| 19 | m | 656 | ARG | NH1-CZ-NH2 | -5.97 | 111.54 | 119.30 |
| 14 | a | 676 | ALA | N-CA-C | 5.97 | 117.45 | 111.07 |
| 8 | N | 323 | TYR | CB-CA-C | -5.97 | 105.86 | 114.87 |
| 8 | P | 355 | SER | CA-C-N | 5.97 | 131.06 | 122.35 |
| 8 | P | 355 | SER | C-N-CA | 5.97 | 131.06 | 122.35 |
| 9 | Q | 573 | HIS | CA-C-N | 5.97 | 129.38 | 120.31 |
| 9 | Q | 573 | HIS | C-N-CA | 5.97 | 129.38 | 120.31 |
| 9 | R | 138 | ASN | O-C-N | 5.97 | 128.22 | 122.07 |
| 10 | W | 344 | SER | CA-C-N | 5.97 | 129.18 | 120.71 |
| 10 | W | 344 | SER | C-N-CA | 5.97 | 129.18 | 120.71 |
| 2 | Z | 1318 | HIS | CE1-NE2-CD2 | -5.97 | 103.03 | 109.00 |
| 12 | v | 582 | GLU | N-CA-C | -5.97 | 98.09 | 110.80 |
| 13 | w | 1432 | LYS | CB-CA-C | -5.97 | 101.51 | 110.88 |
| 18 | l | 15 | VAL | N-CA-C | -5.97 | 99.46 | 108.17 |
| 20 | g | 451 | ASN | N-CA-C | -5.97 | 104.21 | 112.03 |
| 1 | 0 | 297 | HIS | ND1-CE1-NE2 | 5.96 | 114.36 | 108.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | I | 464 | THR | CA-C-N | 5.96 | 128.76 | 120.29 |
| 6 | I | 464 | THR | C-N-CA | 5.96 | 128.76 | 120.29 |
| 8 | N | 299 | ASN | CA-C-N | 5.96 | 128.27 | 120.28 |
| 8 | N | 299 | ASN | C-N-CA | 5.96 | 128.27 | 120.28 |
| 9 | T | 215 | TYR | CA-C-N | 5.96 | 128.27 | 120.28 |
| 9 | T | 215 | TYR | C-N-CA | 5.96 | 128.27 | 120.28 |
| 14 | h | 604 | ALA | CA-C-N | 5.96 | 128.07 | 120.56 |
| 14 | h | 604 | ALA | C-N-CA | 5.96 | 128.07 | 120.56 |
| 14 | h | 1036 | GLY | CA-C-O | -5.96 | 108.28 | 120.80 |
| 16 | j | 547 | ARG | NE-CZ-NH2 | 5.96 | 124.57 | 119.20 |
| 21 | p | 57 | TRP | CG-CD2-CE3 | -5.96 | 127.94 | 133.90 |
| 15 | b | 506 | GLU | N-CA-C | -5.96 | 104.53 | 112.94 |
| 2 | 1 | 767 | ASN | O-C-N | -5.96 | 114.66 | 122.59 |
| 8 | P | 1392 | PHE | CA-C-N | 5.96 | 128.27 | 120.28 |
| 8 | P | 1392 | PHE | C-N-CA | 5.96 | 128.27 | 120.28 |
| 9 | S | 96 | LEU | CA-C-O | 5.96 | 126.87 | 120.55 |
| 2 | Z | 499 | SER | N-CA-C | -5.96 | 98.10 | 110.80 |
| 5 | B | 382 | LYS | CA-C-N | 5.96 | 128.75 | 120.29 |
| 5 | B | 382 | LYS | C-N-CA | 5.96 | 128.75 | 120.29 |
| 5 | B | 386 | LEU | N-CA-C | -5.96 | 105.09 | 112.90 |
| 4 | D | 790 | ASN | N-CA-C | 5.96 | 119.81 | 112.54 |
| 9 | T | 99 | ASN | CA-C-N | 5.96 | 126.52 | 120.38 |
| 9 | T | 99 | ASN | C-N-CA | 5.96 | 126.52 | 120.38 |
| 10 | U | 283 | ILE | CA-CB-CG2 | 5.96 | 120.63 | 110.50 |
| 20 | n | 264 | ASN | CA-CB-CG | -5.96 | 106.64 | 112.60 |
| 15 | b | 307 | LYS | N-CA-C | -5.96 | 105.66 | 113.17 |
| 19 | f | 561 | ASN | N-CA-C | -5.96 | 104.67 | 113.61 |
| 1 | 0 | 361 | ILE | CA-CB-CG1 | -5.96 | 100.27 | 110.40 |
| 8 | N | 995 | LEU | N-CA-C | -5.96 | 104.85 | 114.09 |
| 9 | R | 793 | LYS | CA-C-O | 5.96 | 125.69 | 119.14 |
| 5 | B | 411 | ARG | NE-CZ-NH2 | 5.96 | 124.56 | 119.20 |
| 8 | N | 330 | TYR | N-CA-CB | 5.96 | 119.00 | 110.06 |
| 8 | N | 1439 | LEU | CA-C-O | -5.96 | 114.19 | 120.63 |
| 1 | Y | 1000 | ASP | CA-C-N | 5.96 | 128.57 | 120.77 |
| 1 | Y | 1000 | ASP | C-N-CA | 5.96 | 128.57 | 120.77 |
| 16 | c | 355 | SER | CA-C-N | 5.96 | 129.37 | 120.31 |
| 16 | c | 355 | SER | C-N-CA | 5.96 | 129.37 | 120.31 |
| 20 | g | 585 | LEU | N-CA-C | -5.96 | 104.67 | 113.61 |
| 14 | a | 351 | LEU | N-CA-CB | 5.96 | 119.37 | 109.60 |
| 1 | 0 | 623 | GLY | CA-C-O | 5.96 | 126.97 | 120.66 |
| 1 | 0 | 893 | ILE | CA-C-N | 5.96 | 128.26 | 120.28 |
| 1 | 0 | 893 | ILE | C-N-CA | 5.96 | 128.26 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 1536 | SER | CA-C-N | 5.96 | 128.86 | 120.28 |
| 7 | M | 1536 | SER | C-N-CA | 5.96 | 128.86 | 120.28 |
| 8 | N | 1504 | LEU | CA-C-O | -5.96 | 114.57 | 120.82 |
| 7 | O | 1509 | ASP | N-CA-CB | 5.96 | 118.88 | 109.71 |
| 8 | P | 1048 | LYS | N-CA-C | -5.96 | 98.11 | 110.80 |
| 9 | T | 543 | LYS | N-CA-CB | 5.96 | 119.55 | 110.14 |
| 10 | U | 313 | TRP | N-CA-C | -5.96 | 100.27 | 109.14 |
| 16 | j | 522 | THR | N-CA-C | -5.96 | 106.01 | 113.28 |
| 20 | n | 1111 | GLU | CA-C-N | 5.96 | 128.75 | 120.29 |
| 20 | n | 1111 | GLU | C-N-CA | 5.96 | 128.75 | 120.29 |
| 1 | 0 | 133 | TYR | N-CA-C | -5.96 | 101.71 | 110.52 |
| 4 | D | 642 | THR | N-CA-CB | 5.95 | 119.51 | 110.28 |
| 5 | K | 407 | GLU | CA-C-N | 5.95 | 128.06 | 120.56 |
| 5 | K | 407 | GLU | C-N-CA | 5.95 | 128.06 | 120.56 |
| 7 | M | 1120 | THR | O-C-N | -5.95 | 116.46 | 123.25 |
| 7 | M | 1412 | TYR | CA-C-N | 5.95 | 128.85 | 120.28 |
| 7 | M | 1412 | TYR | C-N-CA | 5.95 | 128.85 | 120.28 |
| 7 | O | 917 | PHE | CA-CB-CG | 5.95 | 119.75 | 113.80 |
| 9 | S | 714 | CYS | CA-C-N | 5.95 | 128.85 | 120.28 |
| 9 | S | 714 | CYS | C-N-CA | 5.95 | 128.85 | 120.28 |
| 12 | u | 39 | GLN | CG-CD-NE2 | 5.95 | 125.33 | 116.40 |
| 19 | m | 353 | ASP | CA-CB-CG | -5.95 | 106.65 | 112.60 |
| 19 | m | 595 | ARG | NE-CZ-NH2 | 5.95 | 124.56 | 119.20 |
| 16 | c | 157 | SER | N-CA-CB | 5.95 | 120.55 | 110.49 |
| 1 | 0 | 274 | VAL | N-CA-C | -5.95 | 100.11 | 108.27 |
| 7 | O | 1655 | SER | N-CA-CB | 5.95 | 118.64 | 110.01 |
| 8 | P | 1560 | MET | N-CA-CB | 5.95 | 118.87 | 110.12 |
| 9 | T | 254 | LEU | CA-C-O | 5.95 | 127.06 | 120.63 |
| 12 | v | 49 | LEU | CB-CA-C | -5.95 | 101.89 | 111.18 |
| 14 | h | 611 | THR | N-CA-C | -5.95 | 105.98 | 113.72 |
| 18 | e | 318 | ILE | N-CA-C | -5.95 | 99.64 | 108.45 |
| 8 | N | 1041 | ASN | N-CA-C | 5.95 | 117.89 | 108.67 |
| 8 | P | 43 | PHE | N-CA-C | -5.95 | 105.67 | 113.17 |
| 8 | P | 1166 | VAL | N-CA-C | 5.95 | 116.44 | 107.75 |
| 9 | Q | 233 | ASP | N-CA-C | -5.95 | 98.12 | 110.80 |
| 9 | T | 568 | ASP | CA-CB-CG | -5.95 | 106.65 | 112.60 |
| 12 | v | 303 | ALA | CB-CA-C | -5.95 | 97.61 | 109.33 |
| 15 | b | 57 | PRO | N-CA-CB | 5.95 | 109.50 | 103.25 |
| 1 | 0 | 706 | GLY | N-CA-C | -5.95 | 104.60 | 112.81 |
| 5 | E | 413 | LEU | CA-C-N | 5.95 | 128.25 | 120.28 |
| 5 | E | 413 | LEU | C-N-CA | 5.95 | 128.25 | 120.28 |
| 8 | N | 1504 | LEU | N-CA-CB | 5.95 | 118.64 | 110.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 729 | MET | N-CA-C | 5.95 | 117.73 | 110.41 |
| 2 | Z | 927 | HIS | CA-CB-CG | 5.95 | 119.75 | 113.80 |
| 2 | Z | 1213 | LEU | N-CA-C | -5.95 | 106.56 | 113.88 |
| 20 | n | 593 | ILE | N-CA-C | 5.95 | 116.73 | 110.72 |
| 14 | a | 101 | SER | N-CA-CB | 5.95 | 119.44 | 109.92 |
| 2 | 1 | 856 | ASN | CA-C-N | 5.95 | 129.35 | 120.31 |
| 2 | 1 | 856 | ASN | C-N-CA | 5.95 | 129.35 | 120.31 |
| 2 | 1 | 1189 | LYS | CA-C-N | 5.95 | 128.25 | 120.28 |
| 2 | 1 | 1189 | LYS | C-N-CA | 5.95 | 128.25 | 120.28 |
| 7 | M | 95 | GLY | CA-C-N | 5.95 | 129.56 | 120.82 |
| 7 | M | 95 | GLY | C-N-CA | 5.95 | 129.56 | 120.82 |
| 20 | n | 624 | THR | CA-CB-OG1 | 5.95 | 118.52 | 109.60 |
| 2 | 1 | 542 | ALA | CA-C-N | 5.95 | 125.96 | 119.90 |
| 2 | 1 | 542 | ALA | C-N-CA | 5.95 | 125.96 | 119.90 |
| 8 | N | 1483 | ILE | CB-CA-C | 5.95 | 117.81 | 110.73 |
| 7 | O | 1044 | SER | N-CA-C | -5.95 | 103.56 | 112.54 |
| 9 | T | 226 | ARG | N-CA-C | -5.95 | 105.29 | 112.54 |
| 12 | v | 375 | VAL | CA-C-N | 5.95 | 129.13 | 122.59 |
| 12 | v | 375 | VAL | C-N-CA | 5.95 | 129.13 | 122.59 |
| 15 | i | 227 | VAL | N-CA-CB | 5.95 | 121.04 | 111.23 |
| 18 | l | 105 | ASN | N-CA-C | -5.95 | 104.68 | 112.41 |
| 19 | m | 522 | LEU | N-CA-C | -5.95 | 97.44 | 108.02 |
| 20 | g | 722 | PHE | CA-C-N | 5.95 | 132.13 | 121.66 |
| 20 | g | 722 | PHE | C-N-CA | 5.95 | 132.13 | 121.66 |
| 1 | Y | 597 | THR | N-CA-C | -5.94 | 100.03 | 109.07 |
| 14 | h | 606 | LYS | N-CA-CB | 5.94 | 120.53 | 110.49 |
| 1 | Y | 1238 | ARG | N-CA-C | -5.94 | 104.22 | 112.30 |
| 20 | n | 388 | GLU | N-CA-C | -5.94 | 100.04 | 109.07 |
| 17 | d | 103 | ASN | CA-CB-CG | -5.94 | 106.66 | 112.60 |
| 1 | 0 | 947 | LEU | N-CA-CB | 5.94 | 120.53 | 110.49 |
| 5 | B | 456 | THR | N-CA-C | -5.94 | 104.44 | 111.03 |
| 9 | T | 502 | ASP | CA-CB-CG | -5.94 | 106.66 | 112.60 |
| 9 | T | 833 | ILE | N-CA-C | -5.94 | 104.94 | 110.53 |
| 10 | W | 327 | ALA | O-C-N | 5.94 | 129.66 | 122.35 |
| 13 | w | 1357 | ASN | CA-C-N | 5.94 | 128.24 | 120.28 |
| 13 | w | 1357 | ASN | C-N-CA | 5.94 | 128.24 | 120.28 |
| 20 | n | 307 | LEU | CA-C-O | -5.94 | 111.64 | 119.06 |
| 21 | s | 80 | TYR | CA-C-O | -5.94 | 114.28 | 120.70 |
| 19 | f | 352 | LEU | CA-C-N | 5.94 | 130.80 | 122.36 |
| 19 | f | 352 | LEU | C-N-CA | 5.94 | 130.80 | 122.36 |
| 14 | a | 240 | ASN | CA-CB-CG | -5.94 | 106.66 | 112.60 |
| 2 | 1 | 1092 | LEU | CB-CA-C | 5.94 | 122.24 | 110.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 143 | ASN | CA-C-N | 5.94 | 128.85 | 120.42 |
| 7 | O | 143 | ASN | C-N-CA | 5.94 | 128.85 | 120.42 |
| 9 | Q | 125 | ILE | CA-C-N | 5.94 | 128.72 | 120.29 |
| 9 | Q | 125 | ILE | C-N-CA | 5.94 | 128.72 | 120.29 |
| 9 | R | 762 | ASN | OD1-CG-ND2 | 5.94 | 128.54 | 122.60 |
| 9 | T | 209 | ARG | N-CA-CB | 5.94 | 119.37 | 110.22 |
| 9 | T | 707 | HIS | CG-CD2-NE2 | 5.94 | 113.14 | 107.20 |
| 12 | u | 96 | GLY | CA-C-N | 5.94 | 129.30 | 120.87 |
| 12 | u | 96 | GLY | C-N-CA | 5.94 | 129.30 | 120.87 |
| 20 | n | 170 | SER | O-C-N | -5.94 | 115.96 | 122.67 |
| 7 | M | 224 | ASP | CA-CB-CG | 5.94 | 118.54 | 112.60 |
| 7 | O | 519 | ASP | CA-CB-CG | 5.94 | 118.54 | 112.60 |
| 9 | T | 121 | ILE | CA-C-O | -5.94 | 114.77 | 120.95 |
| 9 | T | 653 | VAL | N-CA-C | 5.94 | 116.67 | 110.62 |
| 2 | Z | 383 | HIS | CA-C-N | 5.94 | 128.85 | 120.42 |
| 2 | Z | 383 | HIS | C-N-CA | 5.94 | 128.85 | 120.42 |
| 2 | Z | 509 | THR | CA-C-N | 5.94 | 131.06 | 121.98 |
| 2 | Z | 509 | THR | C-N-CA | 5.94 | 131.06 | 121.98 |
| 14 | h | 495 | TYR | CB-CG-CD2 | -5.94 | 111.89 | 120.80 |
| 16 | j | 213 | SER | N-CA-CB | 5.94 | 120.33 | 110.47 |
| 16 | c | 441 | ARG | N-CA-CB | 5.94 | 120.53 | 110.49 |
| 18 | e | 201 | LYS | N-CA-C | -5.94 | 101.69 | 110.48 |
| 19 | f | 157 | ASP | CA-CB-CG | 5.94 | 118.54 | 112.60 |
| 8 | P | 1207 | TRP | O-C-N | 5.94 | 128.18 | 122.07 |
| 9 | Q | 692 | MET | CA-C-N | 5.94 | 131.53 | 121.14 |
| 9 | Q | 692 | MET | C-N-CA | 5.94 | 131.53 | 121.14 |
| 1 | Y | 667 | LEU | CA-C-N | 5.94 | 125.56 | 119.56 |
| 1 | Y | 667 | LEU | C-N-CA | 5.94 | 125.56 | 119.56 |
| 2 | Z | 1307 | VAL | CA-C-O | 5.94 | 124.60 | 118.96 |
| 14 | h | 187 | LYS | N-CA-C | -5.94 | 100.03 | 109.76 |
| 17 | k | 228 | ASP | CA-C-N | 5.94 | 132.88 | 121.54 |
| 17 | k | 228 | ASP | C-N-CA | 5.94 | 132.88 | 121.54 |
| 19 | m | 159 | ASP | CB-CA-C | -5.94 | 100.18 | 110.09 |
| 5 | E | 301 | PRO | CA-C-N | 5.93 | 129.45 | 123.04 |
| 5 | E | 301 | PRO | C-N-CA | 5.93 | 129.45 | 123.04 |
| 7 | M | 695 | ALA | N-CA-C | 5.93 | 117.75 | 111.28 |
| 9 | R | 226 | ARG | NE-CZ-NH1 | 5.93 | 127.43 | 121.50 |
| 1 | Y | 1181 | PHE | CA-C-N | 5.93 | 129.44 | 120.95 |
| 1 | Y | 1181 | PHE | C-N-CA | 5.93 | 129.44 | 120.95 |
| 19 | m | 537 | PHE | CA-CB-CG | -5.93 | 107.86 | 113.80 |
| 14 | a | 390 | GLN | CB-CG-CD | -5.93 | 102.51 | 112.60 |
| 9 | S | 587 | THR | CA-C-N | 5.93 | 130.31 | 121.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | S | 587 | THR | C-N-CA | 5.93 | 130.31 | 121.77 |
| 10 | U | 319 | LYS | N-CA-CB | 5.93 | 119.54 | 109.87 |
| 21 | s | 75 | HIS | ND1-CE1-NE2 | 5.93 | 114.33 | 108.40 |
| 14 | h | 1028 | THR | N-CA-C | -5.93 | 105.38 | 114.16 |
| 2 | 1 | 600 | LYS | CA-C-N | 5.93 | 131.23 | 122.99 |
| 2 | 1 | 600 | LYS | C-N-CA | 5.93 | 131.23 | 122.99 |
| 5 | E | 361 | ARG | N-CA-C | 5.93 | 117.74 | 111.28 |
| 7 | M | 225 | SER | CA-C-N | 5.93 | 128.22 | 120.28 |
| 7 | M | 225 | SER | C-N-CA | 5.93 | 128.22 | 120.28 |
| 8 | N | 338 | SER | CB-CA-C | -5.93 | 99.11 | 109.07 |
| 9 | S | 269 | ASN | CA-C-N | 5.93 | 129.97 | 121.02 |
| 9 | S | 269 | ASN | C-N-CA | 5.93 | 129.97 | 121.02 |
| 1 | Y | 1373 | LYS | CA-C-N | 5.93 | 130.48 | 120.64 |
| 1 | Y | 1373 | LYS | C-N-CA | 5.93 | 130.48 | 120.64 |
| 12 | v | 271 | ASP | CA-CB-CG | -5.93 | 106.67 | 112.60 |
| 20 | g | 507 | ILE | N-CA-CB | -5.93 | 104.61 | 112.26 |
| 14 | a | 100 | ALA | CA-C-N | 5.93 | 129.54 | 120.82 |
| 14 | a | 100 | ALA | C-N-CA | 5.93 | 129.54 | 120.82 |
| 1 | 0 | 1025 | ASN | N-CA-C | -5.93 | 104.70 | 112.41 |
| 6 | C | 334 | SER | CA-C-N | 5.93 | 128.47 | 120.65 |
| 6 | C | 334 | SER | C-N-CA | 5.93 | 128.47 | 120.65 |
| 7 | M | 1049 | LEU | CA-C-N | 5.93 | 132.86 | 121.54 |
| 7 | M | 1049 | LEU | C-N-CA | 5.93 | 132.86 | 121.54 |
| 7 | O | 150 | PHE | CA-C-O | -5.93 | 114.27 | 120.55 |
| 9 | Q | 229 | ASN | CA-CB-CG | 5.93 | 118.53 | 112.60 |
| 6 | I | 452 | ASP | N-CA-C | 5.93 | 117.82 | 111.36 |
| 8 | N | 768 | ALA | N-CA-C | -5.93 | 106.21 | 113.50 |
| 7 | O | 1091 | LEU | N-CA-CB | 5.93 | 118.77 | 109.94 |
| 9 | Q | 781 | CYS | CB-CA-C | -5.93 | 99.29 | 110.67 |
| 9 | T | 577 | ARG | N-CA-CB | 5.93 | 118.60 | 110.01 |
| 15 | i | 568 | VAL | CA-C-N | 5.93 | 130.90 | 121.18 |
| 15 | i | 568 | VAL | C-N-CA | 5.93 | 130.90 | 121.18 |
| 20 | n | 940 | ASP | CA-CB-CG | -5.93 | 106.67 | 112.60 |
| 15 | b | 161 | ARG | NE-CZ-NH1 | 5.93 | 127.43 | 121.50 |
| 20 | g | 106 | TYR | O-C-N | 5.93 | 130.53 | 122.82 |
| 20 | g | 392 | ASP | CA-C-N | 5.93 | 132.86 | 121.54 |
| 20 | g | 392 | ASP | C-N-CA | 5.93 | 132.86 | 121.54 |
| 2 | 1 | 663 | ALA | CA-C-O | -5.92 | 114.27 | 120.55 |
| 7 | M | 537 | PRO | CA-C-N | 5.92 | 128.22 | 120.28 |
| 7 | M | 537 | PRO | C-N-CA | 5.92 | 128.22 | 120.28 |
| 8 | N | 333 | ARG | N-CA-CB | 5.92 | 119.58 | 110.81 |
| 9 | T | 704 | ARG | CA-C-O | 5.92 | 126.53 | 119.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | f | 393 | ALA | CA-C-N | 5.92 | 128.57 | 120.46 |
| 19 | f | 393 | ALA | C-N-CA | 5.92 | 128.57 | 120.46 |
| 20 | g | 598 | ILE | O-C-N | 5.92 | 127.62 | 121.87 |
| 7 | M | 212 | PHE | CA-C-N | 5.92 | 128.57 | 120.46 |
| 7 | M | 212 | PHE | C-N-CA | 5.92 | 128.57 | 120.46 |
| 9 | T | 327 | VAL | CA-CB-CG2 | -5.92 | 100.33 | 110.40 |
| 4 | z | 714 | PHE | CA-C-O | -5.92 | 113.57 | 120.20 |
| 18 | l | 339 | PHE | N-CA-CB | 5.92 | 119.63 | 110.21 |
| 15 | b | 678 | ASP | CA-CB-CG | 5.92 | 118.52 | 112.60 |
| 19 | f | 216 | GLN | CA-CB-CG | 5.92 | 125.95 | 114.10 |
| 20 | g | 235 | ASN | OD1-CG-ND2 | 5.92 | 128.52 | 122.60 |
| 20 | g | 574 | ASN | CA-C-N | 5.92 | 132.85 | 121.54 |
| 20 | g | 574 | ASN | C-N-CA | 5.92 | 132.85 | 121.54 |
| 14 | a | 219 | ASP | N-CA-CB | 5.92 | 120.50 | 110.49 |
| 1 | 0 | 659 | PHE | CA-CB-CG | 5.92 | 119.72 | 113.80 |
| 5 | B | 351 | GLN | N-CA-CB | 5.92 | 118.66 | 109.48 |
| 6 | I | 348 | GLN | OE1-CD-NE2 | 5.92 | 128.52 | 122.60 |
| 7 | M | 786 | THR | CA-C-N | 5.92 | 130.92 | 120.74 |
| 7 | M | 786 | THR | C-N-CA | 5.92 | 130.92 | 120.74 |
| 7 | M | 881 | THR | CA-CB-CG2 | 5.92 | 120.57 | 110.50 |
| 8 | N | 557 | TYR | CB-CG-CD1 | 5.92 | 129.68 | 120.80 |
| 7 | O | 484 | SER | CA-C-N | 5.92 | 128.57 | 120.46 |
| 7 | O | 484 | SER | C-N-CA | 5.92 | 128.57 | 120.46 |
| 9 | Q | 72 | LEU | CA-C-N | 5.92 | 128.22 | 120.28 |
| 9 | Q | 72 | LEU | C-N-CA | 5.92 | 128.22 | 120.28 |
| 9 | R | 657 | VAL | CA-C-N | 5.92 | 128.49 | 120.38 |
| 9 | R | 657 | VAL | C-N-CA | 5.92 | 128.49 | 120.38 |
| 12 | v | 363 | LEU | CA-C-O | -5.92 | 114.31 | 120.70 |
| 18 | l | 23 | HIS | N-CA-C | -5.92 | 98.99 | 109.06 |
| 20 | n | 637 | ASN | CA-CB-CG | -5.92 | 106.68 | 112.60 |
| 19 | f | 209 | CYS | N-CA-C | 5.92 | 118.69 | 111.82 |
| 14 | a | 983 | GLN | N-CA-CB | -5.92 | 101.71 | 110.53 |
| 5 | B | 330 | VAL | O-C-N | -5.92 | 116.51 | 122.67 |
| 7 | M | 1558 | ASP | N-CA-C | -5.92 | 104.59 | 112.94 |
| 7 | O | 1245 | LEU | N-CA-C | 5.92 | 117.73 | 111.28 |
| 2 | 1 | 187 | ASN | CA-CB-CG | 5.92 | 118.52 | 112.60 |
| 4 | D | 703 | GLN | CA-C-N | 5.92 | 128.69 | 120.29 |
| 4 | D | 703 | GLN | C-N-CA | 5.92 | 128.69 | 120.29 |
| 7 | O | 1282 | ALA | CA-C-N | 5.92 | 128.13 | 120.44 |
| 7 | O | 1282 | ALA | C-N-CA | 5.92 | 128.13 | 120.44 |
| 9 | S | 351 | GLN | O-C-N | -5.92 | 115.40 | 122.15 |
| 1 | Y | 185 | THR | CA-C-O | 5.92 | 127.80 | 121.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | u | 241 | THR | N-CA-C | -5.92 | 99.59 | 109.24 |
| 15 | i | 318 | GLY | CA-C-N | 5.92 | 130.74 | 120.68 |
| 15 | i | 318 | GLY | C-N-CA | 5.92 | 130.74 | 120.68 |
| 19 | m | 407 | VAL | N-CA-C | -5.92 | 105.31 | 111.58 |
| 2 | 1 | 389 | ASN | O-C-N | 5.92 | 129.44 | 122.34 |
| 9 | Q | 819 | MET | N-CA-CB | 5.92 | 120.04 | 110.40 |
| 1 | Y | 919 | VAL | N-CA-C | -5.92 | 106.05 | 111.67 |
| 12 | v | 579 | ARG | O-C-N | 5.92 | 128.16 | 122.07 |
| 13 | w | 1123 | GLN | CB-CA-C | -5.92 | 98.65 | 110.42 |
| 15 | i | 494 | THR | N-CA-CB | 5.92 | 119.44 | 110.45 |
| 16 | j | 547 | ARG | N-CA-C | 5.92 | 118.94 | 110.24 |
| 16 | j | 585 | ASN | CA-C-O | -5.92 | 113.88 | 119.80 |
| 15 | b | 303 | PHE | N-CA-C | -5.92 | 105.89 | 113.23 |
| 20 | g | 597 | CYS | N-CA-C | -5.92 | 104.91 | 111.36 |
| 7 | O | 842 | ASN | CA-CB-CG | 5.92 | 118.52 | 112.60 |
| 9 | Q | 326 | THR | N-CA-C | -5.92 | 98.64 | 108.34 |
| 9 | R | 690 | ARG | CA-C-N | 5.92 | 128.48 | 120.44 |
| 9 | R | 690 | ARG | C-N-CA | 5.92 | 128.48 | 120.44 |
| 17 | k | 113 | GLY | CA-C-N | 5.92 | 127.23 | 119.84 |
| 17 | k | 113 | GLY | C-N-CA | 5.92 | 127.23 | 119.84 |
| 20 | n | 453 | ILE | CA-C-N | 5.92 | 129.61 | 121.33 |
| 20 | n | 453 | ILE | C-N-CA | 5.92 | 129.61 | 121.33 |
| 20 | g | 1010 | ASP | CA-C-N | 5.92 | 129.68 | 120.75 |
| 20 | g | 1010 | ASP | C-N-CA | 5.92 | 129.68 | 120.75 |
| 1 | 0 | 1347 | LEU | CB-CA-C | -5.91 | 98.87 | 110.11 |
| 5 | B | 357 | GLY | N-CA-C | -5.91 | 107.00 | 114.16 |
| 9 | R | 821 | GLN | CA-C-N | 5.91 | 132.84 | 121.54 |
| 9 | R | 821 | GLN | C-N-CA | 5.91 | 132.84 | 121.54 |
| 15 | i | 715 | GLU | N-CA-C | -5.91 | 106.11 | 113.38 |
| 19 | f | 181 | PHE | CA-CB-CG | -5.91 | 107.89 | 113.80 |
| 9 | R | 805 | SER | CA-C-O | 5.91 | 126.82 | 120.55 |
| 2 | Z | 192 | HIS | CA-CB-CG | 5.91 | 119.71 | 113.80 |
| 20 | n | 863 | ARG | CA-C-N | 5.91 | 129.67 | 120.68 |
| 20 | n | 863 | ARG | C-N-CA | 5.91 | 129.67 | 120.68 |
| 14 | a | 28 | VAL | N-CA-C | -5.91 | 99.81 | 108.97 |
| 14 | a | 691 | LYS | N-CA-C | -5.91 | 97.53 | 107.99 |
| 1 | 0 | 654 | THR | CA-CB-OG1 | 5.91 | 118.47 | 109.60 |
| 2 | 1 | 595 | SER | N-CA-CB | 5.91 | 119.04 | 110.88 |
| 6 | C | 393 | ASP | CA-C-N | 5.91 | 128.56 | 120.46 |
| 6 | C | 393 | ASP | C-N-CA | 5.91 | 128.56 | 120.46 |
| 5 | H | 396 | SER | CA-C-O | 5.91 | 126.79 | 120.70 |
| 7 | M | 783 | ILE | CA-C-N | 5.91 | 128.51 | 120.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 783 | ILE | C-N-CA | 5.91 | 128.51 | 120.77 |
| 7 | O | 1668 | LYS | N-CA-C | -5.91 | 105.16 | 112.90 |
| 8 | P | 650 | ASP | CA-CB-CG | 5.91 | 118.51 | 112.60 |
| 8 | P | 660 | PHE | N-CA-C | -5.91 | 98.21 | 110.80 |
| 8 | P | 1413 | ASN | OD1-CG-ND2 | 5.91 | 128.51 | 122.60 |
| 9 | Q | 461 | ASP | N-CA-C | -5.91 | 98.21 | 110.80 |
| 12 | v | 162 | LYS | CA-C-N | 5.91 | 127.23 | 119.84 |
| 12 | v | 162 | LYS | C-N-CA | 5.91 | 127.23 | 119.84 |
| 14 | h | 629 | ILE | N-CA-C | -5.91 | 104.75 | 110.42 |
| 20 | n | 359 | THR | CA-C-O | 5.91 | 127.05 | 120.43 |
| 20 | n | 815 | VAL | CA-C-N | 5.91 | 128.12 | 120.44 |
| 20 | n | 815 | VAL | C-N-CA | 5.91 | 128.12 | 120.44 |
| 1 | 0 | 1010 | LEU | N-CA-C | -5.91 | 98.22 | 110.80 |
| 8 | N | 1127 | ASN | OD1-CG-ND2 | -5.91 | 116.69 | 122.60 |
| 7 | O | 137 | ASN | N-CA-CB | 5.91 | 120.47 | 110.49 |
| 8 | P | 449 | ASP | CA-CB-CG | 5.91 | 118.51 | 112.60 |
| 9 | Q | 334 | TRP | N-CA-C | -5.91 | 104.79 | 112.23 |
| 12 | v | 555 | GLU | CA-C-N | 5.91 | 128.48 | 120.44 |
| 12 | v | 555 | GLU | C-N-CA | 5.91 | 128.48 | 120.44 |
| 21 | r | 20 | LEU | CA-C-N | 5.91 | 128.52 | 120.54 |
| 21 | r | 20 | LEU | C-N-CA | 5.91 | 128.52 | 120.54 |
| 2 | 1 | 1000 | LYS | O-C-N | 5.91 | 130.55 | 122.46 |
| 19 | m | 36 | PHE | CA-C-N | 5.91 | 128.47 | 120.44 |
| 19 | m | 36 | PHE | C-N-CA | 5.91 | 128.47 | 120.44 |
| 19 | f | 540 | ASN | OD1-CG-ND2 | 5.91 | 128.51 | 122.60 |
| 2 | 1 | 412 | ILE | CB-CA-C | 5.91 | 118.67 | 110.99 |
| 7 | M | 425 | ASP | CA-CB-CG | -5.91 | 106.69 | 112.60 |
| 7 | M | 1189 | MET | N-CA-CB | 5.91 | 120.47 | 110.49 |
| 8 | N | 1466 | TYR | N-CA-C | 5.91 | 117.72 | 111.28 |
| 8 | P | 1171 | ARG | NE-CZ-NH2 | -5.91 | 113.89 | 119.20 |
| 9 | Q | 213 | GLU | CB-CG-CD | -5.91 | 102.56 | 112.60 |
| 9 | S | 787 | HIS | CE1-NE2-CD2 | -5.91 | 103.09 | 109.00 |
| 14 | h | 539 | GLU | N-CA-C | -5.91 | 104.92 | 111.36 |
| 18 | l | 124 | LYS | N-CA-C | -5.91 | 99.27 | 108.90 |
| 16 | c | 334 | ASP | CB-CA-C | -5.91 | 100.99 | 110.79 |
| 5 | E | 467 | LYS | N-CA-C | 5.90 | 117.39 | 111.07 |
| 6 | F | 461 | HIS | CE1-NE2-CD2 | -5.90 | 103.10 | 109.00 |
| 8 | N | 722 | SER | N-CA-C | -5.90 | 105.42 | 114.16 |
| 9 | T | 708 | VAL | CA-C-O | -5.90 | 114.81 | 120.95 |
| 20 | n | 1110 | ARG | N-CA-CB | 5.90 | 119.00 | 110.20 |
| 16 | c | 244 | VAL | CA-C-O | -5.90 | 114.86 | 121.36 |
| 2 | 1 | 593 | GLN | O-C-N | 5.90 | 129.12 | 122.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1154 | ARG | CA-C-N | 5.90 | 130.13 | 120.63 |
| 7 | O | 1154 | ARG | C-N-CA | 5.90 | 130.13 | 120.63 |
| 2 | Z | 1331 | ASN | OD1-CG-ND2 | -5.90 | 116.70 | 122.60 |
| 16 | c | 282 | GLU | CA-C-O | -5.90 | 114.16 | 120.42 |
| 18 | e | 84 | TRP | CA-C-N | 5.90 | 131.31 | 122.99 |
| 18 | e | 84 | TRP | C-N-CA | 5.90 | 131.31 | 122.99 |
| 14 | a | 959 | GLU | CA-C-N | 5.90 | 132.47 | 122.26 |
| 14 | a | 959 | GLU | C-N-CA | 5.90 | 132.47 | 122.26 |
| 1 | 0 | 1404 | LYS | CA-C-N | 5.90 | 132.81 | 121.54 |
| 1 | 0 | 1404 | LYS | C-N-CA | 5.90 | 132.81 | 121.54 |
| 2 | 1 | 616 | THR | CA-C-O | -5.90 | 114.27 | 120.70 |
| 7 | M | 1124 | GLY | CA-C-N | 5.90 | 128.58 | 120.67 |
| 7 | M | 1124 | GLY | C-N-CA | 5.90 | 128.58 | 120.67 |
| 8 | P | 691 | SER | CA-C-N | 5.90 | 132.05 | 122.67 |
| 8 | P | 691 | SER | C-N-CA | 5.90 | 132.05 | 122.67 |
| 9 | Q | 709 | LYS | CB-CG-CD | 5.90 | 124.87 | 111.30 |
| 9 | R | 689 | ALA | CA-C-N | 5.90 | 128.19 | 120.28 |
| 9 | R | 689 | ALA | C-N-CA | 5.90 | 128.19 | 120.28 |
| 2 | Z | 280 | GLY | CA-C-N | 5.90 | 128.48 | 120.63 |
| 2 | Z | 280 | GLY | C-N-CA | 5.90 | 128.48 | 120.63 |
| 14 | h | 1034 | LEU | CA-C-O | -5.90 | 112.65 | 119.14 |
| 8 | P | 713 | LYS | N-CA-CB | 5.90 | 118.56 | 110.01 |
| 8 | P | 1036 | ASP | CA-C-O | 5.90 | 125.93 | 119.91 |
| 12 | v | 55 | HIS | CE1-NE2-CD2 | -5.90 | 103.10 | 109.00 |
| 19 | m | 165 | ASN | CA-CB-CG | -5.90 | 106.70 | 112.60 |
| 20 | n | 722 | PHE | CB-CG-CD1 | 5.90 | 130.73 | 120.70 |
| 7 | M | 826 | PRO | N-CA-C | -5.90 | 108.55 | 114.68 |
| 8 | P | 60 | GLN | CA-C-N | 5.90 | 128.18 | 120.28 |
| 8 | P | 60 | GLN | C-N-CA | 5.90 | 128.18 | 120.28 |
| 9 | Q | 140 | ILE | CA-C-N | 5.90 | 128.18 | 120.28 |
| 9 | Q | 140 | ILE | C-N-CA | 5.90 | 128.18 | 120.28 |
| 2 | Z | 161 | SER | CA-CB-OG | 5.90 | 122.90 | 111.10 |
| 12 | u | 127 | ILE | CA-CB-CG2 | -5.90 | 100.47 | 110.50 |
| 4 | y | 705 | ASP | CA-C-N | 5.90 | 128.66 | 120.29 |
| 4 | y | 705 | ASP | C-N-CA | 5.90 | 128.66 | 120.29 |
| 14 | h | 671 | ASP | N-CA-C | 5.90 | 119.03 | 110.42 |
| 14 | h | 723 | PHE | CA-CB-CG | 5.90 | 119.70 | 113.80 |
| 19 | m | 300 | ASN | CA-C-N | 5.90 | 128.77 | 120.28 |
| 19 | m | 300 | ASN | C-N-CA | 5.90 | 128.77 | 120.28 |
| 16 | c | 226 | LYS | N-CA-C | -5.90 | 106.09 | 113.28 |
| 20 | g | 814 | LEU | N-CA-C | 5.90 | 117.79 | 111.36 |
| 14 | a | 740 | PHE | CA-CB-CG | -5.90 | 107.90 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 1318 | HIS | N-CA-C | 5.89 | 117.78 | 111.36 |
| 8 | P | 912 | TRP | CB-CG-CD2 | -5.89 | 118.55 | 126.80 |
| 8 | P | 1248 | THR | CA-C-O | 5.89 | 126.73 | 120.36 |
| 9 | T | 91 | GLN | CA-C-N | 5.89 | 128.18 | 120.28 |
| 9 | T | 91 | GLN | C-N-CA | 5.89 | 128.18 | 120.28 |
| 2 | Z | 670 | PRO | CA-C-N | 5.89 | 127.51 | 120.14 |
| 2 | Z | 670 | PRO | C-N-CA | 5.89 | 127.51 | 120.14 |
| 2 | Z | 1283 | PHE | CA-C-O | -5.89 | 115.42 | 121.32 |
| 12 | u | 288 | ASN | CA-C-O | -5.89 | 112.08 | 120.16 |
| 15 | i | 683 | MET | CA-CB-CG | 5.89 | 125.89 | 114.10 |
| 18 | l | 107 | SER | O-C-N | -5.89 | 115.68 | 122.93 |
| 20 | n | 983 | VAL | N-CA-C | -5.89 | 104.72 | 113.39 |
| 21 | s | 39 | ARG | NE-CZ-NH2 | -5.89 | 113.89 | 119.20 |
| 19 | f | 545 | ALA | N-CA-C | -5.89 | 103.50 | 112.99 |
| 20 | g | 516 | LEU | CA-C-O | -5.89 | 112.95 | 118.73 |
| 6 | C | 450 | PHE | CA-C-N | 5.89 | 129.26 | 120.31 |
| 6 | C | 450 | PHE | C-N-CA | 5.89 | 129.26 | 120.31 |
| 7 | M | 211 | ASP | CA-C-N | 5.89 | 128.98 | 120.79 |
| 7 | M | 211 | ASP | C-N-CA | 5.89 | 128.98 | 120.79 |
| 7 | M | 268 | ILE | CA-C-O | 5.89 | 125.33 | 119.97 |
| 7 | M | 632 | SER | N-CA-CB | 5.89 | 118.78 | 110.12 |
| 7 | O | 350 | ARG | CB-CA-C | 5.89 | 118.48 | 110.94 |
| 7 | O | 533 | LEU | N-CA-C | -5.89 | 105.91 | 112.57 |
| 8 | P | 659 | GLU | N-CA-C | -5.89 | 104.94 | 111.36 |
| 9 | R | 40 | GLY | CA-C-O | 5.89 | 128.62 | 121.61 |
| 9 | T | 291 | LYS | N-CA-C | -5.89 | 105.92 | 113.23 |
| 1 | Y | 1078 | LYS | N-CA-C | -5.89 | 105.85 | 113.16 |
| 2 | Z | 674 | GLU | CA-C-N | 5.89 | 128.99 | 120.98 |
| 2 | Z | 674 | GLU | C-N-CA | 5.89 | 128.99 | 120.98 |
| 14 | h | 8 | ASP | N-CA-C | -5.89 | 99.58 | 109.07 |
| 14 | h | 394 | ASP | CA-CB-CG | -5.89 | 106.71 | 112.60 |
| 17 | k | 87 | GLY | O-C-N | 5.89 | 129.34 | 122.45 |
| 17 | k | 209 | ASP | CA-CB-CG | 5.89 | 118.49 | 112.60 |
| 14 | a | 560 | ASN | OD1-CG-ND2 | 5.89 | 128.49 | 122.60 |
| 4 | J | 800 | HIS | CE1-NE2-CD2 | -5.89 | 103.11 | 109.00 |
| 1 | Y | 1050 | ALA | CA-C-O | 5.89 | 126.75 | 119.97 |
| 14 | a | 650 | HIS | CG-CD2-NE2 | 5.89 | 113.09 | 107.20 |
| 5 | H | 437 | TRP | CA-C-N | 5.89 | 128.65 | 120.29 |
| 5 | H | 437 | TRP | C-N-CA | 5.89 | 128.65 | 120.29 |
| 5 | H | 457 | ASN | OD1-CG-ND2 | -5.89 | 116.71 | 122.60 |
| 5 | K | 320 | GLU | N-CA-CB | 5.89 | 120.44 | 110.49 |
| 7 | M | 723 | GLU | N-CA-C | -5.89 | 100.95 | 110.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 183 | TRP | CB-CG-CD2 | 5.89 | 135.05 | 126.80 |
| 15 | i | 241 | GLU | CA-C-N | 5.89 | 131.17 | 121.39 |
| 15 | i | 241 | GLU | C-N-CA | 5.89 | 131.17 | 121.39 |
| 16 | c | 331 | ARG | N-CA-C | 5.89 | 117.37 | 111.07 |
| 19 | f | 278 | GLN | CB-CA-C | -5.89 | 100.51 | 110.64 |
| 20 | g | 877 | GLU | N-CA-C | -5.89 | 104.85 | 112.68 |
| 2 | 1 | 124 | ASN | CA-C-N | 5.89 | 132.03 | 122.67 |
| 2 | 1 | 124 | ASN | C-N-CA | 5.89 | 132.03 | 122.67 |
| 8 | N | 1429 | HIS | CA-C-N | 5.89 | 128.09 | 120.44 |
| 8 | N | 1429 | HIS | C-N-CA | 5.89 | 128.09 | 120.44 |
| 21 | t | 79 | PHE | CA-C-O | -5.89 | 114.97 | 121.33 |
| 2 | 1 | 1161 | HIS | ND1-CE1-NE2 | 5.89 | 114.29 | 108.40 |
| 7 | M | 573 | ASN | CB-CG-OD1 | 5.89 | 132.57 | 120.80 |
| 7 | M | 1358 | VAL | O-C-N | -5.89 | 115.59 | 122.07 |
| 7 | M | 1612 | LEU | O-C-N | 5.89 | 130.42 | 122.59 |
| 7 | O | 793 | TYR | CA-CB-CG | -5.89 | 103.30 | 113.90 |
| 8 | P | 1431 | ILE | N-CA-CB | 5.89 | 118.68 | 112.21 |
| 9 | T | 58 | SER | N-CA-C | -5.89 | 105.68 | 112.92 |
| 20 | g | 424 | VAL | CB-CA-C | -5.89 | 100.58 | 111.18 |
| 7 | M | 153 | THR | CA-C-N | 5.88 | 128.48 | 120.54 |
| 7 | M | 153 | THR | C-N-CA | 5.88 | 128.48 | 120.54 |
| 8 | N | 780 | HIS | CB-CG-ND1 | 5.88 | 131.53 | 122.70 |
| 8 | N | 922 | PHE | CA-CB-CG | -5.88 | 107.92 | 113.80 |
| 1 | Y | 1356 | LYS | N-CA-C | -5.88 | 100.37 | 109.14 |
| 19 | m | 104 | LEU | CA-C-N | 5.88 | 128.17 | 120.28 |
| 19 | m | 104 | LEU | C-N-CA | 5.88 | 128.17 | 120.28 |
| 14 | a | 406 | ARG | N-CA-C | -5.88 | 105.41 | 112.59 |
| 14 | a | 1020 | ASN | CA-CB-CG | -5.88 | 106.72 | 112.60 |
| 4 | A | 747 | THR | O-C-N | 5.88 | 128.36 | 122.12 |
| 16 | j | 468 | GLU | N-CA-C | -5.88 | 104.45 | 111.69 |
| 16 | c | 610 | TRP | CB-CG-CD1 | 5.88 | 135.72 | 126.90 |
| 20 | g | 430 | ASN | N-CA-CB | 5.88 | 120.68 | 111.56 |
| 4 | A | 670 | VAL | O-C-N | -5.88 | 113.76 | 121.82 |
| 4 | G | 687 | GLU | CB-CG-CD | -5.88 | 102.60 | 112.60 |
| 9 | Q | 412 | TYR | N-CA-CB | 5.88 | 120.29 | 110.41 |
| 1 | Y | 384 | GLU | N-CA-C | -5.88 | 100.47 | 109.41 |
| 2 | Z | 1069 | GLN | CA-C-O | 5.88 | 126.61 | 119.38 |
| 13 | w | 1288 | ILE | CA-C-N | 5.88 | 128.44 | 120.44 |
| 13 | w | 1288 | ILE | C-N-CA | 5.88 | 128.44 | 120.44 |
| 19 | m | 684 | ILE | CA-C-N | 5.88 | 130.17 | 120.94 |
| 19 | m | 684 | ILE | C-N-CA | 5.88 | 130.17 | 120.94 |
| 14 | a | 585 | ASP | CA-C-O | -5.88 | 114.31 | 120.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | a | 1000 | TYR | CA-C-N | 5.88 | 128.16 | 120.28 |
| 14 | a | 1000 | TYR | C-N-CA | 5.88 | 128.16 | 120.28 |
| 7 | M | 711 | GLN | CA-C-O | 5.88 | 126.99 | 120.82 |
| 9 | R | 303 | ASN | N-CA-CB | 5.88 | 119.46 | 110.70 |
| 1 | Y | 604 | PRO | N-CA-C | -5.88 | 100.36 | 112.47 |
| 1 | Y | 1276 | LEU | O-C-N | 5.88 | 130.69 | 123.10 |
| 14 | a | 981 | LEU | N-CA-CB | 5.88 | 119.39 | 110.28 |
| 6 | I | 323 | SER | O-C-N | -5.88 | 115.89 | 122.12 |
| 4 | J | 671 | LYS | CA-C-N | 5.88 | 127.69 | 120.22 |
| 4 | J | 671 | LYS | C-N-CA | 5.88 | 127.69 | 120.22 |
| 7 | M | 429 | GLU | CA-C-N | 5.88 | 128.16 | 120.28 |
| 7 | M | 429 | GLU | C-N-CA | 5.88 | 128.16 | 120.28 |
| 8 | N | 714 | LEU | CA-C-N | 5.88 | 128.64 | 120.29 |
| 8 | N | 714 | LEU | C-N-CA | 5.88 | 128.64 | 120.29 |
| 7 | O | 1356 | LEU | N-CA-C | 5.88 | 118.16 | 111.11 |
| 9 | S | 422 | ARG | N-CA-C | -5.88 | 99.07 | 109.06 |
| 2 | Z | 365 | SER | CA-C-O | 5.88 | 126.79 | 120.32 |
| 2 | Z | 453 | PHE | N-CA-CB | 5.88 | 118.59 | 110.01 |
| 14 | h | 839 | GLU | CB-CA-C | -5.88 | 101.91 | 110.96 |
| 15 | i | 262 | ILE | CA-C-O | -5.88 | 113.90 | 120.25 |
| 18 | l | 218 | ILE | N-CA-C | -5.88 | 100.01 | 108.53 |
| 18 | e | 83 | LEU | CB-CA-C | -5.88 | 100.10 | 109.80 |
| 19 | f | 162 | LEU | N-CA-C | -5.88 | 106.14 | 113.55 |
| 20 | g | 757 | LYS | N-CA-C | -5.88 | 105.30 | 112.88 |
| 2 | 1 | 245 | ASN | CA-CB-CG | 5.88 | 118.48 | 112.60 |
| 4 | D | 654 | HIS | CA-C-N | 5.88 | 128.63 | 120.29 |
| 4 | D | 654 | HIS | C-N-CA | 5.88 | 128.63 | 120.29 |
| 9 | S | 229 | ASN | N-CA-CB | 5.88 | 120.42 | 110.49 |
| 9 | S | 410 | ALA | N-CA-C | -5.88 | 104.61 | 113.89 |
| 9 | T | 370 | TYR | N-CA-C | -5.88 | 105.87 | 113.16 |
| 1 | Y | 1281 | THR | CA-CB-OG1 | 5.88 | 118.42 | 109.60 |
| 2 | Z | 285 | GLU | O-C-N | 5.88 | 129.95 | 123.25 |
| 12 | v | 260 | HIS | ND1-CE1-NE2 | 5.88 | 114.28 | 108.40 |
| 20 | n | 135 | ALA | O-C-N | -5.88 | 115.19 | 120.71 |
| 21 | o | 67 | SER | CA-C-O | 5.88 | 126.86 | 119.98 |
| 14 | a | 352 | ILE | CB-CA-C | 5.88 | 119.80 | 113.22 |
| 1 | 0 | 355 | THR | CA-C-N | -5.88 | 115.91 | 123.19 |
| 1 | 0 | 355 | THR | C-N-CA | -5.88 | 115.91 | 123.19 |
| 9 | S | 724 | ARG | NE-CZ-NH2 | 5.88 | 124.49 | 119.20 |
| 9 | T | 330 | GLY | CA-C-O | -5.88 | 112.53 | 119.46 |
| 2 | Z | 186 | ASN | N-CA-C | -5.88 | 105.69 | 112.92 |
| 19 | m | 186 | GLU | CA-C-N | 5.88 | 128.43 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | m | 186 | GLU | C-N-CA | 5.88 | 128.43 | 120.44 |
| 6 | I | 453 | ILE | N-CA-C | 5.87 | 116.61 | 110.62 |
| 7 | O | 219 | HIS | CB-CG-CD2 | -5.87 | 123.56 | 131.20 |
| 8 | P | 615 | LEU | CA-C-N | 5.87 | 130.66 | 120.68 |
| 8 | P | 615 | LEU | C-N-CA | 5.87 | 130.66 | 120.68 |
| 9 | Q | 98 | PRO | N-CA-CB | 5.87 | 109.79 | 103.33 |
| 1 | Y | 1388 | PHE | CA-CB-CG | 5.87 | 119.67 | 113.80 |
| 19 | m | 116 | LEU | O-C-N | 5.87 | 128.35 | 122.12 |
| 20 | g | 461 | ASP | N-CA-CB | 5.87 | 120.68 | 110.81 |
| 4 | A | 648 | LEU | CA-C-N | 5.87 | 129.23 | 120.31 |
| 4 | A | 648 | LEU | C-N-CA | 5.87 | 129.23 | 120.31 |
| 8 | N | 1123 | HIS | CE1-NE2-CD2 | -5.87 | 103.13 | 109.00 |
| 7 | O | 267 | SER | CA-C-N | 5.87 | 130.84 | 122.09 |
| 7 | O | 267 | SER | C-N-CA | 5.87 | 130.84 | 122.09 |
| 1 | Y | 381 | VAL | N-CA-CB | 5.87 | 116.93 | 110.53 |
| 20 | n | 135 | ALA | CA-C-N | 5.87 | 125.98 | 119.87 |
| 20 | n | 135 | ALA | C-N-CA | 5.87 | 125.98 | 119.87 |
| 21 | p | 82 | GLY | CA-C-O | -5.87 | 113.12 | 121.52 |
| 15 | b | 575 | LEU | N-CA-C | -5.87 | 106.16 | 113.38 |
| 19 | f | 642 | ASN | CA-CB-CG | -5.87 | 106.73 | 112.60 |
| 14 | a | 981 | LEU | CA-C-O | -5.87 | 113.22 | 119.97 |
| 2 | 1 | 1214 | ASP | N-CA-C | 5.87 | 119.52 | 111.54 |
| 6 | C | 383 | LYS | O-C-N | 5.87 | 129.49 | 122.27 |
| 7 | M | 893 | HIS | N-CA-C | -5.87 | 103.84 | 111.71 |
| 7 | O | 109 | ARG | NH1-CZ-NH2 | 5.87 | 126.93 | 119.30 |
| 7 | O | 518 | ASN | N-CA-CB | 5.87 | 120.41 | 110.49 |
| 10 | W | 282 | VAL | N-CA-C | -5.87 | 97.13 | 109.34 |
| 1 | Y | 1384 | ILE | N-CA-C | -5.87 | 99.76 | 108.45 |
| 1 | 0 | 276 | HIS | CE1-NE2-CD2 | -5.87 | 103.13 | 109.00 |
| 1 | 0 | 1376 | LYS | N-CA-C | -5.87 | 104.47 | 111.69 |
| 2 | 1 | 1042 | ARG | N-CA-C | -5.87 | 104.52 | 111.03 |
| 5 | E | 357 | GLY | O-C-N | -5.87 | 115.88 | 122.28 |
| 8 | P | 692 | ASN | N-CA-C | -5.87 | 105.43 | 112.59 |
| 9 | R | 309 | ILE | CA-C-O | 5.87 | 126.29 | 119.89 |
| 9 | R | 724 | ARG | N-CA-C | 5.87 | 117.68 | 111.28 |
| 9 | S | 826 | ARG | CA-C-N | 5.87 | 128.14 | 120.28 |
| 9 | S | 826 | ARG | C-N-CA | 5.87 | 128.14 | 120.28 |
| 16 | j | 624 | VAL | N-CA-C | -5.87 | 107.02 | 112.83 |
| 18 | l | 196 | ARG | NE-CZ-NH1 | 5.87 | 127.37 | 121.50 |
| 20 | g | 907 | THR | N-CA-CB | 5.87 | 120.79 | 111.17 |
| 20 | g | 1037 | LEU | N-CA-CB | 5.87 | 118.75 | 110.12 |
| 1 | 0 | 1308 | PHE | CA-C-N | 5.87 | 130.05 | 121.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 1308 | PHE | C-N-CA | 5.87 | 130.05 | 121.31 |
| 9 | T | 543 | LYS | CA-C-N | 5.87 | 128.14 | 120.28 |
| 9 | T | 543 | LYS | C-N-CA | 5.87 | 128.14 | 120.28 |
| 9 | T | 543 | LYS | N-CA-C | 5.87 | 119.26 | 111.75 |
| 14 | h | 19 | GLU | CA-C-N | 5.87 | 125.88 | 119.89 |
| 14 | h | 19 | GLU | C-N-CA | 5.87 | 125.88 | 119.89 |
| 20 | g | 366 | ILE | CA-C-N | 5.87 | 129.94 | 122.37 |
| 20 | g | 366 | ILE | C-N-CA | 5.87 | 129.94 | 122.37 |
| 5 | K | 532 | ALA | N-CA-C | 5.87 | 117.75 | 111.36 |
| 6 | L | 465 | LYS | N-CA-C | -5.87 | 106.17 | 113.38 |
| 8 | N | 1095 | GLU | CA-CB-CG | 5.87 | 125.83 | 114.10 |
| 7 | O | 749 | ILE | CA-C-N | 5.87 | 129.65 | 120.97 |
| 7 | O | 749 | ILE | C-N-CA | 5.87 | 129.65 | 120.97 |
| 8 | P | 49 | THR | N-CA-CB | 5.87 | 120.40 | 110.49 |
| 9 | R | 616 | GLU | CA-C-N | 5.87 | 128.06 | 120.44 |
| 9 | R | 616 | GLU | C-N-CA | 5.87 | 128.06 | 120.44 |
| 2 | Z | 1126 | LYS | N-CA-C | -5.87 | 98.31 | 110.80 |
| 12 | u | 394 | SER | CA-C-N | 5.87 | 128.42 | 120.44 |
| 12 | u | 394 | SER | C-N-CA | 5.87 | 128.42 | 120.44 |
| 7 | M | 65 | LYS | CA-C-O | 5.86 | 126.77 | 120.32 |
| 9 | S | 653 | VAL | CG1-CB-CG2 | -5.86 | 97.90 | 110.80 |
| 2 | Z | 771 | PRO | CA-C-N | 5.86 | 128.06 | 120.44 |
| 2 | Z | 771 | PRO | C-N-CA | 5.86 | 128.06 | 120.44 |
| 2 | Z | 1311 | PHE | CA-C-N | 5.86 | 129.22 | 120.31 |
| 2 | Z | 1311 | PHE | C-N-CA | 5.86 | 129.22 | 120.31 |
| 14 | h | 559 | GLU | N-CA-C | -5.86 | 98.31 | 110.80 |
| 15 | i | 453 | ASP | CA-CB-CG | 5.86 | 118.46 | 112.60 |
| 8 | N | 684 | LYS | N-CA-C | -5.86 | 104.28 | 113.02 |
| 20 | n | 393 | THR | N-CA-C | -5.86 | 100.24 | 109.50 |
| 21 | p | 39 | ARG | NE-CZ-NH2 | 5.86 | 124.48 | 119.20 |
| 20 | g | 561 | LYS | N-CA-C | 5.86 | 117.34 | 111.07 |
| 2 | 1 | 123 | TYR | CB-CG-CD1 | 5.86 | 129.59 | 120.80 |
| 6 | L | 455 | GLU | N-CA-CB | 5.86 | 118.57 | 110.07 |
| 7 | M | 1307 | VAL | N-CA-C | -5.86 | 104.61 | 110.30 |
| 7 | O | 277 | LEU | CA-C-N | 5.86 | 127.94 | 120.56 |
| 7 | O | 277 | LEU | C-N-CA | 5.86 | 127.94 | 120.56 |
| 7 | O | 669 | THR | CA-C-N | 5.86 | 128.06 | 120.44 |
| 7 | O | 669 | THR | C-N-CA | 5.86 | 128.06 | 120.44 |
| 2 | Z | 1326 | SER | O-C-N | 5.86 | 128.33 | 122.12 |
| 12 | v | 581 | PHE | N-CA-C | -5.86 | 105.01 | 114.09 |
| 20 | n | 780 | LEU | CA-C-N | 5.86 | 128.13 | 120.28 |
| 20 | n | 780 | LEU | C-N-CA | 5.86 | 128.13 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | B | 514 | THR | N-CA-CB | 5.86 | 118.83 | 110.16 |
| 7 | M | 1409 | ALA | CA-C-O | -5.86 | 114.67 | 120.82 |
| 7 | O | 155 | LEU | CA-C-N | 5.86 | 128.72 | 120.28 |
| 7 | O | 155 | LEU | C-N-CA | 5.86 | 128.72 | 120.28 |
| 15 | i | 114 | ILE | CA-C-N | 5.86 | 128.13 | 120.28 |
| 15 | i | 114 | ILE | C-N-CA | 5.86 | 128.13 | 120.28 |
| 5 | B | 437 | TRP | CA-CB-CG | 5.86 | 124.73 | 113.60 |
| 8 | N | 592 | ILE | CA-C-N | 5.86 | 128.05 | 120.44 |
| 8 | N | 592 | ILE | C-N-CA | 5.86 | 128.05 | 120.44 |
| 9 | R | 118 | GLU | O-C-N | 5.86 | 128.10 | 122.07 |
| 9 | R | 756 | LYS | CA-C-O | 5.86 | 126.76 | 120.55 |
| 9 | S | 820 | ILE | N-CA-C | -5.86 | 106.78 | 112.29 |
| 11 | V | 302 | ARG | CA-C-O | 5.86 | 130.76 | 120.80 |
| 1 | Y | 1204 | TYR | N-CA-C | -5.86 | 106.17 | 113.38 |
| 2 | Z | 1373 | ASP | CA-C-N | 5.86 | 125.33 | 119.24 |
| 2 | Z | 1373 | ASP | C-N-CA | 5.86 | 125.33 | 119.24 |
| 15 | b | 434 | PHE | CA-CB-CG | -5.86 | 107.94 | 113.80 |
| 18 | e | 13 | HIS | CB-CG-ND1 | 5.86 | 131.49 | 122.70 |
| 2 | 1 | 407 | ALA | CB-CA-C | -5.86 | 101.69 | 110.88 |
| 6 | C | 335 | SER | N-CA-C | -5.86 | 104.59 | 110.97 |
| 7 | O | 1119 | PHE | CA-C-N | 5.86 | 130.57 | 121.26 |
| 7 | O | 1119 | PHE | C-N-CA | 5.86 | 130.57 | 121.26 |
| 7 | O | 1352 | GLU | N-CA-C | 5.86 | 118.44 | 111.71 |
| 9 | Q | 773 | ASN | N-CA-C | -5.86 | 106.78 | 114.04 |
| 2 | Z | 557 | ASN | O-C-N | 5.86 | 130.07 | 122.87 |
| 12 | u | 133 | HIS | ND1-CE1-NE2 | 5.86 | 114.26 | 108.40 |
| 14 | h | 370 | ASP | CA-C-O | 5.86 | 127.03 | 120.94 |
| 15 | i | 590 | VAL | CA-C-N | 5.86 | 128.13 | 120.28 |
| 15 | i | 590 | VAL | C-N-CA | 5.86 | 128.13 | 120.28 |
| 21 | q | 75 | HIS | CE1-NE2-CD2 | -5.86 | 103.14 | 109.00 |
| 5 | B | 404 | ARG | NE-CZ-NH2 | -5.85 | 113.93 | 119.20 |
| 7 | O | 67 | ASN | CA-C-O | -5.85 | 115.12 | 121.44 |
| 8 | P | 599 | THR | N-CA-CB | 5.85 | 119.67 | 109.72 |
| 20 | n | 788 | TRP | CB-CG-CD1 | 5.85 | 135.68 | 126.90 |
| 2 | 1 | 1379 | VAL | N-CA-C | -5.85 | 107.03 | 112.83 |
| 8 | N | 739 | ILE | CA-C-O | -5.85 | 112.50 | 119.58 |
| 9 | R | 716 | LEU | O-C-N | -5.85 | 115.92 | 122.12 |
| 11 | V | 396 | ALA | N-CA-CB | 5.85 | 118.72 | 110.12 |
| 1 | Y | 832 | VAL | CA-C-O | 5.85 | 128.09 | 120.78 |
| 2 | Z | 557 | ASN | CA-CB-CG | -5.85 | 106.75 | 112.60 |
| 12 | u | 321 | ASP | N-CA-CB | -5.85 | 101.21 | 110.28 |
| 20 | n | 1059 | GLN | CA-C-N | 5.85 | 128.60 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | n | 1059 | GLN | C-N-CA | 5.85 | 128.60 | 120.29 |
| 16 | c | 768 | ASN | O-C-N | -5.85 | 114.21 | 121.64 |
| 19 | f | 210 | MET | N-CA-CB | 5.85 | 118.82 | 110.16 |
| 19 | f | 659 | TYR | N-CA-CB | 5.85 | 118.89 | 110.40 |
| 7 | M | 1357 | ALA | N-CA-CB | 5.85 | 119.23 | 110.22 |
| 8 | N | 822 | ASN | O-C-N | -5.85 | 116.41 | 121.85 |
| 9 | Q | 128 | LEU | CA-C-N | 5.85 | 129.20 | 120.31 |
| 9 | Q | 128 | LEU | C-N-CA | 5.85 | 129.20 | 120.31 |
| 11 | X | 401 | ASP | CB-CA-C | -5.85 | 98.78 | 110.42 |
| 1 | Y | 1313 | VAL | CA-CB-CG1 | 5.85 | 120.34 | 110.40 |
| 16 | j | 312 | GLU | N-CA-C | -5.85 | 105.64 | 112.89 |
| 19 | m | 466 | ASN | CA-CB-CG | 5.85 | 118.45 | 112.60 |
| 19 | f | 344 | ARG | NH1-CZ-NH2 | -5.85 | 111.70 | 119.30 |
| 1 | 0 | 1363 | PHE | O-C-N | 5.85 | 128.41 | 122.09 |
| 2 | 1 | 1381 | ASP | N-CA-C | -5.85 | 104.30 | 112.25 |
| 7 | M | 699 | VAL | N-CA-C | 5.85 | 116.58 | 110.62 |
| 8 | P | 363 | ASN | CA-C-O | -5.85 | 112.19 | 119.38 |
| 9 | R | 353 | LEU | O-C-N | 5.85 | 128.32 | 122.12 |
| 1 | Y | 914 | TYR | N-CA-C | -5.85 | 98.34 | 110.80 |
| 2 | Z | 1124 | ASP | N-CA-C | -5.85 | 98.34 | 110.80 |
| 12 | v | 77 | GLY | N-CA-C | -5.85 | 107.18 | 115.43 |
| 16 | j | 657 | CYS | N-CA-C | 5.85 | 119.67 | 112.54 |
| 17 | k | 256 | VAL | N-CA-CB | 5.85 | 119.55 | 110.14 |
| 18 | l | 245 | ILE | CB-CA-C | 5.85 | 119.70 | 112.45 |
| 21 | p | 18 | ASP | O-C-N | -5.85 | 115.92 | 122.12 |
| 20 | g | 716 | ASN | N-CA-CB | 5.85 | 120.37 | 110.49 |
| 2 | 1 | 1290 | ASN | CA-CB-CG | -5.85 | 106.75 | 112.60 |
| 9 | T | 234 | ILE | N-CA-C | -5.85 | 106.58 | 113.42 |
| 2 | Z | 713 | ALA | N-CA-C | 5.85 | 117.65 | 111.28 |
| 12 | u | 254 | GLN | O-C-N | 5.85 | 128.09 | 122.07 |
| 18 | e | 44 | ASN | N-CA-C | -5.85 | 98.75 | 108.34 |
| 1 | 0 | 519 | THR | CA-C-O | -5.84 | 114.28 | 121.06 |
| 8 | N | 419 | ASP | N-CA-C | -5.84 | 105.03 | 113.21 |
| 8 | N | 912 | TRP | CB-CG-CD2 | 5.84 | 134.98 | 126.80 |
| 8 | N | 1285 | PHE | CA-C-N | 5.84 | 129.66 | 120.89 |
| 8 | N | 1285 | PHE | C-N-CA | 5.84 | 129.66 | 120.89 |
| 8 | P | 1397 | ASN | CA-C-N | 5.84 | 132.49 | 121.97 |
| 8 | P | 1397 | ASN | C-N-CA | 5.84 | 132.49 | 121.97 |
| 9 | S | 601 | PRO | CA-C-N | 5.84 | 132.86 | 121.41 |
| 9 | S | 601 | PRO | C-N-CA | 5.84 | 132.86 | 121.41 |
| 12 | v | 143 | VAL | CA-CB-CG2 | -5.84 | 100.47 | 110.40 |
| 13 | w | 1438 | GLU | CA-C-N | 5.84 | 128.04 | 120.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 13 | w | 1438 | GLU | C-N-CA | 5.84 | 128.04 | 120.56 |
| 15 | b | 728 | LEU | CA-C-N | 5.84 | 130.62 | 120.68 |
| 15 | b | 728 | LEU | C-N-CA | 5.84 | 130.62 | 120.68 |
| 2 | 1 | 452 | LYS | O-C-N | 5.84 | 130.40 | 122.57 |
| 7 | M | 707 | LEU | N-CA-CB | 5.84 | 118.44 | 109.91 |
| 7 | O | 470 | ASP | CA-C-N | 5.84 | 131.55 | 122.26 |
| 7 | O | 470 | ASP | C-N-CA | 5.84 | 131.55 | 122.26 |
| 12 | u | 432 | ASN | CA-C-O | -5.84 | 113.07 | 120.55 |
| 6 | C | 348 | GLN | CA-C-O | -5.84 | 114.36 | 120.55 |
| 7 | O | 75 | ILE | N-CA-CB | 5.84 | 119.34 | 110.58 |
| 2 | Z | 379 | ILE | CA-CB-CG1 | 5.84 | 120.33 | 110.40 |
| 16 | j | 486 | LEU | CA-C-N | 5.84 | 129.19 | 120.31 |
| 16 | j | 486 | LEU | C-N-CA | 5.84 | 129.19 | 120.31 |
| 15 | b | 707 | SER | N-CA-C | -5.84 | 103.43 | 110.44 |
| 15 | b | 720 | LEU | CA-C-O | -5.84 | 112.16 | 120.16 |
| 18 | e | 312 | TRP | CB-CG-CD1 | -5.84 | 118.14 | 126.90 |
| 20 | g | 778 | ASN | CA-CB-CG | -5.84 | 106.76 | 112.60 |
| 1 | 0 | 1266 | CYS | CA-C-N | 5.84 | 128.03 | 120.44 |
| 1 | 0 | 1266 | CYS | C-N-CA | 5.84 | 128.03 | 120.44 |
| 1 | 0 | 1441 | ASN | CA-C-N | 5.84 | 128.69 | 120.28 |
| 1 | 0 | 1441 | ASN | C-N-CA | 5.84 | 128.69 | 120.28 |
| 2 | 1 | 232 | ILE | CA-CB-CG1 | 5.84 | 120.33 | 110.40 |
| 7 | M | 640 | PHE | CB-CA-C | -5.84 | 101.71 | 110.88 |
| 7 | M | 1390 | GLN | OE1-CD-NE2 | 5.84 | 128.44 | 122.60 |
| 8 | N | 131 | ASP | CB-CA-C | -5.84 | 99.00 | 110.10 |
| 7 | O | 1288 | ASN | CA-C-N | 5.84 | 128.46 | 120.46 |
| 7 | O | 1288 | ASN | C-N-CA | 5.84 | 128.46 | 120.46 |
| 12 | v | 113 | HIS | ND1-CE1-NE2 | 5.84 | 114.24 | 108.40 |
| 21 | s | 79 | PHE | CA-CB-CG | -5.84 | 107.96 | 113.80 |
| 8 | N | 263 | SER | CA-C-N | 5.84 | 128.10 | 120.28 |
| 8 | N | 263 | SER | C-N-CA | 5.84 | 128.10 | 120.28 |
| 1 | Y | 1438 | ASP | CA-C-O | -5.84 | 112.23 | 119.18 |
| 21 | t | 28 | SER | CA-C-N | 5.84 | 128.10 | 120.28 |
| 21 | t | 28 | SER | C-N-CA | 5.84 | 128.10 | 120.28 |
| 7 | O | 1189 | MET | CA-CB-CG | 5.84 | 125.77 | 114.10 |
| 8 | P | 1232 | HIS | CG-CD2-NE2 | 5.84 | 113.04 | 107.20 |
| 9 | S | 621 | HIS | CE1-NE2-CD2 | -5.84 | 103.16 | 109.00 |
| 1 | Y | 769 | ARG | CD-NE-CZ | -5.84 | 116.23 | 124.40 |
| 2 | Z | 593 | GLN | CA-C-O | 5.84 | 126.49 | 119.43 |
| 14 | h | 269 | HIS | CE1-NE2-CD2 | -5.84 | 103.16 | 109.00 |
| 16 | j | 235 | LYS | N-CA-C | 5.84 | 117.72 | 111.36 |
| 16 | j | 602 | PHE | N-CA-C | 5.84 | 117.05 | 109.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | m | 272 | PRO | CA-C-O | -5.84 | 114.78 | 121.96 |
| 17 | d | 153 | TRP | N-CA-CB | 5.84 | 118.61 | 110.26 |
| 14 | a | 64 | ASN | CA-CB-CG | 5.84 | 118.44 | 112.60 |
| 14 | a | 658 | HIS | N-CA-C | 5.84 | 117.64 | 111.28 |
| 2 | 1 | 1196 | ASN | CA-C-O | -5.83 | 114.77 | 121.19 |
| 19 | m | 13 | THR | CA-C-N | 5.83 | 128.68 | 120.28 |
| 19 | m | 13 | THR | C-N-CA | 5.83 | 128.68 | 120.28 |
| 14 | a | 594 | GLY | CA-C-N | 5.83 | 129.93 | 121.18 |
| 14 | a | 594 | GLY | C-N-CA | 5.83 | 129.93 | 121.18 |
| 14 | a | 764 | LEU | CB-CA-C | 5.83 | 120.03 | 110.17 |
| 2 | 1 | 965 | GLY | CA-C-O | -5.83 | 113.88 | 120.30 |
| 5 | K | 411 | ARG | NE-CZ-NH2 | -5.83 | 113.95 | 119.20 |
| 5 | K | 540 | LYS | CB-CA-C | -5.83 | 99.14 | 109.70 |
| 8 | N | 1514 | VAL | N-CA-C | -5.83 | 107.06 | 112.83 |
| 11 | V | 281 | SER | CA-C-N | 5.83 | 129.57 | 120.82 |
| 11 | V | 281 | SER | C-N-CA | 5.83 | 129.57 | 120.82 |
| 1 | Y | 971 | ILE | CA-C-O | -5.83 | 114.88 | 120.95 |
| 14 | h | 944 | ILE | N-CA-C | 5.83 | 116.49 | 110.36 |
| 19 | m | 120 | TRP | CA-CB-CG | 5.83 | 124.68 | 113.60 |
| 20 | n | 466 | TYR | CB-CA-C | 5.83 | 120.51 | 109.37 |
| 20 | n | 1000 | SER | CA-C-N | 5.83 | 129.18 | 120.31 |
| 20 | n | 1000 | SER | C-N-CA | 5.83 | 129.18 | 120.31 |
| 21 | r | 18 | ASP | CB-CA-C | -5.83 | 101.11 | 110.79 |
| 20 | g | 799 | GLU | CA-CB-CG | 5.83 | 125.77 | 114.10 |
| 14 | a | 624 | SER | CA-C-N | 5.83 | 128.03 | 120.56 |
| 14 | a | 624 | SER | C-N-CA | 5.83 | 128.03 | 120.56 |
| 2 | 1 | 581 | SER | CA-C-O | -5.83 | 113.69 | 122.38 |
| 2 | 1 | 1074 | ARG | NE-CZ-NH2 | -5.83 | 113.95 | 119.20 |
| 7 | M | 1493 | LYS | N-CA-C | 5.83 | 118.11 | 111.11 |
| 7 | O | 1165 | ILE | CA-C-N | 5.83 | 128.68 | 120.28 |
| 7 | O | 1165 | ILE | C-N-CA | 5.83 | 128.68 | 120.28 |
| 7 | O | 1332 | PHE | CA-CB-CG | -5.83 | 107.97 | 113.80 |
| 9 | Q | 442 | LEU | O-C-N | 5.83 | 130.35 | 122.59 |
| 9 | R | 435 | TRP | CB-CG-CD2 | 5.83 | 134.97 | 126.80 |
| 11 | X | 390 | ASN | CA-CB-CG | 5.83 | 118.43 | 112.60 |
| 2 | Z | 1100 | PHE | CA-CB-CG | -5.83 | 107.97 | 113.80 |
| 12 | u | 645 | VAL | N-CA-C | -5.83 | 104.83 | 110.72 |
| 4 | y | 808 | ASP | CA-C-N | 5.83 | 128.02 | 120.44 |
| 4 | y | 808 | ASP | C-N-CA | 5.83 | 128.02 | 120.44 |
| 19 | m | 642 | ASN | CA-CB-CG | 5.83 | 118.43 | 112.60 |
| 20 | g | 180 | SER | CA-C-O | 5.83 | 126.79 | 120.43 |
| 2 | 1 | 1386 | ARG | CA-CB-CG | 5.83 | 125.76 | 114.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | v | 389 | TRP | CA-CB-CG | 5.83 | 124.68 | 113.60 |
| 1 | 0 | 958 | LYS | N-CA-C | -5.83 | 105.78 | 114.64 |
| 2 | 1 | 140 | ARG | NE-CZ-NH1 | 5.83 | 127.33 | 121.50 |
| 6 | C | 381 | GLU | N-CA-CB | 5.83 | 120.06 | 110.39 |
| 7 | M | 1120 | THR | CA-C-N | 5.83 | 129.55 | 120.75 |
| 7 | M | 1120 | THR | C-N-CA | 5.83 | 129.55 | 120.75 |
| 8 | N | 1348 | VAL | CA-C-N | 5.83 | 128.09 | 120.28 |
| 8 | N | 1348 | VAL | C-N-CA | 5.83 | 128.09 | 120.28 |
| 8 | P | 88 | PHE | CD1-CG-CD2 | -5.83 | 109.86 | 118.60 |
| 9 | S | 654 | ILE | CA-C-N | 5.83 | 129.93 | 120.60 |
| 9 | S | 654 | ILE | C-N-CA | 5.83 | 129.93 | 120.60 |
| 9 | T | 547 | TYR | N-CA-C | -5.83 | 104.34 | 113.02 |
| 2 | Z | 1331 | ASN | CB-CG-ND2 | 5.83 | 125.14 | 116.40 |
| 12 | u | 219 | ASN | CA-C-N | 5.83 | 129.56 | 120.82 |
| 12 | u | 219 | ASN | C-N-CA | 5.83 | 129.56 | 120.82 |
| 12 | v | 76 | SER | N-CA-C | -5.83 | 98.38 | 110.80 |
| 13 | x | 1294 | LYS | CA-C-O | 5.83 | 126.71 | 120.24 |
| 20 | n | 879 | ALA | N-CA-C | -5.83 | 101.49 | 108.25 |
| 14 | a | 570 | LEU | CA-C-N | 5.83 | 128.34 | 120.65 |
| 14 | a | 570 | LEU | C-N-CA | 5.83 | 128.34 | 120.65 |
| 4 | D | 648 | LEU | N-CA-CB | 5.83 | 118.46 | 110.01 |
| 8 | N | 1205 | LYS | N-CA-C | 5.83 | 119.86 | 112.87 |
| 9 | S | 25 | LEU | CA-C-O | 5.83 | 126.60 | 120.42 |
| 9 | T | 372 | LYS | N-CA-CB | 5.83 | 120.94 | 111.27 |
| 12 | v | 601 | ARG | CA-C-N | 5.83 | 128.01 | 120.44 |
| 12 | v | 601 | ARG | C-N-CA | 5.83 | 128.01 | 120.44 |
| 20 | g | 1089 | LEU | N-CA-C | -5.83 | 105.01 | 111.36 |
| 2 | 1 | 710 | TYR | O-C-N | 5.83 | 128.07 | 122.07 |
| 2 | 1 | 864 | LYS | N-CA-CB | 5.83 | 118.46 | 110.01 |
| 4 | G | 778 | LYS | CB-CG-CD | 5.83 | 124.70 | 111.30 |
| 8 | N | 218 | ASN | CA-C-N | 5.83 | 130.67 | 122.46 |
| 8 | N | 218 | ASN | C-N-CA | 5.83 | 130.67 | 122.46 |
| 8 | N | 457 | LEU | N-CA-CB | 5.83 | 120.34 | 110.49 |
| 7 | O | 358 | LYS | CG-CD-CE | 5.83 | 124.70 | 111.30 |
| 9 | R | 295 | ASN | N-CA-CB | 5.83 | 120.34 | 110.49 |
| 9 | S | 637 | ILE | N-CA-C | -5.83 | 107.31 | 112.90 |
| 10 | U | 323 | SER | CA-C-O | 5.83 | 127.12 | 121.00 |
| 1 | Y | 631 | GLN | N-CA-C | -5.83 | 105.67 | 112.89 |
| 2 | Z | 927 | HIS | ND1-CE1-NE2 | 5.83 | 114.23 | 108.40 |
| 17 | k | 236 | GLN | N-CA-CB | 5.83 | 120.30 | 110.46 |
| 19 | m | 535 | ARG | CA-C-N | 5.83 | 128.01 | 120.44 |
| 19 | m | 535 | ARG | C-N-CA | 5.83 | 128.01 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | o | 16 | ILE | CA-CB-CG1 | 5.83 | 120.30 | 110.40 |
| 20 | g | 307 | LEU | N-CA-C | -5.83 | 106.81 | 114.04 |
| 20 | g | 998 | ASN | N-CA-C | -5.83 | 100.49 | 109.52 |
| 14 | a | 157 | ASP | CA-CB-CG | 5.83 | 118.42 | 112.60 |
| 14 | a | 279 | TYR | N-CA-CB | 5.83 | 120.34 | 110.49 |
| 2 | 1 | 506 | ILE | N-CA-C | -5.82 | 99.32 | 108.23 |
| 8 | N | 1205 | LYS | CA-C-N | 5.82 | 131.91 | 121.66 |
| 8 | N | 1205 | LYS | C-N-CA | 5.82 | 131.91 | 121.66 |
| 7 | O | 631 | LEU | CD1-CG-CD2 | -5.82 | 97.99 | 110.80 |
| 7 | O | 1452 | SER | CA-C-N | 5.82 | 128.36 | 120.44 |
| 7 | O | 1452 | SER | C-N-CA | 5.82 | 128.36 | 120.44 |
| 9 | T | 783 | SER | CA-C-N | 5.82 | 128.40 | 120.54 |
| 9 | T | 783 | SER | C-N-CA | 5.82 | 128.40 | 120.54 |
| 2 | Z | 872 | ASN | OD1-CG-ND2 | 5.82 | 128.42 | 122.60 |
| 12 | v | 119 | GLU | CB-CA-C | -5.82 | 99.03 | 110.10 |
| 14 | h | 869 | HIS | CE1-NE2-CD2 | -5.82 | 103.18 | 109.00 |
| 16 | j | 191 | ASP | CA-CB-CG | -5.82 | 106.78 | 112.60 |
| 16 | j | 262 | LYS | N-CA-C | 5.82 | 118.58 | 111.82 |
| 16 | j | 320 | VAL | CA-C-O | 5.82 | 127.26 | 121.09 |
| 20 | g | 101 | ASP | N-CA-C | -5.82 | 100.90 | 109.81 |
| 7 | M | 967 | THR | CB-CA-C | 5.82 | 120.10 | 110.90 |
| 8 | P | 441 | PRO | O-C-N | 5.82 | 130.50 | 122.64 |
| 8 | P | 1033 | PHE | CA-CB-CG | -5.82 | 107.98 | 113.80 |
| 1 | Y | 646 | SER | N-CA-CB | 5.82 | 120.50 | 111.24 |
| 18 | e | 2 | GLN | CA-C-N | 5.82 | 125.83 | 119.89 |
| 18 | e | 2 | GLN | C-N-CA | 5.82 | 125.83 | 119.89 |
| 5 | E | 310 | ALA | N-CA-C | -5.82 | 100.65 | 108.86 |
| 5 | K | 344 | SER | N-CA-CB | 5.82 | 120.73 | 110.37 |
| 4 | z | 767 | VAL | CB-CA-C | -5.82 | 104.52 | 111.97 |
| 15 | b | 71 | LEU | N-CA-CB | 5.82 | 120.33 | 110.49 |
| 16 | c | 290 | GLU | CA-C-O | 5.82 | 126.66 | 119.97 |
| 5 | E | 335 | TRP | CB-CG-CD1 | 5.82 | 135.63 | 126.90 |
| 1 | Y | 429 | GLU | N-CA-CB | 5.82 | 120.58 | 110.98 |
| 19 | m | 123 | MET | O-C-N | -5.82 | 114.53 | 122.33 |
| 16 | c | 167 | LYS | N-CA-C | -5.82 | 105.80 | 114.64 |
| 1 | 0 | 1069 | ASN | CA-CB-CG | 5.82 | 118.42 | 112.60 |
| 2 | 1 | 344 | GLN | N-CA-CB | 5.82 | 120.32 | 110.49 |
| 8 | P | 691 | SER | CA-C-O | 5.82 | 128.83 | 120.51 |
| 17 | k | 250 | GLU | N-CA-C | -5.82 | 105.49 | 112.59 |
| 19 | f | 413 | ILE | CA-C-N | 5.82 | 128.35 | 120.44 |
| 19 | f | 413 | ILE | C-N-CA | 5.82 | 128.35 | 120.44 |
| 19 | f | 610 | GLU | N-CA-C | 5.82 | 118.40 | 110.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 204 | VAL | N-CA-C | -5.82 | 99.16 | 107.77 |
| 8 | N | 65 | SER | N-CA-CB | 5.82 | 120.32 | 110.49 |
| 8 | P | 279 | ILE | N-CA-CB | 5.82 | 120.83 | 111.23 |
| 8 | P | 1409 | ALA | CA-C-N | 5.82 | 128.00 | 120.44 |
| 8 | P | 1409 | ALA | C-N-CA | 5.82 | 128.00 | 120.44 |
| 9 | Q | 461 | ASP | CA-C-N | 5.82 | 134.31 | 122.04 |
| 9 | Q | 461 | ASP | C-N-CA | 5.82 | 134.31 | 122.04 |
| 9 | Q | 716 | LEU | CA-C-N | 5.82 | 128.07 | 120.28 |
| 9 | Q | 716 | LEU | C-N-CA | 5.82 | 128.07 | 120.28 |
| 9 | S | 135 | ASP | CA-C-O | -5.82 | 114.39 | 120.55 |
| 1 | Y | 1196 | ILE | CA-C-O | 5.82 | 126.98 | 120.64 |
| 12 | v | 230 | SER | CA-C-O | -5.82 | 112.91 | 120.00 |
| 17 | k | 19 | TYR | CA-C-O | -5.82 | 113.28 | 119.97 |
| 14 | a | 289 | THR | CA-C-N | 5.82 | 129.82 | 121.50 |
| 14 | a | 289 | THR | C-N-CA | 5.82 | 129.82 | 121.50 |
| 7 | M | 1339 | ILE | CA-C-N | 5.81 | 128.07 | 120.28 |
| 7 | M | 1339 | ILE | C-N-CA | 5.81 | 128.07 | 120.28 |
| 1 | Y | 390 | PRO | CA-C-O | -5.81 | 114.92 | 121.43 |
| 2 | Z | 619 | GLU | N-CA-C | -5.81 | 106.35 | 113.50 |
| 17 | k | 74 | SER | CA-C-N | 5.81 | 128.07 | 120.28 |
| 17 | k | 74 | SER | C-N-CA | 5.81 | 128.07 | 120.28 |
| 19 | m | 113 | ASN | CA-CB-CG | -5.81 | 106.79 | 112.60 |
| 5 | H | 508 | LYS | N-CA-C | 5.81 | 117.62 | 111.28 |
| 9 | Q | 772 | PRO | CB-CA-C | -5.81 | 101.97 | 111.56 |
| 9 | R | 40 | GLY | O-C-N | -5.81 | 117.29 | 123.45 |
| 15 | i | 705 | LYS | CA-C-N | 5.81 | 132.64 | 121.54 |
| 15 | i | 705 | LYS | C-N-CA | 5.81 | 132.64 | 121.54 |
| 20 | n | 90 | ILE | CA-C-N | 5.81 | 132.37 | 122.37 |
| 20 | n | 90 | ILE | C-N-CA | 5.81 | 132.37 | 122.37 |
| 20 | n | 840 | PRO | CA-C-O | -5.81 | 114.82 | 121.56 |
| 20 | n | 984 | PHE | CA-C-N | 5.81 | 129.15 | 120.31 |
| 20 | n | 984 | PHE | C-N-CA | 5.81 | 129.15 | 120.31 |
| 2 | 1 | 1115 | LEU | CA-C-N | 5.81 | 128.54 | 120.29 |
| 2 | 1 | 1115 | LEU | C-N-CA | 5.81 | 128.54 | 120.29 |
| 4 | D | 777 | ASN | N-CA-C | -5.81 | 100.92 | 109.81 |
| 1 | Y | 624 | PHE | CA-CB-CG | -5.81 | 107.99 | 113.80 |
| 2 | 1 | 213 | THR | CA-C-N | 5.81 | 128.65 | 120.28 |
| 2 | 1 | 213 | THR | C-N-CA | 5.81 | 128.65 | 120.28 |
| 7 | M | 1525 | LEU | CA-C-N | 5.81 | 127.88 | 120.56 |
| 7 | M | 1525 | LEU | C-N-CA | 5.81 | 127.88 | 120.56 |
| 8 | N | 349 | PHE | N-CA-CB | 5.81 | 118.76 | 110.16 |
| 9 | Q | 53 | VAL | O-C-N | -5.81 | 116.24 | 121.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | Q | 413 | LYS | N-CA-C | -5.81 | 105.29 | 112.90 |
| 1 | Y | 209 | HIS | CE1-NE2-CD2 | -5.81 | 103.19 | 109.00 |
| 2 | Z | 1386 | ARG | N-CA-CB | 5.81 | 120.31 | 110.49 |
| 18 | e | 173 | TRP | N-CA-CB | 5.81 | 119.46 | 110.46 |
| 20 | g | 618 | LEU | N-CA-C | -5.81 | 104.95 | 112.68 |
| 20 | g | 719 | ASN | N-CA-C | -5.81 | 106.36 | 113.50 |
| 14 | a | 658 | HIS | O-C-N | -5.81 | 115.96 | 122.12 |
| 8 | N | 914 | ASP | N-CA-C | -5.81 | 106.54 | 113.97 |
| 8 | N | 1216 | LYS | N-CA-C | 5.81 | 119.62 | 112.54 |
| 7 | O | 763 | HIS | CA-C-O | -5.81 | 113.10 | 119.08 |
| 7 | O | 1656 | SER | N-CA-C | 5.81 | 117.69 | 111.36 |
| 8 | P | 577 | MET | CA-CB-CG | -5.81 | 102.48 | 114.10 |
| 9 | S | 501 | MET | CB-CA-C | -5.81 | 100.17 | 111.03 |
| 2 | Z | 639 | GLU | N-CA-C | -5.81 | 106.03 | 113.23 |
| 2 | Z | 1173 | LEU | N-CA-C | 5.81 | 117.28 | 111.07 |
| 12 | u | 664 | ARG | N-CA-CB | 5.81 | 119.28 | 110.28 |
| 12 | v | 341 | ASN | CB-CA-C | -5.81 | 103.63 | 112.11 |
| 12 | v | 364 | ILE | CA-CB-CG1 | 5.81 | 120.27 | 110.40 |
| 14 | h | 477 | GLN | CA-C-N | 5.81 | 127.10 | 119.84 |
| 14 | h | 477 | GLN | C-N-CA | 5.81 | 127.10 | 119.84 |
| 15 | i | 49 | VAL | CA-C-N | 5.81 | 127.10 | 119.84 |
| 15 | i | 49 | VAL | C-N-CA | 5.81 | 127.10 | 119.84 |
| 20 | n | 838 | GLU | N-CA-CB | 5.81 | 118.62 | 110.90 |
| 20 | n | 895 | SER | N-CA-CB | 5.81 | 121.79 | 111.69 |
| 19 | f | 159 | ASP | N-CA-C | -5.81 | 106.17 | 113.72 |
| 19 | f | 400 | ASN | O-C-N | -5.81 | 114.67 | 121.23 |
| 19 | f | 685 | SER | N-CA-C | 5.81 | 117.79 | 110.24 |
| 20 | g | 479 | VAL | N-CA-CB | 5.81 | 118.78 | 111.46 |
| 6 | I | 316 | LEU | CA-C-N | 5.81 | 128.53 | 120.29 |
| 6 | I | 316 | LEU | C-N-CA | 5.81 | 128.53 | 120.29 |
| 8 | N | 750 | PHE | CB-CG-CD2 | 5.81 | 130.57 | 120.70 |
| 8 | P | 113 | VAL | N-CA-C | 5.81 | 116.58 | 110.72 |
| 20 | n | 341 | ASP | CA-CB-CG | 5.81 | 118.41 | 112.60 |
| 18 | e | 68 | TYR | N-CA-C | -5.81 | 104.60 | 112.26 |
| 20 | g | 1016 | PHE | N-CA-CB | 5.81 | 120.30 | 110.49 |
| 1 | 0 | 685 | VAL | N-CA-CB | 5.80 | 117.34 | 110.55 |
| 5 | K | 469 | ARG | CD-NE-CZ | -5.80 | 116.27 | 124.40 |
| 7 | M | 773 | LYS | CA-C-N | 5.80 | 128.06 | 120.28 |
| 7 | M | 773 | LYS | C-N-CA | 5.80 | 128.06 | 120.28 |
| 1 | Y | 834 | ILE | N-CA-C | -5.80 | 100.06 | 108.36 |
| 20 | n | 540 | HIS | ND1-CE1-NE2 | 5.80 | 114.20 | 108.40 |
| 15 | b | 177 | GLU | CB-CG-CD | 5.80 | 122.47 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | b | 413 | ASP | N-CA-CB | 5.80 | 120.30 | 110.49 |
| 15 | b | 508 | LEU | CA-C-O | -5.80 | 112.35 | 117.98 |
| 20 | g | 1043 | ARG | NE-CZ-NH2 | -5.80 | 113.97 | 119.20 |
| 2 | 1 | 149 | GLU | CB-CG-CD | -5.80 | 102.73 | 112.60 |
| 14 | h | 68 | ILE | CA-C-O | 5.80 | 127.97 | 120.95 |
| 15 | i | 683 | MET | CG-SD-CE | -5.80 | 88.13 | 100.90 |
| 20 | n | 674 | ASN | N-CA-C | -5.80 | 105.69 | 112.89 |
| 8 | P | 111 | HIS | CE1-NE2-CD2 | -5.80 | 103.20 | 109.00 |
| 9 | S | 417 | ARG | O-C-N | 5.80 | 129.61 | 123.11 |
| 9 | T | 345 | LEU | CA-C-N | 5.80 | 128.71 | 120.53 |
| 9 | T | 345 | LEU | C-N-CA | 5.80 | 128.71 | 120.53 |
| 21 | s | 41 | ILE | CB-CA-C | -5.80 | 104.55 | 111.97 |
| 7 | O | 967 | THR | O-C-N | -5.80 | 116.10 | 122.07 |
| 9 | Q | 505 | HIS | ND1-CE1-NE2 | 5.80 | 114.20 | 108.40 |
| 16 | j | 305 | ARG | CA-C-O | 5.80 | 125.96 | 119.41 |
| 20 | n | 1027 | ASN | OD1-CG-ND2 | -5.80 | 116.80 | 122.60 |
| 15 | b | 76 | TYR | CA-CB-CG | 5.80 | 124.34 | 113.90 |
| 16 | c | 174 | ARG | NE-CZ-NH2 | 5.80 | 124.42 | 119.20 |
| 5 | E | 358 | LEU | N-CA-C | 5.80 | 117.27 | 111.07 |
| 8 | N | 386 | SER | CA-C-N | 5.80 | 130.69 | 121.18 |
| 8 | N | 386 | SER | C-N-CA | 5.80 | 130.69 | 121.18 |
| 15 | i | 243 | GLN | CA-C-N | 5.80 | 130.40 | 120.72 |
| 15 | i | 243 | GLN | C-N-CA | 5.80 | 130.40 | 120.72 |
| 20 | n | 922 | LEU | N-CA-C | 5.80 | 117.40 | 111.14 |
| 2 | 1 | 1066 | ASN | N-CA-CB | 5.80 | 118.56 | 110.56 |
| 2 | 1 | 1281 | VAL | CA-C-O | 5.80 | 125.65 | 119.91 |
| 6 | C | 296 | ALA | CA-C-O | -5.80 | 112.12 | 119.31 |
| 4 | D | 769 | ILE | N-CA-C | 5.80 | 116.53 | 110.62 |
| 7 | M | 845 | ASP | N-CA-CB | 5.80 | 118.58 | 109.94 |
| 7 | M | 1593 | ASN | CA-C-O | -5.80 | 114.37 | 120.63 |
| 8 | N | 595 | ILE | CA-C-N | 5.80 | 128.63 | 120.28 |
| 8 | N | 595 | ILE | C-N-CA | 5.80 | 128.63 | 120.28 |
| 8 | P | 1077 | ARG | N-CA-C | 5.80 | 118.38 | 111.71 |
| 12 | v | 422 | ARG | N-CA-C | -5.80 | 100.14 | 108.60 |
| 13 | x | 1354 | ALA | N-CA-CB | 5.80 | 118.41 | 110.01 |
| 4 | z | 808 | ASP | N-CA-CB | 5.80 | 118.41 | 110.01 |
| 21 | r | 56 | THR | CA-CB-OG1 | 5.80 | 118.29 | 109.60 |
| 15 | b | 277 | THR | CA-C-O | 5.80 | 126.50 | 119.78 |
| 2 | 1 | 925 | ARG | NE-CZ-NH2 | -5.79 | 113.98 | 119.20 |
| 15 | b | 165 | GLN | N-CA-CB | 5.79 | 120.28 | 110.49 |
| 1 | 0 | 445 | ARG | NE-CZ-NH2 | -5.79 | 113.98 | 119.20 |
| 1 | 0 | 1278 | LEU | N-CA-C | -5.79 | 104.88 | 112.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 1305 | SER | N-CA-CB | 5.79 | 120.28 | 110.49 |
| 5 | E | 343 | PRO | N-CA-CB | -5.79 | 97.17 | 103.25 |
| 7 | O | 546 | TYR | N-CA-C | -5.79 | 106.05 | 113.23 |
| 9 | R | 799 | LYS | N-CA-C | 5.79 | 118.54 | 111.82 |
| 2 | Z | 633 | HIS | CG-CD2-NE2 | 5.79 | 112.99 | 107.20 |
| 12 | u | 62 | HIS | ND1-CE1-NE2 | 5.79 | 114.19 | 108.40 |
| 12 | v | 538 | ARG | CA-C-N | 5.79 | 128.40 | 120.46 |
| 12 | v | 538 | ARG | C-N-CA | 5.79 | 128.40 | 120.46 |
| 15 | b | 618 | ASN | CA-CB-CG | 5.79 | 118.39 | 112.60 |
| 14 | a | 386 | LEU | O-C-N | 5.79 | 128.26 | 122.12 |
| 1 | 0 | 980 | SER | CA-C-O | 5.79 | 126.53 | 119.64 |
| 8 | N | 744 | LEU | N-CA-C | -5.79 | 106.22 | 113.28 |
| 12 | u | 433 | ASP | CA-CB-CG | 5.79 | 118.39 | 112.60 |
| 15 | i | 226 | GLN | CA-C-O | 5.79 | 126.67 | 120.24 |
| 14 | a | 936 | TYR | CA-C-O | 5.79 | 128.13 | 121.47 |
| 1 | 0 | 424 | SER | N-CA-C | -5.79 | 99.22 | 109.06 |
| 1 | 0 | 1074 | MET | N-CA-C | -5.79 | 104.04 | 113.19 |
| 7 | M | 909 | LEU | N-CA-CB | 5.79 | 120.28 | 110.49 |
| 8 | N | 1429 | HIS | CE1-NE2-CD2 | -5.79 | 103.21 | 109.00 |
| 8 | P | 906 | TYR | N-CA-C | 5.79 | 117.67 | 111.36 |
| 9 | T | 50 | ARG | N-CA-C | -5.79 | 105.99 | 114.39 |
| 2 | Z | 430 | VAL | N-CA-C | -5.79 | 100.07 | 108.87 |
| 20 | g | 1046 | VAL | N-CA-C | 5.79 | 116.53 | 110.62 |
| 7 | M | 251 | ASP | N-CA-C | -5.79 | 106.14 | 113.43 |
| 7 | M | 1483 | THR | CA-C-N | 5.79 | 128.84 | 120.79 |
| 7 | M | 1483 | THR | C-N-CA | 5.79 | 128.84 | 120.79 |
| 7 | O | 751 | PRO | N-CA-CB | 5.79 | 109.27 | 103.48 |
| 7 | O | 1345 | PHE | CA-CB-CG | -5.79 | 108.01 | 113.80 |
| 8 | P | 768 | ALA | CA-C-O | -5.79 | 114.41 | 120.55 |
| 8 | P | 1405 | ASN | N-CA-CB | 5.79 | 118.74 | 110.06 |
| 10 | U | 248 | TRP | CB-CG-CD1 | -5.79 | 118.22 | 126.90 |
| 1 | Y | 608 | ILE | CA-C-O | 5.79 | 126.41 | 120.39 |
| 2 | Z | 1239 | ASN | N-CA-C | 5.79 | 117.59 | 111.28 |
| 15 | i | 403 | HIS | ND1-CE1-NE2 | 5.79 | 114.19 | 108.40 |
| 21 | t | 66 | GLY | N-CA-C | -5.79 | 101.85 | 110.71 |
| 19 | f | 469 | ARG | CB-CA-C | 5.79 | 121.94 | 110.42 |
| 6 | I | 309 | PRO | N-CD-CG | 5.79 | 111.88 | 103.20 |
| 4 | J | 708 | GLU | CA-C-O | -5.79 | 112.96 | 119.79 |
| 7 | M | 1081 | GLU | CB-CG-CD | 5.79 | 122.44 | 112.60 |
| 1 | Y | 214 | VAL | N-CA-C | -5.79 | 99.20 | 107.77 |
| 13 | w | 1290 | ASP | CA-C-N | 5.79 | 130.38 | 120.72 |
| 13 | w | 1290 | ASP | C-N-CA | 5.79 | 130.38 | 120.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 1373 | LYS | O-C-N | 5.79 | 128.34 | 122.09 |
| 6 | C | 307 | SER | CB-CA-C | -5.79 | 97.90 | 109.99 |
| 7 | M | 507 | ALA | CA-C-N | 5.79 | 128.03 | 120.28 |
| 7 | M | 507 | ALA | C-N-CA | 5.79 | 128.03 | 120.28 |
| 8 | N | 857 | LEU | CA-C-N | 5.79 | 128.03 | 120.28 |
| 8 | N | 857 | LEU | C-N-CA | 5.79 | 128.03 | 120.28 |
| 8 | P | 1452 | SER | N-CA-C | 5.79 | 117.28 | 110.97 |
| 9 | R | 226 | ARG | NE-CZ-NH2 | -5.79 | 113.99 | 119.20 |
| 9 | S | 759 | ASP | N-CA-CB | 5.79 | 119.21 | 110.30 |
| 1 | Y | 113 | HIS | CB-CA-C | -5.79 | 101.80 | 110.88 |
| 1 | Y | 230 | HIS | CA-CB-CG | 5.79 | 119.59 | 113.80 |
| 1 | Y | 512 | LYS | CA-CB-CG | 5.79 | 125.67 | 114.10 |
| 14 | h | 71 | HIS | CB-CG-ND1 | 5.79 | 131.38 | 122.70 |
| 14 | h | 641 | ASP | CA-CB-CG | -5.79 | 106.81 | 112.60 |
| 18 | l | 21 | GLY | O-C-N | 5.79 | 129.78 | 122.43 |
| 19 | m | 179 | ILE | CA-C-N | 5.79 | 129.10 | 120.31 |
| 19 | m | 179 | ILE | C-N-CA | 5.79 | 129.10 | 120.31 |
| 14 | a | 625 | ILE | CA-C-N | 5.79 | 129.10 | 120.31 |
| 14 | a | 625 | ILE | C-N-CA | 5.79 | 129.10 | 120.31 |
| 7 | M | 1526 | ILE | CA-CB-CG2 | -5.78 | 100.67 | 110.50 |
| 8 | P | 77 | ASN | CA-C-N | 5.78 | 131.90 | 122.65 |
| 8 | P | 77 | ASN | C-N-CA | 5.78 | 131.90 | 122.65 |
| 9 | Q | 510 | LEU | N-CA-C | -5.78 | 106.87 | 114.04 |
| 9 | S | 800 | GLY | O-C-N | -5.78 | 116.58 | 122.19 |
| 19 | m | 184 | ILE | N-CA-C | -5.78 | 104.88 | 110.72 |
| 19 | m | 579 | GLN | O-C-N | -5.78 | 116.11 | 122.07 |
| 20 | n | 576 | ASN | N-CA-CB | 5.78 | 119.42 | 110.80 |
| 20 | g | 86 | LEU | CA-C-N | 5.78 | 128.92 | 120.71 |
| 20 | g | 86 | LEU | C-N-CA | 5.78 | 128.92 | 120.71 |
| 20 | g | 1000 | SER | N-CA-C | -5.78 | 105.72 | 112.89 |
| 19 | m | 76 | HIS | ND1-CE1-NE2 | 5.78 | 114.18 | 108.40 |
| 17 | d | 203 | HIS | CE1-NE2-CD2 | -5.78 | 103.22 | 109.00 |
| 2 | 1 | 646 | TYR | CB-CG-CD2 | 5.78 | 129.47 | 120.80 |
| 7 | M | 1498 | LEU | N-CA-C | -5.78 | 100.53 | 109.14 |
| 8 | P | 939 | LEU | N-CA-C | -5.78 | 103.50 | 110.44 |
| 9 | Q | 546 | ARG | CA-CB-CG | 5.78 | 125.66 | 114.10 |
| 9 | S | 428 | VAL | N-CA-C | -5.78 | 107.11 | 112.83 |
| 9 | S | 787 | HIS | CG-CD2-NE2 | 5.78 | 112.98 | 107.20 |
| 2 | Z | 762 | LEU | N-CA-C | -5.78 | 105.06 | 111.36 |
| 4 | y | 664 | SER | CA-C-N | 5.78 | 127.95 | 120.44 |
| 4 | y | 664 | SER | C-N-CA | 5.78 | 127.95 | 120.44 |
| 15 | i | 290 | GLU | N-CA-CB | 5.78 | 118.72 | 110.16 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | i | 668 | ALA | O-C-N | -5.78 | 115.85 | 123.13 |
| 20 | n | 146 | MET | N-CA-CB | 5.78 | 120.26 | 110.49 |
| 20 | n | 443 | TRP | N-CA-C | -5.78 | 98.49 | 110.80 |
| 20 | g | 431 | SER | CB-CA-C | 5.78 | 122.94 | 112.30 |
| 14 | a | 958 | TRP | CA-C-O | -5.78 | 114.58 | 120.71 |
| 2 | 1 | 259 | ASN | N-CA-C | -5.78 | 99.77 | 108.96 |
| 7 | M | 676 | ASP | N-CA-C | 5.78 | 117.58 | 111.28 |
| 12 | v | 406 | ALA | N-CA-C | -5.78 | 106.27 | 113.38 |
| 15 | i | 467 | ASN | OD1-CG-ND2 | 5.78 | 128.38 | 122.60 |
| 15 | i | 664 | VAL | O-C-N | -5.78 | 115.88 | 121.83 |
| 19 | m | 16 | SER | N-CA-C | -5.78 | 105.33 | 112.90 |
| 20 | n | 898 | ASP | CA-CB-CG | 5.78 | 118.38 | 112.60 |
| 18 | e | 14 | ASP | CA-CB-CG | 5.78 | 118.38 | 112.60 |
| 20 | g | 802 | ILE | CA-C-O | -5.78 | 114.94 | 120.95 |
| 1 | 0 | 382 | ILE | N-CA-C | -5.78 | 99.90 | 108.45 |
| 6 | L | 374 | GLN | CG-CD-OE1 | -5.78 | 109.25 | 120.80 |
| 7 | M | 438 | VAL | N-CA-C | 5.78 | 116.51 | 110.62 |
| 7 | O | 1646 | LEU | CA-C-N | 5.78 | 128.02 | 120.28 |
| 7 | O | 1646 | LEU | C-N-CA | 5.78 | 128.02 | 120.28 |
| 9 | T | 67 | THR | N-CA-C | 5.78 | 117.25 | 111.07 |
| 2 | Z | 712 | SER | CB-CA-C | -5.78 | 101.20 | 110.79 |
| 16 | j | 164 | ILE | CA-CB-CG1 | 5.78 | 120.22 | 110.40 |
| 19 | m | 403 | SER | N-CA-C | -5.78 | 103.79 | 111.24 |
| 21 | q | 28 | SER | N-CA-C | 5.78 | 117.66 | 111.36 |
| 20 | g | 74 | THR | CB-CA-C | 5.78 | 119.26 | 109.84 |
| 14 | a | 625 | ILE | N-CA-CB | 5.78 | 117.97 | 110.57 |
| 7 | M | 420 | THR | O-C-N | -5.78 | 116.00 | 122.93 |
| 9 | T | 716 | LEU | CA-C-N | 5.78 | 128.02 | 120.28 |
| 9 | T | 716 | LEU | C-N-CA | 5.78 | 128.02 | 120.28 |
| 1 | Y | 1099 | ASP | CA-CB-CG | -5.78 | 106.83 | 112.60 |
| 12 | u | 178 | ARG | N-CA-C | -5.78 | 100.48 | 109.72 |
| 13 | x | 1272 | ILE | CB-CA-C | -5.78 | 104.58 | 111.97 |
| 15 | b | 349 | TYR | CB-CG-CD1 | 5.78 | 129.46 | 120.80 |
| 14 | a | 807 | ILE | CA-C-N | 5.78 | 128.29 | 120.44 |
| 14 | a | 807 | ILE | C-N-CA | 5.78 | 128.29 | 120.44 |
| 7 | M | 1064 | THR | CA-C-N | 5.77 | 130.33 | 122.19 |
| 7 | M | 1064 | THR | C-N-CA | 5.77 | 130.33 | 122.19 |
| 7 | O | 276 | ALA | CA-C-N | 5.77 | 128.29 | 120.44 |
| 7 | O | 276 | ALA | C-N-CA | 5.77 | 128.29 | 120.44 |
| 15 | b | 117 | ASP | O-C-N | 5.77 | 128.73 | 122.15 |
| 1 | 0 | 1415 | ILE | O-C-N | -5.77 | 116.43 | 122.20 |
| 5 | B | 405 | ASN | CA-C-N | 5.77 | 130.22 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | B | 405 | ASN | C-N-CA | 5.77 | 130.22 | 120.29 |
| 20 | n | 465 | LEU | CA-C-N | 5.77 | 131.60 | 122.94 |
| 20 | n | 465 | LEU | C-N-CA | 5.77 | 131.60 | 122.94 |
| 21 | t | 73 | LYS | N-CA-CB | 5.77 | 118.60 | 109.71 |
| 19 | f | 340 | GLU | O-C-N | -5.77 | 115.16 | 122.26 |
| 1 | Y | 197 | ASN | CA-C-N | 5.77 | 128.01 | 120.28 |
| 1 | Y | 197 | ASN | C-N-CA | 5.77 | 128.01 | 120.28 |
| 4 | z | 667 | GLN | N-CA-C | -5.77 | 104.89 | 111.07 |
| 20 | n | 649 | PHE | CA-C-N | 5.77 | 130.49 | 120.68 |
| 20 | n | 649 | PHE | C-N-CA | 5.77 | 130.49 | 120.68 |
| 14 | a | 288 | VAL | N-CA-C | -5.77 | 100.09 | 108.17 |
| 1 | 0 | 205 | ASP | N-CA-C | -5.77 | 100.73 | 109.85 |
| 1 | 0 | 446 | LEU | N-CA-C | -5.77 | 99.78 | 109.07 |
| 1 | 0 | 1306 | GLU | CA-C-O | 5.77 | 125.55 | 119.03 |
| 7 | M | 1005 | PHE | CA-CB-CG | 5.77 | 119.57 | 113.80 |
| 8 | N | 1257 | LEU | CA-C-O | -5.77 | 114.43 | 120.55 |
| 7 | O | 1657 | ASP | N-CA-CB | 5.77 | 118.90 | 110.30 |
| 21 | o | 8 | THR | O-C-N | 5.77 | 126.76 | 121.80 |
| 21 | p | 42 | ALA | CB-CA-C | -5.77 | 101.21 | 110.79 |
| 2 | 1 | 1165 | ASP | CA-CB-CG | 5.77 | 118.37 | 112.60 |
| 6 | F | 470 | LEU | CA-C-O | -5.77 | 114.75 | 120.80 |
| 6 | I | 439 | ILE | O-C-N | -5.77 | 116.91 | 122.16 |
| 8 | N | 936 | LEU | O-C-N | 5.77 | 128.23 | 122.12 |
| 12 | u | 30 | GLN | CB-CG-CD | -5.77 | 102.80 | 112.60 |
| 15 | i | 538 | ILE | N-CA-CB | -5.77 | 102.70 | 110.54 |
| 16 | j | 209 | GLN | OE1-CD-NE2 | 5.77 | 128.37 | 122.60 |
| 20 | n | 415 | SER | N-CA-C | -5.77 | 103.98 | 113.50 |
| 14 | a | 484 | TYR | N-CA-CB | 5.77 | 118.59 | 109.71 |
| 14 | a | 770 | PHE | N-CA-C | -5.77 | 106.29 | 113.38 |
| 9 | S | 787 | HIS | ND1-CE1-NE2 | 5.77 | 114.17 | 108.40 |
| 2 | Z | 705 | LEU | N-CA-CB | 5.77 | 120.23 | 110.49 |
| 20 | n | 786 | LEU | N-CA-C | -5.77 | 106.28 | 113.55 |
| 20 | g | 392 | ASP | CA-C-O | -5.77 | 114.39 | 121.02 |
| 14 | a | 942 | ILE | N-CA-C | -5.77 | 106.67 | 113.42 |
| 1 | 0 | 581 | PRO | CA-C-N | 5.76 | 130.65 | 121.66 |
| 1 | 0 | 581 | PRO | C-N-CA | 5.76 | 130.65 | 121.66 |
| 5 | E | 300 | ASP | CA-C-O | -5.76 | 114.17 | 119.76 |
| 7 | O | 780 | ILE | CA-C-N | 5.76 | 128.00 | 120.28 |
| 7 | O | 780 | ILE | C-N-CA | 5.76 | 128.00 | 120.28 |
| 14 | h | 183 | LEU | N-CA-C | -5.76 | 100.31 | 109.59 |
| 15 | i | 657 | TYR | O-C-N | -5.76 | 114.92 | 122.59 |
| 16 | j | 770 | SER | N-CA-CB | 5.76 | 120.30 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 17 | k | 94 | VAL | N-CA-C | -5.76 | 99.87 | 108.46 |
| 1 | 0 | 199 | ASN | N-CA-C | -5.76 | 106.47 | 112.93 |
| 7 | M | 695 | ALA | N-CA-CB | 5.76 | 118.59 | 110.12 |
| 8 | P | 1130 | PHE | CB-CA-C | -5.76 | 100.11 | 110.37 |
| 8 | P | 1563 | LEU | O-C-N | 5.76 | 130.15 | 122.43 |
| 1 | Y | 213 | LYS | CA-C-N | 5.76 | 131.16 | 122.98 |
| 1 | Y | 213 | LYS | C-N-CA | 5.76 | 131.16 | 122.98 |
| 1 | Y | 457 | ILE | CA-CB-CG1 | 5.76 | 120.20 | 110.40 |
| 6 | L | 292 | HIS | CG-CD2-NE2 | 5.76 | 112.96 | 107.20 |
| 8 | P | 837 | ASP | O-C-N | -5.76 | 115.14 | 122.34 |
| 9 | Q | 702 | ILE | O-C-N | -5.76 | 115.37 | 122.57 |
| 12 | v | 126 | SER | CA-C-N | 5.76 | 128.99 | 122.48 |
| 12 | v | 126 | SER | C-N-CA | 5.76 | 128.99 | 122.48 |
| 16 | j | 460 | ASN | CA-C-O | 5.76 | 126.53 | 120.42 |
| 14 | a | 568 | LYS | N-CA-C | 5.76 | 117.56 | 111.28 |
| 14 | a | 748 | PHE | N-CA-CB | 5.76 | 120.23 | 110.49 |
| 1 | 0 | 1238 | ARG | NE-CZ-NH1 | -5.76 | 115.74 | 121.50 |
| 2 | 1 | 405 | LYS | N-CA-CB | 5.76 | 120.22 | 110.49 |
| 6 | L | 463 | LYS | CA-C-N | 5.76 | 129.06 | 120.31 |
| 6 | L | 463 | LYS | C-N-CA | 5.76 | 129.06 | 120.31 |
| 7 | M | 1194 | LEU | N-CA-C | -5.76 | 106.11 | 113.02 |
| 7 | M | 1252 | VAL | CA-C-N | 5.76 | 128.00 | 120.28 |
| 7 | M | 1252 | VAL | C-N-CA | 5.76 | 128.00 | 120.28 |
| 8 | N | 163 | ASP | CA-CB-CG | 5.76 | 118.36 | 112.60 |
| 7 | O | 893 | HIS | CG-CD2-NE2 | 5.76 | 112.96 | 107.20 |
| 2 | Z | 1008 | ILE | CA-C-N | 5.76 | 128.00 | 120.28 |
| 2 | Z | 1008 | ILE | C-N-CA | 5.76 | 128.00 | 120.28 |
| 13 | w | 1224 | GLU | CA-C-O | -5.76 | 114.74 | 120.90 |
| 14 | h | 871 | HIS | ND1-CE1-NE2 | 5.76 | 114.16 | 108.40 |
| 18 | l | 337 | ASN | N-CA-CB | 5.76 | 120.22 | 110.49 |
| 1 | 0 | 1011 | ARG | NE-CZ-NH1 | 5.76 | 127.26 | 121.50 |
| 1 | 0 | 1319 | GLU | N-CA-C | 5.76 | 118.30 | 111.33 |
| 5 | B | 392 | LEU | CA-C-N | 5.76 | 132.54 | 121.54 |
| 5 | B | 392 | LEU | C-N-CA | 5.76 | 132.54 | 121.54 |
| 5 | B | 537 | TYR | CA-C-O | 5.76 | 126.63 | 119.78 |
| 5 | H | 351 | GLN | N-CA-C | 5.76 | 118.62 | 110.50 |
| 9 | S | 160 | GLY | CA-C-N | 5.76 | 128.35 | 120.46 |
| 9 | S | 160 | GLY | C-N-CA | 5.76 | 128.35 | 120.46 |
| 14 | h | 361 | SER | N-CA-C | -5.76 | 100.38 | 108.96 |
| 20 | n | 121 | THR | N-CA-CB | 5.76 | 119.75 | 110.65 |
| 5 | B | 458 | GLU | N-CA-C | 5.76 | 117.23 | 111.07 |
| 5 | E | 301 | PRO | N-CA-CB | -5.76 | 97.21 | 103.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | J | 665 | TRP | CA-CB-CG | 5.76 | 124.54 | 113.60 |
| 4 | J | 697 | LEU | CA-C-O | -5.76 | 112.72 | 119.05 |
| 8 | P | 86 | ASP | O-C-N | -5.76 | 114.70 | 121.32 |
| 9 | R | 775 | LEU | N-CA-C | 5.76 | 118.33 | 111.71 |
| 9 | T | 151 | HIS | N-CA-CB | 5.76 | 119.30 | 110.61 |
| 12 | v | 72 | ILE | O-C-N | 5.76 | 129.16 | 123.00 |
| 15 | i | 88 | TYR | N-CA-CB | 5.76 | 119.11 | 110.53 |
| 7 | M | 766 | GLN | N-CA-C | -5.75 | 106.42 | 113.50 |
| 7 | M | 1536 | SER | O-C-N | 5.75 | 128.31 | 122.09 |
| 8 | P | 330 | TYR | O-C-N | 5.75 | 128.22 | 122.12 |
| 9 | R | 73 | LEU | N-CA-C | 5.75 | 117.55 | 111.28 |
| 12 | v | 449 | ASN | N-CA-C | -5.75 | 101.22 | 110.14 |
| 14 | h | 87 | ALA | N-CA-C | -5.75 | 106.09 | 113.23 |
| 21 | o | 27 | ILE | CB-CA-C | 5.75 | 119.91 | 112.14 |
| 19 | f | 645 | ASP | CA-CB-CG | 5.75 | 118.36 | 112.60 |
| 4 | A | 769 | ILE | O-C-N | 5.75 | 127.45 | 121.87 |
| 4 | A | 809 | ASP | N-CA-CB | 5.75 | 118.67 | 110.16 |
| 7 | M | 740 | LEU | O-C-N | 5.75 | 130.38 | 123.36 |
| 8 | P | 1189 | ASP | CA-CB-CG | 5.75 | 118.35 | 112.60 |
| 11 | X | 276 | TYR | CA-C-O | -5.75 | 114.72 | 120.64 |
| 2 | Z | 725 | GLU | N-CA-C | -5.75 | 106.26 | 113.28 |
| 13 | w | 1309 | ASP | CA-C-O | -5.75 | 114.32 | 120.42 |
| 4 | y | 811 | SER | N-CA-C | 5.75 | 117.63 | 111.36 |
| 2 | 1 | 622 | GLU | N-CA-C | -5.75 | 106.49 | 112.93 |
| 8 | N | 1565 | ASN | N-CA-C | -5.75 | 104.64 | 111.03 |
| 7 | O | 866 | GLN | CA-CB-CG | 5.75 | 125.60 | 114.10 |
| 8 | P | 915 | ASP | CA-CB-CG | 5.75 | 118.35 | 112.60 |
| 9 | S | 370 | TYR | O-C-N | -5.75 | 114.94 | 122.59 |
| 2 | Z | 958 | ASN | N-CA-CB | 5.75 | 120.21 | 110.49 |
| 19 | m | 202 | LEU | CA-C-O | 5.75 | 126.17 | 119.32 |
| 16 | c | 296 | LEU | N-CA-C | -5.75 | 106.10 | 113.23 |
| 19 | f | 327 | VAL | CA-C-N | 5.75 | 127.99 | 120.28 |
| 19 | f | 327 | VAL | C-N-CA | 5.75 | 127.99 | 120.28 |
| 9 | R | 235 | ALA | CB-CA-C | -5.75 | 101.85 | 110.88 |
| 1 | 0 | 1339 | LYS | N-CA-C | -5.75 | 105.53 | 113.18 |
| 2 | 1 | 996 | VAL | CA-C-N | 5.75 | 127.98 | 120.28 |
| 2 | 1 | 996 | VAL | C-N-CA | 5.75 | 127.98 | 120.28 |
| 7 | M | 978 | ILE | CA-C-O | -5.75 | 114.76 | 120.85 |
| 7 | M | 1137 | ASN | CA-CB-CG | 5.75 | 118.35 | 112.60 |
| 8 | N | 1349 | TYR | CA-CB-CG | -5.75 | 103.55 | 113.90 |
| 2 | Z | 490 | SER | CA-C-N | 5.75 | 129.05 | 120.31 |
| 2 | Z | 490 | SER | C-N-CA | 5.75 | 129.05 | 120.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 769 | HIS | CA-CB-CG | -5.75 | 108.05 | 113.80 |
| 14 | h | 734 | HIS | CE1-NE2-CD2 | -5.75 | 103.25 | 109.00 |
| 20 | n | 252 | PHE | CA-CB-CG | 5.75 | 119.55 | 113.80 |
| 18 | e | 237 | ASP | N-CA-C | -5.75 | 105.93 | 113.17 |
| 19 | f | 334 | ARG | NE-CZ-NH2 | 5.75 | 124.37 | 119.20 |
| 7 | M | 1066 | ASP | N-CA-C | -5.75 | 100.58 | 109.14 |
| 7 | O | 158 | ILE | CA-C-N | 5.75 | 127.91 | 120.44 |
| 7 | O | 158 | ILE | C-N-CA | 5.75 | 127.91 | 120.44 |
| 7 | O | 1106 | PHE | CA-CB-CG | -5.75 | 108.05 | 113.80 |
| 8 | P | 322 | HIS | CE1-NE2-CD2 | -5.75 | 103.25 | 109.00 |
| 9 | T | 411 | VAL | N-CA-C | 5.75 | 118.23 | 111.05 |
| 9 | T | 766 | ASN | N-CA-C | -5.75 | 106.03 | 113.16 |
| 2 | Z | 820 | ASP | CA-CB-CG | 5.75 | 118.35 | 112.60 |
| 4 | y | 813 | SER | CA-C-O | 5.75 | 127.05 | 120.90 |
| 14 | h | 252 | THR | CA-C-N | 5.75 | 129.03 | 120.87 |
| 14 | h | 252 | THR | C-N-CA | 5.75 | 129.03 | 120.87 |
| 19 | m | 192 | ALA | N-CA-C | -5.75 | 101.67 | 109.54 |
| 15 | b | 209 | LEU | O-C-N | 5.75 | 129.34 | 122.27 |
| 20 | g | 621 | TYR | N-CA-C | -5.75 | 100.67 | 109.41 |
| 20 | g | 817 | THR | CA-C-N | 5.75 | 132.18 | 123.04 |
| 20 | g | 817 | THR | C-N-CA | 5.75 | 132.18 | 123.04 |
| 1 | 0 | 706 | GLY | O-C-N | 5.75 | 129.26 | 123.11 |
| 8 | P | 809 | PRO | CB-CA-C | 5.75 | 116.63 | 111.40 |
| 2 | Z | 434 | PHE | N-CA-CB | 5.75 | 120.00 | 110.63 |
| 20 | n | 638 | SER | N-CA-CB | 5.75 | 118.21 | 111.09 |
| 7 | M | 1388 | CYS | N-CA-C | 5.74 | 118.31 | 111.71 |
| 7 | O | 1329 | LEU | O-C-N | -5.74 | 115.60 | 122.15 |
| 9 | S | 56 | LEU | CA-C-N | 5.74 | 131.67 | 120.99 |
| 9 | S | 56 | LEU | C-N-CA | 5.74 | 131.67 | 120.99 |
| 12 | u | 161 | GLU | CA-C-N | 5.74 | 128.65 | 120.49 |
| 12 | u | 161 | GLU | C-N-CA | 5.74 | 128.65 | 120.49 |
| 19 | m | 674 | ALA | CA-C-N | 5.74 | 130.74 | 122.35 |
| 19 | m | 674 | ALA | C-N-CA | 5.74 | 130.74 | 122.35 |
| 14 | a | 1009 | SER | N-CA-C | -5.74 | 105.66 | 114.16 |
| 7 | M | 814 | ASN | CA-CB-CG | 5.74 | 118.34 | 112.60 |
| 7 | O | 150 | PHE | CA-CB-CG | -5.74 | 108.06 | 113.80 |
| 7 | O | 705 | ASP | CA-CB-CG | 5.74 | 118.34 | 112.60 |
| 9 | R | 511 | ALA | CA-C-N | 5.74 | 127.97 | 120.28 |
| 9 | R | 511 | ALA | C-N-CA | 5.74 | 127.97 | 120.28 |
| 14 | h | 952 | ASN | CA-C-N | 5.74 | 128.55 | 120.28 |
| 14 | h | 952 | ASN | C-N-CA | 5.74 | 128.55 | 120.28 |
| 7 | M | 137 | ASN | CA-CB-CG | 5.74 | 118.34 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 571 | ASN | CA-C-O | -5.74 | 114.50 | 120.70 |
| 8 | P | 77 | ASN | N-CA-C | -5.74 | 99.42 | 108.14 |
| 8 | P | 1252 | LEU | N-CA-CB | 5.74 | 118.56 | 110.12 |
| 1 | Y | 782 | ARG | CA-C-N | -5.74 | 112.88 | 122.64 |
| 1 | Y | 782 | ARG | C-N-CA | -5.74 | 112.88 | 122.64 |
| 12 | v | 79 | LEU | CA-C-O | -5.74 | 114.67 | 121.16 |
| 16 | j | 514 | GLU | CA-C-N | 5.74 | 131.24 | 122.69 |
| 16 | j | 514 | GLU | C-N-CA | 5.74 | 131.24 | 122.69 |
| 15 | b | 105 | SER | CA-C-N | 5.74 | 127.90 | 120.44 |
| 15 | b | 105 | SER | C-N-CA | 5.74 | 127.90 | 120.44 |
| 20 | g | 122 | VAL | N-CA-CB | 5.74 | 119.25 | 111.21 |
| 5 | H | 336 | ASP | CA-C-N | 5.74 | 127.90 | 120.44 |
| 5 | H | 336 | ASP | C-N-CA | 5.74 | 127.90 | 120.44 |
| 6 | I | 378 | HIS | N-CA-CB | 5.74 | 118.65 | 110.16 |
| 8 | N | 769 | PHE | CA-CB-CG | 5.74 | 119.54 | 113.80 |
| 9 | R | 333 | ILE | N-CA-C | 5.74 | 118.22 | 111.05 |
| 9 | S | 493 | ASP | N-CA-CB | 5.74 | 118.94 | 110.56 |
| 9 | T | 325 | LEU | O-C-N | -5.74 | 116.39 | 123.33 |
| 9 | T | 546 | ARG | NE-CZ-NH2 | 5.74 | 124.36 | 119.20 |
| 13 | w | 1432 | LYS | N-CA-C | 5.74 | 117.21 | 111.07 |
| 14 | h | 494 | PHE | CA-CB-CG | -5.74 | 108.06 | 113.80 |
| 16 | j | 217 | PHE | N-CA-C | -5.74 | 106.04 | 113.16 |
| 20 | n | 1102 | PHE | O-C-N | -5.74 | 116.10 | 121.72 |
| 19 | f | 442 | LEU | N-CA-C | -5.74 | 105.94 | 113.17 |
| 20 | g | 546 | ILE | O-C-N | -5.74 | 114.56 | 121.10 |
| 2 | 1 | 109 | PRO | CA-C-O | -5.74 | 114.78 | 121.95 |
| 7 | M | 736 | PHE | CB-CG-CD2 | 5.74 | 130.45 | 120.70 |
| 10 | U | 254 | ILE | N-CA-CB | 5.74 | 119.33 | 111.41 |
| 4 | y | 808 | ASP | O-C-N | 5.74 | 128.29 | 122.09 |
| 19 | m | 310 | THR | CA-CB-CG2 | 5.74 | 120.25 | 110.50 |
| 16 | c | 660 | VAL | CA-C-N | 5.74 | 130.30 | 120.72 |
| 16 | c | 660 | VAL | C-N-CA | 5.74 | 130.30 | 120.72 |
| 19 | f | 232 | ASN | CA-C-N | 5.74 | 131.88 | 122.07 |
| 19 | f | 232 | ASN | C-N-CA | 5.74 | 131.88 | 122.07 |
| 6 | L | 378 | HIS | CA-C-O | 5.74 | 126.63 | 120.55 |
| 7 | M | 1458 | LEU | N-CA-CB | 5.74 | 120.18 | 110.49 |
| 7 | M | 1618 | SER | CA-C-O | -5.74 | 114.80 | 120.82 |
| 7 | M | 1675 | THR | N-CA-CB | 5.74 | 118.33 | 110.01 |
| 8 | N | 205 | PRO | CA-C-N | 5.74 | 129.53 | 120.47 |
| 8 | N | 205 | PRO | C-N-CA | 5.74 | 129.53 | 120.47 |
| 7 | O | 1626 | VAL | CA-C-N | 5.74 | 128.44 | 120.29 |
| 7 | O | 1626 | VAL | C-N-CA | 5.74 | 128.44 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | T | 474 | PHE | CA-CB-CG | -5.74 | 108.06 | 113.80 |
| 2 | Z | 614 | TYR | CA-C-N | 5.74 | 129.01 | 120.87 |
| 2 | Z | 614 | TYR | C-N-CA | 5.74 | 129.01 | 120.87 |
| 12 | v | 383 | GLN | N-CA-CB | 5.74 | 119.77 | 110.42 |
| 12 | v | 526 | GLU | N-CA-C | 5.74 | 117.61 | 111.36 |
| 14 | h | 1028 | THR | CA-CB-OG1 | 5.74 | 118.20 | 109.60 |
| 15 | i | 469 | PHE | CA-C-N | 5.74 | 132.54 | 121.18 |
| 15 | i | 469 | PHE | C-N-CA | 5.74 | 132.54 | 121.18 |
| 15 | b | 165 | GLN | OE1-CD-NE2 | -5.74 | 116.86 | 122.60 |
| 8 | N | 1516 | PRO | CA-C-N | 5.73 | 127.96 | 120.28 |
| 8 | N | 1516 | PRO | C-N-CA | 5.73 | 127.96 | 120.28 |
| 2 | Z | 755 | TYR | CA-C-N | 5.73 | 127.96 | 120.28 |
| 2 | Z | 755 | TYR | C-N-CA | 5.73 | 127.96 | 120.28 |
| 19 | m | 671 | LEU | CB-CA-C | -5.73 | 99.66 | 110.67 |
| 20 | n | 390 | ILE | O-C-N | -5.73 | 116.36 | 122.61 |
| 20 | n | 552 | THR | CA-C-O | 5.73 | 125.36 | 119.05 |
| 14 | a | 436 | HIS | CE1-NE2-CD2 | -5.73 | 103.27 | 109.00 |
| 8 | N | 1081 | ILE | CB-CA-C | 5.73 | 120.42 | 112.05 |
| 7 | O | 721 | SER | CA-C-N | 5.73 | 132.49 | 121.54 |
| 7 | O | 721 | SER | C-N-CA | 5.73 | 132.49 | 121.54 |
| 13 | w | 1120 | SER | N-CA-CB | 5.73 | 120.36 | 111.24 |
| 14 | h | 572 | ASP | N-CA-CB | 5.73 | 119.17 | 110.28 |
| 19 | m | 459 | LYS | CG-CD-CE | 5.73 | 124.48 | 111.30 |
| 1 | 0 | 121 | LEU | CA-C-N | 5.73 | 132.49 | 121.54 |
| 1 | 0 | 121 | LEU | C-N-CA | 5.73 | 132.49 | 121.54 |
| 7 | M | 1670 | ILE | CA-C-N | 5.73 | 127.78 | 120.56 |
| 7 | M | 1670 | ILE | C-N-CA | 5.73 | 127.78 | 120.56 |
| 8 | N | 1350 | LEU | CA-C-N | 5.73 | 129.69 | 121.55 |
| 8 | N | 1350 | LEU | C-N-CA | 5.73 | 129.69 | 121.55 |
| 8 | P | 704 | ASP | CA-C-N | 5.73 | 132.49 | 121.54 |
| 8 | P | 704 | ASP | C-N-CA | 5.73 | 132.49 | 121.54 |
| 9 | T | 125 | ILE | CA-C-N | 5.73 | 127.96 | 120.28 |
| 9 | T | 125 | ILE | C-N-CA | 5.73 | 127.96 | 120.28 |
| 13 | w | 1125 | ASP | N-CA-C | 5.73 | 117.53 | 111.28 |
| 15 | i | 388 | ASN | N-CA-C | -5.73 | 98.59 | 110.80 |
| 20 | n | 801 | CYS | N-CA-C | -5.73 | 106.25 | 113.18 |
| 21 | q | 89 | PHE | N-CA-CB | 5.73 | 121.23 | 111.66 |
| 14 | a | 900 | VAL | N-CA-CB | -5.73 | 104.87 | 112.26 |
| 1 | 0 | 897 | ILE | CA-C-N | 5.73 | 129.02 | 120.31 |
| 1 | 0 | 897 | ILE | C-N-CA | 5.73 | 129.02 | 120.31 |
| 6 | F | 299 | ILE | O-C-N | 5.73 | 127.86 | 121.90 |
| 12 | u | 572 | SER | CB-CA-C | -5.73 | 101.89 | 110.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | u | 633 | GLU | N-CA-CB | 5.73 | 118.64 | 110.16 |
| 2 | 1 | 235 | ILE | N-CA-CB | 5.73 | 117.36 | 110.31 |
| 2 | 1 | 402 | ARG | N-CA-C | -5.73 | 105.49 | 112.88 |
| 7 | O | 1166 | HIS | CE1-NE2-CD2 | -5.73 | 103.27 | 109.00 |
| 7 | O | 1362 | ASP | CA-CB-CG | 5.73 | 118.33 | 112.60 |
| 1 | Y | 1340 | TRP | CA-C-O | -5.73 | 113.38 | 119.97 |
| 12 | v | 244 | ILE | N-CA-C | 5.73 | 117.15 | 110.62 |
| 12 | v | 436 | ASN | N-CA-C | -5.73 | 100.59 | 109.24 |
| 14 | h | 192 | VAL | CA-C-N | 5.73 | 129.93 | 120.94 |
| 14 | h | 192 | VAL | C-N-CA | 5.73 | 129.93 | 120.94 |
| 16 | c | 193 | GLU | N-CA-C | 5.73 | 117.60 | 111.36 |
| 16 | c | 545 | LYS | CA-C-O | 5.73 | 127.01 | 121.00 |
| 20 | g | 809 | LYS | CA-C-N | 5.73 | 131.08 | 123.00 |
| 20 | g | 809 | LYS | C-N-CA | 5.73 | 131.08 | 123.00 |
| 1 | 0 | 180 | ASN | CA-C-N | 5.73 | 131.23 | 122.93 |
| 1 | 0 | 180 | ASN | C-N-CA | 5.73 | 131.23 | 122.93 |
| 2 | 1 | 958 | ASN | N-CA-CB | 5.73 | 120.17 | 110.49 |
| 7 | O | 1292 | ARG | N-CA-C | 5.73 | 117.52 | 111.28 |
| 8 | P | 659 | GLU | CB-CG-CD | -5.73 | 102.87 | 112.60 |
| 9 | R | 418 | CYS | N-CA-C | -5.73 | 97.83 | 108.02 |
| 10 | U | 331 | ASN | CA-CB-CG | -5.73 | 106.87 | 112.60 |
| 2 | Z | 242 | HIS | CB-CG-ND1 | 5.73 | 131.29 | 122.70 |
| 12 | v | 332 | GLU | N-CA-C | -5.73 | 100.07 | 109.40 |
| 13 | w | 1298 | TYR | CA-C-N | 5.73 | 127.89 | 120.56 |
| 13 | w | 1298 | TYR | C-N-CA | 5.73 | 127.89 | 120.56 |
| 4 | G | 703 | GLN | OE1-CD-NE2 | -5.72 | 116.88 | 122.60 |
| 7 | M | 1628 | GLY | N-CA-C | -5.72 | 105.86 | 112.50 |
| 9 | S | 834 | ASN | N-CA-CB | 5.72 | 120.17 | 110.49 |
| 2 | Z | 847 | LEU | N-CA-C | -5.72 | 102.01 | 110.48 |
| 14 | h | 493 | TRP | CB-CG-CD2 | -5.72 | 118.78 | 126.80 |
| 16 | j | 455 | GLN | CG-CD-NE2 | -5.72 | 107.81 | 116.40 |
| 2 | 1 | 633 | HIS | CE1-NE2-CD2 | -5.72 | 103.28 | 109.00 |
| 9 | R | 236 | ASN | N-CA-C | 5.72 | 117.52 | 111.28 |
| 9 | R | 820 | ILE | CA-C-O | 5.72 | 125.58 | 119.91 |
| 12 | u | 117 | ASP | CA-CB-CG | 5.72 | 118.32 | 112.60 |
| 12 | u | 153 | MET | N-CA-C | -5.72 | 99.08 | 108.41 |
| 12 | u | 311 | GLN | CA-C-N | 5.72 | 132.47 | 121.54 |
| 12 | u | 311 | GLN | C-N-CA | 5.72 | 132.47 | 121.54 |
| 13 | x | 1401 | LEU | CB-CA-C | -5.72 | 101.90 | 110.88 |
| 21 | o | 75 | HIS | CB-CG-ND1 | 5.72 | 131.28 | 122.70 |
| 5 | B | 288 | ILE | N-CA-C | -5.72 | 107.17 | 112.83 |
| 8 | P | 876 | LEU | O-C-N | -5.72 | 115.86 | 122.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1019 | THR | CA-C-N | 5.72 | 130.39 | 121.35 |
| 8 | P | 1019 | THR | C-N-CA | 5.72 | 130.39 | 121.35 |
| 9 | S | 759 | ASP | CA-C-N | 5.72 | 129.00 | 120.31 |
| 9 | S | 759 | ASP | C-N-CA | 5.72 | 129.00 | 120.31 |
| 12 | u | 285 | PHE | O-C-N | -5.72 | 115.83 | 122.87 |
| 12 | v | 569 | LYS | CA-C-N | 5.72 | 128.30 | 120.46 |
| 12 | v | 569 | LYS | C-N-CA | 5.72 | 128.30 | 120.46 |
| 17 | d | 182 | VAL | CA-C-O | 5.72 | 127.15 | 121.09 |
| 20 | g | 801 | CYS | CA-C-N | 5.72 | 128.30 | 120.46 |
| 20 | g | 801 | CYS | C-N-CA | 5.72 | 128.30 | 120.46 |
| 2 | 1 | 370 | SER | N-CA-C | -5.72 | 101.64 | 109.71 |
| 7 | M | 1157 | TRP | O-C-N | 5.72 | 127.96 | 122.07 |
| 8 | N | 374 | VAL | N-CA-C | -5.72 | 107.19 | 113.43 |
| 7 | O | 1119 | PHE | CB-CA-C | -5.72 | 98.50 | 110.17 |
| 7 | O | 1300 | LEU | N-CA-CB | 5.72 | 119.44 | 109.72 |
| 1 | Y | 148 | PHE | CA-C-O | 5.72 | 127.44 | 121.38 |
| 14 | h | 387 | VAL | CA-C-O | 5.72 | 125.86 | 120.14 |
| 18 | l | 45 | TRP | CG-CD2-CE3 | -5.72 | 128.18 | 133.90 |
| 19 | m | 147 | SER | CA-C-N | 5.72 | 129.67 | 121.55 |
| 19 | m | 147 | SER | C-N-CA | 5.72 | 129.67 | 121.55 |
| 21 | t | 22 | GLU | CA-C-N | 5.72 | 127.94 | 120.28 |
| 21 | t | 22 | GLU | C-N-CA | 5.72 | 127.94 | 120.28 |
| 19 | f | 114 | LYS | CB-CA-C | -5.72 | 101.50 | 110.94 |
| 19 | f | 221 | PRO | N-CA-C | -5.72 | 106.68 | 114.80 |
| 20 | g | 528 | GLU | O-C-N | 5.72 | 130.26 | 122.37 |
| 14 | a | 81 | PHE | O-C-N | -5.72 | 116.64 | 123.27 |
| 1 | 0 | 577 | PHE | O-C-N | -5.72 | 116.62 | 123.31 |
| 8 | N | 70 | LYS | N-CA-CB | 5.72 | 120.15 | 110.49 |
| 7 | O | 480 | ARG | N-CA-C | 5.72 | 117.51 | 111.28 |
| 9 | Q | 329 | ASN | N-CA-C | 5.72 | 119.32 | 111.54 |
| 9 | T | 438 | MET | CG-SD-CE | -5.72 | 88.32 | 100.90 |
| 19 | m | 687 | ALA | N-CA-CB | 5.72 | 120.15 | 110.49 |
| 20 | n | 529 | HIS | CA-C-N | 5.72 | 131.81 | 121.92 |
| 20 | n | 529 | HIS | C-N-CA | 5.72 | 131.81 | 121.92 |
| 1 | 0 | 832 | VAL | CA-CB-CG1 | 5.72 | 120.12 | 110.40 |
| 1 | 0 | 1089 | LEU | CA-C-N | 5.72 | 130.88 | 121.39 |
| 1 | 0 | 1089 | LEU | C-N-CA | 5.72 | 130.88 | 121.39 |
| 4 | G | 637 | LEU | CA-C-N | 5.72 | 128.21 | 120.44 |
| 4 | G | 637 | LEU | C-N-CA | 5.72 | 128.21 | 120.44 |
| 9 | Q | 123 | MET | N-CA-C | 5.72 | 117.19 | 111.07 |
| 9 | Q | 262 | SER | N-CA-C | -5.72 | 105.04 | 113.61 |
| 9 | Q | 441 | MET | CA-C-N | 5.72 | 132.46 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | Q | 441 | MET | C-N-CA | 5.72 | 132.46 | 121.54 |
| 9 | S | 91 | GLN | CA-C-O | -5.72 | 114.82 | 120.82 |
| 9 | S | 325 | LEU | N-CA-C | -5.72 | 99.73 | 108.76 |
| 1 | Y | 856 | TYR | N-CA-CB | -5.72 | 101.98 | 110.61 |
| 14 | h | 912 | ASP | CA-CB-CG | -5.72 | 106.88 | 112.60 |
| 16 | j | 271 | TRP | CB-CG-CD1 | -5.72 | 118.33 | 126.90 |
| 20 | g | 525 | GLU | N-CA-CB | 5.72 | 118.44 | 109.69 |
| 1 | 0 | 162 | HIS | CA-C-N | 5.71 | 128.41 | 120.29 |
| 1 | 0 | 162 | HIS | C-N-CA | 5.71 | 128.41 | 120.29 |
| 2 | 1 | 904 | TYR | CA-C-N | 5.71 | 128.51 | 120.28 |
| 2 | 1 | 904 | TYR | C-N-CA | 5.71 | 128.51 | 120.28 |
| 5 | B | 329 | HIS | N-CA-C | 5.71 | 122.97 | 110.80 |
| 5 | K | 383 | SER | CA-C-N | 5.71 | 131.14 | 121.14 |
| 5 | K | 383 | SER | C-N-CA | 5.71 | 131.14 | 121.14 |
| 7 | M | 1496 | ASP | O-C-N | -5.71 | 116.62 | 123.31 |
| 7 | O | 3 | TRP | CA-C-O | -5.71 | 114.49 | 119.18 |
| 9 | T | 276 | GLN | O-C-N | -5.71 | 114.99 | 122.59 |
| 20 | n | 662 | ASN | CA-CB-CG | 5.71 | 118.31 | 112.60 |
| 20 | n | 973 | LYS | N-CA-C | -5.71 | 105.23 | 114.09 |
| 21 | o | 78 | TYR | N-CA-C | -5.71 | 98.97 | 108.34 |
| 20 | g | 717 | CYS | N-CA-C | -5.71 | 105.95 | 114.64 |
| 1 | 0 | 192 | LEU | N-CA-C | -5.71 | 100.58 | 109.72 |
| 1 | 0 | 1154 | ASP | N-CA-CB | 5.71 | 120.14 | 110.49 |
| 8 | N | 839 | ILE | N-CA-C | -5.71 | 107.27 | 111.90 |
| 7 | O | 197 | LEU | O-C-N | 5.71 | 128.19 | 122.08 |
| 1 | Y | 362 | ASP | N-CA-C | -5.71 | 99.88 | 108.96 |
| 1 | Y | 1294 | ILE | N-CA-CB | 5.71 | 119.13 | 112.33 |
| 2 | Z | 840 | THR | CA-C-N | 5.71 | 127.94 | 120.28 |
| 2 | Z | 840 | THR | C-N-CA | 5.71 | 127.94 | 120.28 |
| 1 | 0 | 269 | ASP | CA-CB-CG | 5.71 | 118.31 | 112.60 |
| 7 | M | 64 | PHE | N-CA-CB | 5.71 | 120.25 | 111.46 |
| 7 | M | 1465 | GLN | CA-C-N | 5.71 | 128.40 | 120.29 |
| 7 | M | 1465 | GLN | C-N-CA | 5.71 | 128.40 | 120.29 |
| 9 | Q | 677 | PRO | N-CA-CB | 5.71 | 109.25 | 103.25 |
| 2 | Z | 974 | ILE | N-CA-C | 5.71 | 116.36 | 110.36 |
| 2 | Z | 1345 | TRP | CE2-CD2-CE3 | 5.71 | 124.51 | 118.80 |
| 20 | g | 345 | GLN | OE1-CD-NE2 | -5.71 | 116.89 | 122.60 |
| 14 | a | 389 | LEU | CA-C-N | 5.71 | 131.51 | 122.60 |
| 14 | a | 389 | LEU | C-N-CA | 5.71 | 131.51 | 122.60 |
| 2 | 1 | 1181 | THR | N-CA-C | -5.71 | 105.90 | 112.92 |
| 5 | B | 319 | THR | CA-C-N | 5.71 | 132.45 | 121.54 |
| 5 | B | 319 | THR | C-N-CA | 5.71 | 132.45 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 365 | LEU | N-CA-C | 5.71 | 118.28 | 111.71 |
| 9 | Q | 302 | VAL | N-CA-C | 5.71 | 118.19 | 111.05 |
| 9 | T | 61 | LYS | CA-C-N | 5.71 | 130.34 | 121.26 |
| 9 | T | 61 | LYS | C-N-CA | 5.71 | 130.34 | 121.26 |
| 2 | Z | 929 | ASP | N-CA-C | 5.71 | 119.78 | 113.21 |
| 12 | u | 400 | SER | CA-C-O | 5.71 | 129.17 | 122.03 |
| 14 | h | 501 | THR | N-CA-C | -5.71 | 104.51 | 113.02 |
| 16 | c | 551 | ASN | CB-CA-C | -5.71 | 103.28 | 112.07 |
| 19 | f | 232 | ASN | CA-C-O | 5.71 | 124.80 | 118.52 |
| 5 | K | 469 | ARG | NE-CZ-NH1 | 5.71 | 127.21 | 121.50 |
| 8 | N | 1385 | LEU | CA-C-N | 5.71 | 128.19 | 120.65 |
| 8 | N | 1385 | LEU | C-N-CA | 5.71 | 128.19 | 120.65 |
| 8 | N | 1519 | CYS | N-CA-C | 5.71 | 117.50 | 111.28 |
| 8 | N | 1555 | VAL | CA-C-N | 5.71 | 127.93 | 120.28 |
| 8 | N | 1555 | VAL | C-N-CA | 5.71 | 127.93 | 120.28 |
| 7 | O | 48 | ARG | CA-C-N | 5.71 | 127.86 | 120.44 |
| 7 | O | 48 | ARG | C-N-CA | 5.71 | 127.86 | 120.44 |
| 8 | P | 15 | PHE | CA-C-N | 5.71 | 132.44 | 121.54 |
| 8 | P | 15 | PHE | C-N-CA | 5.71 | 132.44 | 121.54 |
| 8 | P | 1042 | SER | N-CA-C | -5.71 | 106.32 | 113.28 |
| 9 | Q | 466 | ILE | CA-C-N | 5.71 | 131.72 | 122.76 |
| 9 | Q | 466 | ILE | C-N-CA | 5.71 | 131.72 | 122.76 |
| 9 | R | 438 | MET | N-CA-C | 5.71 | 117.19 | 110.97 |
| 1 | Y | 1418 | THR | O-C-N | 5.71 | 129.89 | 123.27 |
| 2 | Z | 214 | PHE | CA-CB-CG | -5.71 | 108.09 | 113.80 |
| 14 | h | 750 | LEU | CA-C-N | 5.71 | 129.82 | 120.63 |
| 14 | h | 750 | LEU | C-N-CA | 5.71 | 129.82 | 120.63 |
| 19 | m | 552 | ARG | CA-C-O | 5.71 | 126.03 | 119.35 |
| 20 | n | 850 | TYR | CB-CG-CD1 | 5.71 | 129.36 | 120.80 |
| 17 | d | 270 | ALA | N-CA-C | -5.71 | 98.20 | 108.48 |
| 20 | g | 229 | PHE | N-CA-C | -5.71 | 99.98 | 109.46 |
| 20 | g | 304 | PRO | N-CA-CB | 5.71 | 108.38 | 103.36 |
| 20 | g | 728 | ALA | CB-CA-C | -5.71 | 101.15 | 110.85 |
| 5 | H | 436 | MET | CA-C-O | -5.71 | 114.37 | 120.42 |
| 8 | P | 135 | PHE | N-CA-C | -5.71 | 106.17 | 113.02 |
| 8 | P | 673 | SER | CA-C-N | 5.71 | 128.20 | 120.38 |
| 8 | P | 673 | SER | C-N-CA | 5.71 | 128.20 | 120.38 |
| 9 | Q | 456 | ARG | NE-CZ-NH2 | -5.71 | 114.06 | 119.20 |
| 1 | Y | 111 | LEU | O-C-N | -5.71 | 116.07 | 122.12 |
| 2 | Z | 457 | SER | CA-C-O | -5.71 | 111.10 | 120.80 |
| 2 | Z | 1113 | ASP | CA-C-N | 5.71 | 127.75 | 120.56 |
| 2 | Z | 1113 | ASP | C-N-CA | 5.71 | 127.75 | 120.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 169 | VAL | CA-CB-CG2 | -5.71 | 100.70 | 110.40 |
| 14 | h | 378 | TRP | O-C-N | 5.71 | 129.83 | 122.81 |
| 18 | l | 32 | HIS | CE1-NE2-CD2 | -5.71 | 103.29 | 109.00 |
| 2 | 1 | 946 | GLU | CA-C-N | 5.71 | 128.50 | 120.28 |
| 2 | 1 | 946 | GLU | C-N-CA | 5.71 | 128.50 | 120.28 |
| 2 | Z | 581 | SER | N-CA-C | -5.71 | 106.36 | 113.38 |
| 12 | u | 690 | ASP | O-C-N | 5.71 | 128.65 | 122.15 |
| 14 | h | 153 | GLN | O-C-N | 5.71 | 129.78 | 123.33 |
| 14 | h | 383 | ASN | N-CA-C | -5.71 | 105.63 | 112.59 |
| 18 | l | 167 | SER | N-CA-C | -5.71 | 100.99 | 109.83 |
| 18 | l | 240 | ILE | N-CA-C | -5.71 | 100.12 | 108.11 |
| 1 | 0 | 671 | LEU | N-CA-CB | 5.70 | 119.20 | 110.70 |
| 2 | 1 | 153 | GLN | CA-C-O | -5.70 | 112.53 | 119.32 |
| 6 | I | 398 | VAL | CA-C-N | 5.70 | 127.92 | 120.28 |
| 6 | I | 398 | VAL | C-N-CA | 5.70 | 127.92 | 120.28 |
| 19 | m | 399 | ILE | N-CA-CB | 5.70 | 117.48 | 110.64 |
| 19 | m | 611 | SER | CA-C-N | 5.70 | 132.43 | 121.54 |
| 19 | m | 611 | SER | C-N-CA | 5.70 | 132.43 | 121.54 |
| 21 | r | 58 | HIS | CE1-NE2-CD2 | -5.70 | 103.30 | 109.00 |
| 15 | b | 510 | HIS | CG-CD2-NE2 | 5.70 | 112.90 | 107.20 |
| 16 | c | 135 | ALA | N-CA-C | 5.70 | 118.44 | 111.82 |
| 20 | g | 949 | TYR | CA-C-O | -5.70 | 113.66 | 120.10 |
| 14 | a | 994 | ILE | O-C-N | 5.70 | 127.83 | 121.90 |
| 8 | N | 1218 | SER | N-CA-C | -5.70 | 98.66 | 110.80 |
| 7 | O | 1190 | TYR | O-C-N | 5.70 | 129.88 | 122.87 |
| 9 | R | 650 | TYR | N-CA-CB | 5.70 | 119.91 | 111.01 |
| 1 | Y | 1199 | ILE | N-CA-C | -5.70 | 107.18 | 112.43 |
| 17 | k | 221 | TYR | O-C-N | -5.70 | 116.59 | 123.03 |
| 20 | n | 938 | ASN | N-CA-C | -5.70 | 104.09 | 113.50 |
| 2 | 1 | 1065 | ALA | O-C-N | 5.70 | 128.19 | 122.03 |
| 4 | D | 655 | PHE | O-C-N | 5.70 | 128.65 | 122.15 |
| 6 | F | 318 | SER | CB-CA-C | -5.70 | 101.33 | 110.79 |
| 7 | M | 1021 | HIS | O-C-N | -5.70 | 116.16 | 122.09 |
| 8 | N | 1613 | ASN | O-C-N | 5.70 | 127.94 | 122.07 |
| 9 | R | 229 | ASN | CA-CB-CG | 5.70 | 118.30 | 112.60 |
| 9 | S | 367 | PHE | CA-CB-CG | -5.70 | 108.10 | 113.80 |
| 9 | S | 371 | PHE | CA-C-O | 5.70 | 126.59 | 120.55 |
| 1 | Y | 113 | HIS | O-C-N | -5.70 | 116.20 | 122.07 |
| 1 | Y | 657 | GLU | CA-C-N | 5.70 | 128.27 | 120.46 |
| 1 | Y | 657 | GLU | C-N-CA | 5.70 | 128.27 | 120.46 |
| 2 | Z | 219 | GLU | CA-C-N | 5.70 | 132.43 | 121.54 |
| 2 | Z | 219 | GLU | C-N-CA | 5.70 | 132.43 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 1110 | ARG | N-CA-CB | 5.70 | 118.60 | 110.16 |
| 14 | a | 954 | ARG | N-CA-CB | 5.70 | 118.28 | 110.01 |
| 1 | 0 | 986 | THR | N-CA-C | 5.70 | 118.43 | 111.82 |
| 7 | M | 1627 | LYS | CA-C-N | 5.70 | 126.27 | 119.94 |
| 7 | M | 1627 | LYS | C-N-CA | 5.70 | 126.27 | 119.94 |
| 7 | O | 1493 | LYS | CA-C-O | 5.70 | 126.59 | 120.55 |
| 9 | R | 535 | ALA | O-C-N | 5.70 | 129.97 | 122.33 |
| 10 | U | 263 | ALA | CA-C-O | -5.70 | 114.51 | 120.55 |
| 13 | w | 1441 | LEU | N-CA-C | 5.70 | 117.49 | 111.28 |
| 4 | y | 639 | ASP | CB-CA-C | -5.70 | 101.93 | 110.88 |
| 21 | q | 75 | HIS | ND1-CE1-NE2 | 5.70 | 114.10 | 108.40 |
| 14 | a | 957 | ASP | N-CA-C | -5.70 | 98.66 | 110.80 |
| 2 | 1 | 1286 | HIS | ND1-CE1-NE2 | 5.70 | 114.10 | 108.40 |
| 8 | N | 591 | MET | CG-SD-CE | -5.70 | 88.37 | 100.90 |
| 8 | N | 770 | HIS | CE1-NE2-CD2 | -5.70 | 103.30 | 109.00 |
| 7 | O | 835 | LYS | N-CA-CB | 5.70 | 120.12 | 110.49 |
| 2 | Z | 613 | CYS | N-CA-C | -5.70 | 100.85 | 109.85 |
| 12 | v | 698 | ASN | O-C-N | 5.70 | 127.94 | 122.07 |
| 14 | h | 958 | TRP | O-C-N | 5.70 | 130.08 | 123.41 |
| 15 | i | 307 | LYS | CB-CA-C | 5.70 | 120.53 | 110.85 |
| 17 | k | 88 | ARG | N-CA-C | -5.70 | 100.40 | 109.23 |
| 5 | H | 324 | TYR | CA-CB-CG | 5.70 | 124.15 | 113.90 |
| 9 | Q | 154 | GLU | CA-C-N | 5.70 | 127.74 | 120.56 |
| 9 | Q | 154 | GLU | C-N-CA | 5.70 | 127.74 | 120.56 |
| 9 | T | 53 | VAL | CB-CA-C | -5.70 | 105.64 | 112.19 |
| 9 | T | 773 | ASN | N-CA-CB | 5.70 | 118.27 | 110.01 |
| 1 | Y | 380 | TYR | CB-CG-CD2 | 5.70 | 129.34 | 120.80 |
| 1 | Y | 939 | ASP | N-CA-C | 5.70 | 117.49 | 111.28 |
| 12 | u | 362 | SER | O-C-N | -5.70 | 118.28 | 123.41 |
| 14 | h | 200 | ASN | CA-CB-CG | 5.70 | 118.30 | 112.60 |
| 17 | k | 10 | GLU | N-CA-C | -5.70 | 106.00 | 113.12 |
| 16 | c | 241 | PHE | CA-CB-CG | -5.70 | 108.10 | 113.80 |
| 16 | c | 265 | HIS | ND1-CE1-NE2 | 5.70 | 114.09 | 108.40 |
| 8 | N | 975 | GLN | N-CA-C | -5.69 | 100.29 | 108.60 |
| 18 | l | 191 | ALA | CA-C-N | 5.69 | 129.77 | 121.80 |
| 18 | l | 191 | ALA | C-N-CA | 5.69 | 129.77 | 121.80 |
| 15 | b | 194 | GLY | O-C-N | 5.69 | 129.38 | 122.32 |
| 2 | 1 | 1319 | LEU | CA-C-N | 5.69 | 130.22 | 120.72 |
| 2 | 1 | 1319 | LEU | C-N-CA | 5.69 | 130.22 | 120.72 |
| 8 | N | 614 | ILE | CA-C-O | -5.69 | 114.32 | 120.47 |
| 9 | T | 158 | ASN | CB-CA-C | -5.69 | 101.91 | 110.90 |
| 9 | T | 340 | LEU | N-CA-C | 5.69 | 118.42 | 111.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 180 | LEU | N-CA-CB | 5.69 | 118.83 | 110.35 |
| 2 | Z | 444 | GLY | CA-C-N | 5.69 | 130.31 | 121.26 |
| 2 | Z | 444 | GLY | C-N-CA | 5.69 | 130.31 | 121.26 |
| 12 | u | 27 | PHE | N-CA-CB | 5.69 | 122.12 | 111.53 |
| 15 | b | 427 | LYS | N-CA-C | -5.69 | 104.56 | 112.30 |
| 1 | 0 | 225 | VAL | N-CA-C | -5.69 | 101.51 | 107.60 |
| 4 | D | 763 | SER | N-CA-C | 5.69 | 117.56 | 111.36 |
| 7 | M | 356 | ILE | CB-CA-C | 5.69 | 116.58 | 111.00 |
| 7 | M | 766 | GLN | N-CA-CB | 5.69 | 118.90 | 110.53 |
| 7 | M | 785 | TYR | O-C-N | -5.69 | 115.56 | 122.22 |
| 8 | N | 1076 | SER | CA-C-O | -5.69 | 114.85 | 120.82 |
| 9 | R | 76 | SER | CB-CA-C | -5.69 | 99.10 | 110.42 |
| 11 | X | 270 | ALA | CB-CA-C | -5.69 | 99.54 | 110.24 |
| 2 | Z | 428 | THR | N-CA-C | -5.69 | 104.54 | 113.02 |
| 12 | v | 142 | ILE | CA-C-N | 5.69 | 130.01 | 122.95 |
| 12 | v | 142 | ILE | C-N-CA | 5.69 | 130.01 | 122.95 |
| 19 | m | 170 | ASP | CA-C-N | 5.69 | 129.97 | 120.64 |
| 19 | m | 170 | ASP | C-N-CA | 5.69 | 129.97 | 120.64 |
| 19 | m | 546 | LEU | N-CA-C | -5.69 | 104.54 | 113.02 |
| 15 | b | 156 | GLU | O-C-N | 5.69 | 128.24 | 122.09 |
| 4 | J | 810 | ASN | CA-C-N | 5.69 | 127.84 | 120.44 |
| 4 | J | 810 | ASN | C-N-CA | 5.69 | 127.84 | 120.44 |
| 8 | P | 475 | TYR | CB-CG-CD1 | 5.69 | 129.33 | 120.80 |
| 13 | w | 1310 | VAL | CA-C-O | -5.69 | 115.03 | 120.95 |
| 20 | n | 305 | THR | OG1-CB-CG2 | 5.69 | 120.68 | 109.30 |
| 19 | f | 291 | ASN | CA-C-O | -5.69 | 114.52 | 120.55 |
| 1 | 0 | 1443 | VAL | CB-CA-C | -5.69 | 104.69 | 111.97 |
| 2 | 1 | 365 | SER | O-C-N | -5.69 | 116.73 | 123.22 |
| 2 | 1 | 1222 | ILE | CA-C-O | -5.69 | 114.82 | 120.85 |
| 4 | J | 702 | ARG | CB-CG-CD | 5.69 | 124.38 | 111.30 |
| 7 | M | 48 | ARG | CA-C-N | 5.69 | 127.83 | 120.44 |
| 7 | M | 48 | ARG | C-N-CA | 5.69 | 127.83 | 120.44 |
| 8 | N | 56 | ASN | CB-CG-ND2 | -5.69 | 107.87 | 116.40 |
| 8 | N | 444 | ASN | OD1-CG-ND2 | 5.69 | 128.29 | 122.60 |
| 9 | Q | 67 | THR | CA-C-N | 5.69 | 127.90 | 120.28 |
| 9 | Q | 67 | THR | C-N-CA | 5.69 | 127.90 | 120.28 |
| 9 | Q | 371 | PHE | CA-CB-CG | -5.69 | 108.11 | 113.80 |
| 10 | W | 262 | ILE | N-CA-C | -5.69 | 106.77 | 112.17 |
| 2 | Z | 640 | ALA | O-C-N | 5.69 | 128.63 | 122.15 |
| 13 | x | 1431 | MET | CA-C-N | 5.69 | 127.83 | 120.44 |
| 13 | x | 1431 | MET | C-N-CA | 5.69 | 127.83 | 120.44 |
| 4 | z | 640 | LEU | N-CA-C | 5.69 | 117.16 | 111.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 715 | THR | CA-C-N | 5.69 | 132.41 | 121.54 |
| 14 | h | 715 | THR | C-N-CA | 5.69 | 132.41 | 121.54 |
| 18 | e | 105 | ASN | CB-CG-OD1 | 5.69 | 132.18 | 120.80 |
| 14 | a | 615 | SER | N-CA-C | -5.69 | 106.38 | 113.38 |
| 4 | J | 754 | ASN | CA-C-O | -5.69 | 114.52 | 120.55 |
| 14 | h | 233 | TYR | CB-CG-CD2 | -5.69 | 112.27 | 120.80 |
| 17 | d | 249 | LYS | N-CA-C | -5.69 | 100.71 | 109.52 |
| 18 | e | 106 | ASP | N-CA-CB | 5.69 | 120.10 | 110.49 |
| 20 | g | 635 | VAL | CA-C-N | 5.69 | 129.76 | 121.80 |
| 20 | g | 635 | VAL | C-N-CA | 5.69 | 129.76 | 121.80 |
| 2 | 1 | 1249 | PRO | N-CA-CB | 5.68 | 109.81 | 103.44 |
| 9 | S | 555 | GLU | N-CA-C | 5.68 | 117.15 | 111.07 |
| 2 | Z | 209 | PRO | CB-CA-C | 5.68 | 118.79 | 111.46 |
| 20 | n | 470 | LYS | N-CA-C | -5.68 | 106.51 | 113.50 |
| 16 | c | 180 | GLN | CA-C-O | 5.68 | 126.27 | 120.24 |
| 20 | g | 987 | LEU | CA-C-N | 5.68 | 127.72 | 120.56 |
| 20 | g | 987 | LEU | C-N-CA | 5.68 | 127.72 | 120.56 |
| 2 | 1 | 340 | GLU | CA-C-N | 5.68 | 132.39 | 121.54 |
| 2 | 1 | 340 | GLU | C-N-CA | 5.68 | 132.39 | 121.54 |
| 2 | 1 | 913 | ALA | N-CA-CB | 5.68 | 120.09 | 110.49 |
| 6 | C | 303 | GLU | N-CA-C | -5.68 | 105.55 | 112.88 |
| 5 | H | 306 | THR | N-CA-CB | 5.68 | 119.63 | 110.42 |
| 9 | Q | 766 | ASN | CA-CB-CG | 5.68 | 118.28 | 112.60 |
| 9 | R | 22 | LEU | N-CA-CB | 5.68 | 118.25 | 110.01 |
| 9 | T | 247 | GLY | CA-C-O | -5.68 | 115.38 | 121.35 |
| 1 | Y | 1326 | LYS | N-CA-C | 5.68 | 119.47 | 112.54 |
| 16 | c | 319 | SER | N-CA-CB | -5.68 | 101.55 | 110.30 |
| 2 | 1 | 643 | THR | CA-CB-OG1 | 5.68 | 118.12 | 109.60 |
| 8 | P | 570 | GLN | N-CA-C | -5.68 | 105.93 | 112.92 |
| 9 | Q | 758 | GLN | N-CA-C | -5.68 | 104.93 | 112.94 |
| 1 | Y | 107 | TYR | CB-CA-C | 5.68 | 120.22 | 110.79 |
| 13 | w | 1352 | VAL | CA-C-N | 5.68 | 127.89 | 120.28 |
| 13 | w | 1352 | VAL | C-N-CA | 5.68 | 127.89 | 120.28 |
| 20 | g | 234 | ARG | NH1-CZ-NH2 | -5.68 | 111.92 | 119.30 |
| 1 | 0 | 236 | THR | CA-C-N | 5.68 | 129.69 | 120.60 |
| 1 | 0 | 236 | THR | C-N-CA | 5.68 | 129.69 | 120.60 |
| 2 | 1 | 946 | GLU | CA-C-O | 5.68 | 125.39 | 119.14 |
| 5 | K | 437 | TRP | CA-C-O | -5.68 | 111.84 | 119.11 |
| 7 | M | 31 | ASP | O-C-N | -5.68 | 115.68 | 122.15 |
| 7 | M | 1140 | GLU | CA-C-O | -5.68 | 115.15 | 121.23 |
| 7 | M | 1538 | LEU | CA-C-N | 5.68 | 129.60 | 121.02 |
| 7 | M | 1538 | LEU | C-N-CA | 5.68 | 129.60 | 121.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 937 | LEU | CA-C-N | 5.68 | 130.19 | 120.71 |
| 7 | O | 937 | LEU | C-N-CA | 5.68 | 130.19 | 120.71 |
| 7 | O | 1005 | PHE | CA-C-N | 5.68 | 127.89 | 120.28 |
| 7 | O | 1005 | PHE | C-N-CA | 5.68 | 127.89 | 120.28 |
| 8 | P | 111 | HIS | ND1-CG-CD2 | -5.68 | 100.42 | 106.10 |
| 9 | R | 644 | TYR | O-C-N | 5.68 | 128.14 | 122.12 |
| 11 | V | 373 | ASN | CA-C-N | 5.68 | 130.22 | 122.04 |
| 11 | V | 373 | ASN | C-N-CA | 5.68 | 130.22 | 122.04 |
| 17 | k | 288 | LYS | N-CA-CB | 5.68 | 118.38 | 109.69 |
| 21 | t | 76 | PHE | N-CA-C | 5.68 | 118.70 | 108.48 |
| 17 | d | 213 | SER | CA-C-O | -5.68 | 114.51 | 120.02 |
| 19 | f | 410 | SER | CA-C-O | 5.68 | 126.50 | 119.97 |
| 14 | a | 186 | LEU | N-CA-C | -5.68 | 97.98 | 107.80 |
| 5 | K | 385 | GLN | CA-C-N | 5.68 | 127.82 | 120.44 |
| 5 | K | 385 | GLN | C-N-CA | 5.68 | 127.82 | 120.44 |
| 6 | L | 456 | ARG | NE-CZ-NH2 | -5.68 | 114.09 | 119.20 |
| 9 | R | 643 | LEU | N-CA-C | 5.68 | 117.47 | 111.28 |
| 2 | Z | 438 | ILE | N-CA-CB | 5.68 | 119.67 | 110.13 |
| 16 | j | 635 | ASP | CA-CB-CG | 5.68 | 118.28 | 112.60 |
| 5 | B | 313 | TYR | CA-C-N | 5.68 | 129.54 | 121.42 |
| 5 | B | 313 | TYR | C-N-CA | 5.68 | 129.54 | 121.42 |
| 4 | D | 661 | LYS | CA-C-O | -5.68 | 114.86 | 120.82 |
| 5 | H | 469 | ARG | NE-CZ-NH2 | -5.68 | 114.09 | 119.20 |
| 6 | I | 356 | GLN | N-CA-C | -5.68 | 101.25 | 109.59 |
| 7 | O | 147 | ALA | N-CA-C | 5.68 | 117.47 | 111.28 |
| 7 | O | 518 | ASN | N-CA-C | -5.68 | 98.71 | 110.80 |
| 9 | Q | 564 | GLU | CA-C-N | 5.68 | 130.78 | 121.87 |
| 9 | Q | 564 | GLU | C-N-CA | 5.68 | 130.78 | 121.87 |
| 9 | S | 40 | GLY | N-CA-C | -5.68 | 99.73 | 113.18 |
| 9 | S | 823 | ARG | NE-CZ-NH2 | -5.68 | 114.09 | 119.20 |
| 9 | T | 276 | GLN | CA-C-N | 5.68 | 128.16 | 120.44 |
| 9 | T | 276 | GLN | C-N-CA | 5.68 | 128.16 | 120.44 |
| 11 | X | 388 | SER | O-C-N | -5.68 | 117.14 | 123.04 |
| 12 | u | 141 | CYS | CB-CA-C | -5.68 | 99.90 | 109.72 |
| 13 | x | 1359 | THR | CA-C-N | 5.68 | 127.82 | 120.44 |
| 13 | x | 1359 | THR | C-N-CA | 5.68 | 127.82 | 120.44 |
| 14 | h | 443 | LEU | N-CA-CB | 5.68 | 118.24 | 110.01 |
| 19 | m | 244 | ARG | CA-C-O | -5.68 | 114.53 | 120.55 |
| 15 | b | 403 | HIS | CE1-NE2-CD2 | -5.68 | 103.32 | 109.00 |
| 15 | b | 488 | LEU | CA-C-N | 5.68 | 128.24 | 120.46 |
| 15 | b | 488 | LEU | C-N-CA | 5.68 | 128.24 | 120.46 |
| 19 | f | 216 | GLN | OE1-CD-NE2 | 5.68 | 128.28 | 122.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 1122 | THR | CA-CB-OG1 | 5.68 | 118.11 | 109.60 |
| 1 | 0 | 530 | ILE | CB-CA-C | 5.67 | 118.46 | 111.25 |
| 1 | 0 | 1160 | HIS | CA-C-N | 5.67 | 127.89 | 120.28 |
| 1 | 0 | 1160 | HIS | C-N-CA | 5.67 | 127.89 | 120.28 |
| 1 | 0 | 1320 | ILE | N-CA-C | -5.67 | 106.24 | 113.22 |
| 7 | O | 241 | PHE | N-CA-CB | 5.67 | 119.04 | 110.30 |
| 9 | S | 824 | MET | CA-C-O | -5.67 | 115.12 | 120.34 |
| 9 | T | 640 | SER | CB-CA-C | -5.67 | 101.37 | 110.79 |
| 1 | Y | 1437 | SER | N-CA-CB | 5.67 | 119.50 | 110.65 |
| 2 | Z | 882 | ASP | O-C-N | -5.67 | 115.29 | 122.27 |
| 12 | v | 420 | ILE | N-CA-CB | 5.67 | 117.12 | 110.82 |
| 14 | h | 371 | GLU | CA-C-N | 5.67 | 128.82 | 120.82 |
| 14 | h | 371 | GLU | C-N-CA | 5.67 | 128.82 | 120.82 |
| 14 | h | 931 | ASP | N-CA-CB | 5.67 | 118.92 | 110.29 |
| 18 | l | 37 | LYS | CA-C-N | 5.67 | 129.41 | 121.24 |
| 18 | l | 37 | LYS | C-N-CA | 5.67 | 129.41 | 121.24 |
| 19 | f | 391 | HIS | CA-C-N | 5.67 | 128.35 | 120.29 |
| 19 | f | 391 | HIS | C-N-CA | 5.67 | 128.35 | 120.29 |
| 20 | g | 389 | SER | CA-C-N | 5.67 | 128.70 | 120.98 |
| 20 | g | 389 | SER | C-N-CA | 5.67 | 128.70 | 120.98 |
| 18 | e | 59 | VAL | CA-CB-CG2 | 5.67 | 120.05 | 110.40 |
| 4 | A | 819 | ASN | CA-CB-CG | 5.67 | 118.27 | 112.60 |
| 4 | G | 709 | ASN | CA-CB-CG | 5.67 | 118.27 | 112.60 |
| 5 | H | 362 | ASN | CA-C-O | -5.67 | 114.54 | 120.55 |
| 9 | S | 210 | GLU | O-C-N | 5.67 | 127.91 | 122.07 |
| 9 | T | 586 | PHE | CA-CB-CG | 5.67 | 119.47 | 113.80 |
| 10 | U | 279 | ASP | CB-CA-C | 5.67 | 119.85 | 111.06 |
| 1 | Y | 519 | THR | CA-CB-OG1 | 5.67 | 118.11 | 109.60 |
| 1 | Y | 911 | ASN | OD1-CG-ND2 | 5.67 | 128.27 | 122.60 |
| 20 | n | 586 | ASP | O-C-N | -5.67 | 114.87 | 122.19 |
| 1 | 0 | 896 | MET | N-CA-C | 5.67 | 117.46 | 111.28 |
| 1 | 0 | 1209 | LYS | O-C-N | -5.67 | 116.32 | 123.12 |
| 2 | 1 | 199 | HIS | ND1-CE1-NE2 | 5.67 | 114.07 | 108.40 |
| 4 | A | 664 | SER | N-CA-C | -5.67 | 105.18 | 111.36 |
| 12 | u | 151 | ILE | N-CA-CB | 5.67 | 118.60 | 111.46 |
| 12 | v | 174 | GLY | N-CA-C | -5.67 | 99.74 | 113.18 |
| 16 | j | 328 | ASN | CA-C-O | 5.67 | 127.44 | 120.92 |
| 19 | f | 667 | LEU | N-CA-C | -5.67 | 105.10 | 111.28 |
| 6 | I | 329 | ASP | CB-CA-C | -5.67 | 101.98 | 110.88 |
| 7 | M | 1435 | LYS | N-CA-CB | 5.67 | 120.07 | 110.49 |
| 2 | Z | 789 | ASP | CA-CB-CG | 5.67 | 118.27 | 112.60 |
| 12 | u | 597 | GLU | N-CA-CB | 5.67 | 118.45 | 110.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 365 | ILE | N-CA-CB | 5.67 | 119.36 | 112.10 |
| 15 | b | 104 | PHE | CA-C-O | 5.67 | 126.77 | 120.82 |
| 15 | b | 461 | MET | N-CA-C | -5.67 | 104.58 | 113.02 |
| 1 | 0 | 199 | ASN | CA-C-N | 5.67 | 131.85 | 122.33 |
| 1 | 0 | 199 | ASN | C-N-CA | 5.67 | 131.85 | 122.33 |
| 2 | 1 | 813 | ASN | CA-C-N | 5.67 | 130.04 | 120.64 |
| 2 | 1 | 813 | ASN | C-N-CA | 5.67 | 130.04 | 120.64 |
| 2 | 1 | 908 | GLU | CA-C-N | 5.67 | 131.06 | 121.14 |
| 2 | 1 | 908 | GLU | C-N-CA | 5.67 | 131.06 | 121.14 |
| 5 | B | 347 | THR | CA-CB-OG1 | 5.67 | 118.10 | 109.60 |
| 4 | J | 809 | ASP | CA-C-N | 5.67 | 128.34 | 120.29 |
| 4 | J | 809 | ASP | C-N-CA | 5.67 | 128.34 | 120.29 |
| 6 | L | 463 | LYS | N-CA-CB | 5.67 | 118.22 | 110.01 |
| 7 | M | 1062 | SER | CA-C-N | 5.67 | 128.22 | 120.46 |
| 7 | M | 1062 | SER | C-N-CA | 5.67 | 128.22 | 120.46 |
| 8 | N | 143 | SER | CA-C-N | 5.67 | 128.47 | 120.42 |
| 8 | N | 143 | SER | C-N-CA | 5.67 | 128.47 | 120.42 |
| 7 | O | 475 | LYS | N-CA-C | 5.67 | 117.46 | 111.28 |
| 9 | S | 793 | LYS | O-C-N | -5.67 | 115.51 | 122.25 |
| 10 | W | 346 | SER | CB-CA-C | -5.67 | 101.72 | 110.62 |
| 1 | Y | 183 | TRP | CG-CD2-CE3 | -5.67 | 128.23 | 133.90 |
| 15 | i | 324 | ILE | CA-C-N | 5.67 | 128.75 | 120.71 |
| 15 | i | 324 | ILE | C-N-CA | 5.67 | 128.75 | 120.71 |
| 16 | j | 551 | ASN | CA-CB-CG | -5.67 | 106.93 | 112.60 |
| 17 | k | 13 | HIS | CG-CD2-NE2 | 5.67 | 112.87 | 107.20 |
| 21 | q | 68 | TYR | N-CA-C | -5.67 | 97.63 | 107.49 |
| 19 | f | 271 | ILE | CA-CB-CG1 | 5.67 | 120.03 | 110.40 |
| 6 | F | 313 | ALA | CA-C-N | 5.67 | 127.87 | 120.28 |
| 6 | F | 313 | ALA | C-N-CA | 5.67 | 127.87 | 120.28 |
| 7 | M | 1305 | SER | N-CA-C | 5.67 | 118.18 | 111.33 |
| 7 | O | 488 | PHE | CA-C-O | 5.67 | 128.61 | 120.51 |
| 7 | O | 845 | ASP | CA-CB-CG | 5.67 | 118.27 | 112.60 |
| 7 | O | 1021 | HIS | O-C-N | 5.67 | 128.12 | 122.12 |
| 9 | Q | 724 | ARG | CA-C-O | -5.67 | 113.45 | 119.97 |
| 2 | Z | 1290 | ASN | CA-C-O | 5.67 | 126.14 | 119.06 |
| 18 | l | 32 | HIS | CG-CD2-NE2 | 5.67 | 112.86 | 107.20 |
| 18 | l | 327 | LYS | O-C-N | -5.67 | 116.70 | 123.27 |
| 20 | g | 438 | SER | N-CA-C | -5.67 | 105.48 | 112.90 |
| 20 | g | 551 | ASN | OD1-CG-ND2 | 5.67 | 128.26 | 122.60 |
| 2 | 1 | 787 | ALA | N-CA-C | -5.66 | 100.17 | 109.40 |
| 8 | P | 1392 | PHE | CA-CB-CG | -5.66 | 108.14 | 113.80 |
| 11 | V | 293 | HIS | CE1-NE2-CD2 | -5.66 | 103.34 | 109.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | u | 213 | PRO | CA-C-O | -5.66 | 114.87 | 121.95 |
| 12 | v | 314 | ILE | N-CA-CB | 5.66 | 119.00 | 111.64 |
| 12 | v | 351 | ILE | CB-CA-C | -5.66 | 104.49 | 112.14 |
| 17 | k | 63 | HIS | ND1-CE1-NE2 | 5.66 | 114.06 | 108.40 |
| 19 | m | 73 | ARG | CA-C-N | 5.66 | 128.14 | 120.44 |
| 19 | m | 73 | ARG | C-N-CA | 5.66 | 128.14 | 120.44 |
| 16 | c | 468 | GLU | N-CA-CB | -5.66 | 101.76 | 110.20 |
| 20 | g | 818 | LEU | CA-C-N | 5.66 | 132.36 | 121.54 |
| 20 | g | 818 | LEU | C-N-CA | 5.66 | 132.36 | 121.54 |
| 14 | a | 361 | SER | N-CA-C | -5.66 | 100.52 | 108.96 |
| 10 | U | 318 | TYR | N-CA-C | -5.66 | 103.53 | 110.61 |
| 1 | Y | 315 | THR | N-CA-C | -5.66 | 98.74 | 110.80 |
| 2 | Z | 1012 | VAL | O-C-N | 5.66 | 127.46 | 121.91 |
| 1 | 0 | 1330 | PHE | CA-CB-CG | -5.66 | 108.14 | 113.80 |
| 2 | 1 | 646 | TYR | CB-CG-CD1 | -5.66 | 112.31 | 120.80 |
| 2 | 1 | 656 | HIS | CE1-NE2-CD2 | -5.66 | 103.34 | 109.00 |
| 4 | D | 700 | ILE | CA-CB-CG1 | 5.66 | 120.02 | 110.40 |
| 5 | H | 288 | ILE | N-CA-C | -5.66 | 107.36 | 112.12 |
| 7 | M | 925 | HIS | CA-CB-CG | -5.66 | 108.14 | 113.80 |
| 7 | M | 1224 | GLU | N-CA-C | 5.66 | 117.84 | 110.43 |
| 8 | P | 1050 | SER | N-CA-CB | 5.66 | 120.06 | 110.49 |
| 9 | R | 102 | LYS | N-CA-C | -5.66 | 105.96 | 112.92 |
| 9 | S | 289 | LEU | N-CA-C | -5.66 | 106.25 | 114.12 |
| 9 | S | 570 | GLU | N-CA-C | -5.66 | 105.72 | 113.30 |
| 2 | Z | 1250 | SER | O-C-N | -5.66 | 117.06 | 121.47 |
| 2 | Z | 1286 | HIS | ND1-CE1-NE2 | 5.66 | 114.06 | 108.40 |
| 12 | u | 532 | SER | N-CA-C | 5.66 | 117.45 | 111.28 |
| 14 | h | 796 | ASP | N-CA-C | -5.66 | 106.72 | 113.97 |
| 16 | j | 578 | PRO | N-CA-CB | -5.66 | 97.10 | 103.44 |
| 20 | n | 402 | PRO | N-CD-CG | -5.66 | 94.71 | 103.20 |
| 16 | c | 489 | HIS | N-CA-CB | 5.66 | 118.63 | 110.20 |
| 8 | N | 155 | ILE | CA-CB-CG1 | 5.66 | 120.02 | 110.40 |
| 8 | P | 48 | LYS | N-CA-C | -5.66 | 99.19 | 108.41 |
| 8 | P | 1389 | LEU | CA-C-N | 5.66 | 127.86 | 120.28 |
| 8 | P | 1389 | LEU | C-N-CA | 5.66 | 127.86 | 120.28 |
| 9 | S | 73 | LEU | O-C-N | 5.66 | 128.12 | 122.12 |
| 1 | Y | 957 | ASP | N-CA-C | -5.66 | 104.79 | 112.26 |
| 17 | k | 74 | SER | O-C-N | 5.66 | 129.20 | 123.26 |
| 18 | l | 192 | ILE | CA-C-O | 5.66 | 127.42 | 120.74 |
| 16 | c | 176 | PRO | CA-C-N | 5.66 | 128.75 | 120.71 |
| 16 | c | 176 | PRO | C-N-CA | 5.66 | 128.75 | 120.71 |
| 7 | O | 1328 | ILE | N-CA-CB | 5.66 | 120.56 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | Q | 280 | GLN | OE1-CD-NE2 | 5.66 | 128.26 | 122.60 |
| 14 | h | 8 | ASP | CA-C-O | 5.66 | 126.55 | 120.38 |
| 18 | l | 292 | LEU | CA-C-O | 5.66 | 127.42 | 120.92 |
| 21 | r | 21 | LYS | CA-C-N | 5.66 | 127.86 | 120.28 |
| 21 | r | 21 | LYS | C-N-CA | 5.66 | 127.86 | 120.28 |
| 20 | g | 1034 | LYS | CA-C-N | 5.66 | 127.86 | 120.28 |
| 20 | g | 1034 | LYS | C-N-CA | 5.66 | 127.86 | 120.28 |
| 1 | 0 | 110 | HIS | ND1-CE1-NE2 | 5.66 | 114.06 | 108.40 |
| 1 | 0 | 948 | ASP | N-CA-C | -5.66 | 103.45 | 110.41 |
| 2 | 1 | 1091 | SER | CA-C-O | 5.66 | 127.41 | 121.19 |
| 6 | L | 325 | TYR | CA-C-N | 5.66 | 127.86 | 120.28 |
| 6 | L | 325 | TYR | C-N-CA | 5.66 | 127.86 | 120.28 |
| 7 | M | 692 | TYR | CA-C-N | 5.66 | 128.42 | 120.28 |
| 7 | M | 692 | TYR | C-N-CA | 5.66 | 128.42 | 120.28 |
| 8 | N | 1047 | LEU | CA-C-O | -5.66 | 115.01 | 121.40 |
| 7 | O | 256 | HIS | CA-CB-CG | 5.66 | 119.46 | 113.80 |
| 7 | O | 1538 | LEU | CA-C-N | 5.66 | 129.56 | 121.02 |
| 7 | O | 1538 | LEU | C-N-CA | 5.66 | 129.56 | 121.02 |
| 14 | h | 527 | SER | N-CA-C | 5.66 | 119.44 | 112.54 |
| 21 | r | 50 | ASP | CB-CA-C | -5.66 | 101.40 | 110.79 |
| 15 | b | 398 | ILE | CA-C-N | 5.66 | 127.86 | 120.28 |
| 15 | b | 398 | ILE | C-N-CA | 5.66 | 127.86 | 120.28 |
| 18 | e | 51 | TRP | CA-CB-CG | 5.66 | 124.34 | 113.60 |
| 20 | g | 328 | HIS | CA-C-N | 5.66 | 127.21 | 120.14 |
| 20 | g | 328 | HIS | C-N-CA | 5.66 | 127.21 | 120.14 |
| 7 | O | 450 | LEU | N-CA-C | 5.65 | 118.17 | 111.33 |
| 8 | P | 805 | LEU | CA-C-O | -5.65 | 112.42 | 120.51 |
| 9 | T | 319 | SER | CA-C-N | 5.65 | 128.90 | 120.87 |
| 9 | T | 319 | SER | C-N-CA | 5.65 | 128.90 | 120.87 |
| 2 | Z | 560 | LEU | CA-C-N | 5.65 | 131.44 | 122.62 |
| 2 | Z | 560 | LEU | C-N-CA | 5.65 | 131.44 | 122.62 |
| 20 | g | 713 | ASP | CA-CB-CG | 5.65 | 118.25 | 112.60 |
| 14 | a | 442 | TYR | N-CA-C | -5.65 | 105.03 | 111.14 |
| 6 | C | 455 | GLU | N-CA-CB | 5.65 | 118.21 | 110.01 |
| 4 | G | 760 | SER | N-CA-C | 5.65 | 117.25 | 111.14 |
| 7 | O | 1038 | LEU | N-CA-C | 5.65 | 117.62 | 110.33 |
| 9 | Q | 132 | ALA | O-C-N | 5.65 | 127.89 | 122.07 |
| 9 | Q | 346 | ILE | CA-C-O | -5.65 | 115.07 | 120.95 |
| 9 | R | 246 | ASN | CA-C-N | 5.65 | 129.26 | 122.03 |
| 9 | R | 246 | ASN | C-N-CA | 5.65 | 129.26 | 122.03 |
| 9 | S | 647 | ALA | CA-C-N | 5.65 | 130.20 | 122.34 |
| 9 | S | 647 | ALA | C-N-CA | 5.65 | 130.20 | 122.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | T | 573 | HIS | ND1-CE1-NE2 | 5.65 | 114.05 | 108.40 |
| 2 | Z | 879 | THR | N-CA-CB | 5.65 | 120.04 | 110.49 |
| 12 | u | 658 | LEU | CA-C-O | 5.65 | 126.21 | 119.60 |
| 15 | b | 499 | ALA | CA-C-N | 5.65 | 127.79 | 120.44 |
| 15 | b | 499 | ALA | C-N-CA | 5.65 | 127.79 | 120.44 |
| 1 | 0 | 671 | LEU | N-CA-C | -5.65 | 106.28 | 112.72 |
| 7 | O | 1374 | LYS | CA-C-N | 5.65 | 126.10 | 119.94 |
| 7 | O | 1374 | LYS | C-N-CA | 5.65 | 126.10 | 119.94 |
| 10 | U | 348 | ALA | N-CA-C | -5.65 | 104.14 | 111.71 |
| 14 | h | 294 | GLU | CA-C-N | 5.65 | 132.33 | 121.54 |
| 14 | h | 294 | GLU | C-N-CA | 5.65 | 132.33 | 121.54 |
| 20 | n | 459 | GLY | N-CA-C | -5.65 | 99.79 | 113.18 |
| 17 | d | 136 | THR | CA-C-O | 5.65 | 127.41 | 121.19 |
| 5 | E | 510 | VAL | CA-C-N | 5.65 | 127.85 | 120.28 |
| 5 | E | 510 | VAL | C-N-CA | 5.65 | 127.85 | 120.28 |
| 1 | Y | 975 | ILE | O-C-N | -5.65 | 117.63 | 121.98 |
| 12 | v | 564 | LEU | CA-C-N | 5.65 | 127.78 | 120.44 |
| 12 | v | 564 | LEU | C-N-CA | 5.65 | 127.78 | 120.44 |
| 19 | f | 55 | ASN | CA-CB-CG | 5.65 | 118.25 | 112.60 |
| 1 | 0 | 854 | ILE | CA-C-N | 5.65 | 132.33 | 121.54 |
| 1 | 0 | 854 | ILE | C-N-CA | 5.65 | 132.33 | 121.54 |
| 7 | M | 186 | LEU | CA-C-N | 5.65 | 128.16 | 120.54 |
| 7 | M | 186 | LEU | C-N-CA | 5.65 | 128.16 | 120.54 |
| 8 | N | 297 | THR | N-CA-CB | 5.65 | 118.42 | 110.12 |
| 8 | N | 1192 | LEU | CA-C-N | 5.65 | 128.12 | 120.38 |
| 8 | N | 1192 | LEU | C-N-CA | 5.65 | 128.12 | 120.38 |
| 7 | O | 1425 | LYS | N-CA-CB | 5.65 | 118.16 | 109.91 |
| 7 | O | 1556 | ASP | N-CA-C | 5.65 | 122.29 | 109.81 |
| 8 | P | 796 | SER | O-C-N | -5.65 | 115.08 | 122.59 |
| 9 | T | 571 | LEU | CA-C-N | 5.65 | 127.78 | 120.44 |
| 9 | T | 571 | LEU | C-N-CA | 5.65 | 127.78 | 120.44 |
| 4 | y | 665 | TRP | CA-C-N | 5.65 | 127.85 | 120.28 |
| 4 | y | 665 | TRP | C-N-CA | 5.65 | 127.85 | 120.28 |
| 19 | m | 694 | VAL | CA-C-O | 5.65 | 125.50 | 119.91 |
| 20 | g | 862 | PHE | N-CA-C | -5.65 | 104.98 | 112.94 |
| 20 | g | 949 | TYR | O-C-N | 5.65 | 128.83 | 122.22 |
| 20 | g | 1079 | PRO | N-CA-C | 5.65 | 120.07 | 111.15 |
| 14 | a | 82 | TYR | N-CA-C | -5.65 | 99.08 | 108.23 |
| 8 | P | 1461 | ILE | N-CA-CB | 5.65 | 116.78 | 110.51 |
| 4 | y | 624 | PRO | N-CA-CB | 5.65 | 109.54 | 103.33 |
| 14 | h | 1005 | ASN | N-CA-C | -5.65 | 106.27 | 114.12 |
| 21 | p | 36 | GLN | OE1-CD-NE2 | 5.65 | 128.25 | 122.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 270 | VAL | CB-CA-C | 5.64 | 120.55 | 111.29 |
| 1 | 0 | 1160 | HIS | O-C-N | 5.64 | 128.58 | 122.15 |
| 1 | 0 | 1219 | ARG | NE-CZ-NH2 | -5.64 | 114.12 | 119.20 |
| 2 | 1 | 577 | PHE | CA-C-N | 5.64 | 128.73 | 120.71 |
| 2 | 1 | 577 | PHE | C-N-CA | 5.64 | 128.73 | 120.71 |
| 4 | G | 773 | SER | CB-CA-C | -5.64 | 101.42 | 110.79 |
| 7 | M | 719 | ILE | O-C-N | 5.64 | 129.38 | 122.72 |
| 7 | M | 1183 | TYR | CB-CG-CD2 | -5.64 | 112.33 | 120.80 |
| 7 | M | 1439 | GLU | N-CA-C | 5.64 | 117.88 | 111.11 |
| 8 | P | 506 | ALA | CA-C-N | 5.64 | 126.19 | 120.38 |
| 8 | P | 506 | ALA | C-N-CA | 5.64 | 126.19 | 120.38 |
| 8 | P | 1233 | PHE | N-CA-C | -5.64 | 105.60 | 112.88 |
| 9 | R | 162 | LEU | CA-C-N | 5.64 | 128.19 | 120.46 |
| 9 | R | 162 | LEU | C-N-CA | 5.64 | 128.19 | 120.46 |
| 9 | T | 435 | TRP | CA-C-O | -5.64 | 114.57 | 120.55 |
| 11 | X | 346 | LYS | N-CA-CB | 5.64 | 120.10 | 110.50 |
| 15 | i | 473 | LEU | N-CA-C | 5.64 | 117.11 | 111.07 |
| 19 | m | 281 | ASP | CA-CB-CG | 5.64 | 118.25 | 112.60 |
| 5 | H | 302 | ASN | N-CA-C | -5.64 | 103.82 | 111.55 |
| 5 | H | 449 | ASP | CA-CB-CG | 5.64 | 118.24 | 112.60 |
| 7 | M | 152 | HIS | CA-C-N | 5.64 | 127.78 | 120.44 |
| 7 | M | 152 | HIS | C-N-CA | 5.64 | 127.78 | 120.44 |
| 9 | S | 678 | ASP | N-CA-CB | 5.64 | 119.76 | 110.39 |
| 9 | S | 738 | GLN | CA-C-O | -5.64 | 113.26 | 120.31 |
| 9 | T | 94 | GLN | O-C-N | 5.64 | 128.10 | 122.12 |
| 10 | W | 338 | THR | CA-C-N | 5.64 | 128.88 | 120.87 |
| 10 | W | 338 | THR | C-N-CA | 5.64 | 128.88 | 120.87 |
| 2 | Z | 749 | ARG | O-C-N | -5.64 | 114.83 | 121.32 |
| 13 | w | 1123 | GLN | CA-C-N | 5.64 | 129.27 | 120.75 |
| 13 | w | 1123 | GLN | C-N-CA | 5.64 | 129.27 | 120.75 |
| 13 | w | 1353 | SER | N-CA-CB | 5.64 | 118.41 | 110.12 |
| 13 | w | 1364 | ASN | CA-C-N | 5.64 | 129.58 | 120.55 |
| 13 | w | 1364 | ASN | C-N-CA | 5.64 | 129.58 | 120.55 |
| 20 | g | 875 | PHE | CA-CB-CG | 5.64 | 119.44 | 113.80 |
| 6 | I | 292 | HIS | CG-CD2-NE2 | 5.64 | 112.84 | 107.20 |
| 9 | R | 338 | PHE | O-C-N | -5.64 | 114.77 | 122.33 |
| 9 | R | 770 | ASN | CA-CB-CG | -5.64 | 106.96 | 112.60 |
| 9 | S | 789 | LEU | CA-C-O | 5.64 | 126.46 | 119.97 |
| 9 | T | 434 | ASP | CA-CB-CG | 5.64 | 118.24 | 112.60 |
| 11 | V | 395 | LEU | N-CA-C | 5.64 | 117.51 | 111.36 |
| 20 | n | 447 | VAL | O-C-N | -5.64 | 117.11 | 123.03 |
| 14 | a | 314 | THR | CA-C-O | 5.64 | 127.96 | 121.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 696 | PHE | CA-C-N | 5.64 | 128.10 | 120.38 |
| 7 | M | 696 | PHE | C-N-CA | 5.64 | 128.10 | 120.38 |
| 9 | R | 352 | VAL | CA-C-N | 5.64 | 127.84 | 120.28 |
| 9 | R | 352 | VAL | C-N-CA | 5.64 | 127.84 | 120.28 |
| 11 | V | 289 | SER | CB-CA-C | -5.64 | 101.03 | 110.56 |
| 1 | Y | 211 | ILE | N-CA-C | -5.64 | 99.42 | 107.77 |
| 12 | v | 351 | ILE | O-C-N | 5.64 | 127.34 | 121.87 |
| 13 | w | 1338 | GLN | CA-C-O | -5.64 | 114.90 | 120.82 |
| 14 | h | 1001 | LEU | N-CA-C | -5.64 | 105.74 | 113.30 |
| 21 | r | 77 | VAL | CA-C-O | 5.64 | 126.26 | 120.96 |
| 15 | b | 145 | ASN | N-CA-C | -5.64 | 106.53 | 113.41 |
| 20 | g | 823 | GLN | CB-CG-CD | -5.64 | 103.01 | 112.60 |
| 14 | a | 133 | LEU | CA-C-N | 5.64 | 125.61 | 120.03 |
| 14 | a | 133 | LEU | C-N-CA | 5.64 | 125.61 | 120.03 |
| 1 | 0 | 1448 | MET | CA-C-N | 5.64 | 128.63 | 120.79 |
| 1 | 0 | 1448 | MET | C-N-CA | 5.64 | 128.63 | 120.79 |
| 7 | M | 194 | SER | O-C-N | 5.64 | 128.10 | 122.12 |
| 7 | M | 939 | THR | CA-C-N | 5.64 | 127.83 | 120.28 |
| 7 | M | 939 | THR | C-N-CA | 5.64 | 127.83 | 120.28 |
| 8 | N | 59 | ARG | N-CA-CB | 5.64 | 120.02 | 110.49 |
| 7 | O | 963 | ASN | CA-CB-CG | -5.64 | 106.96 | 112.60 |
| 9 | Q | 279 | GLU | CA-C-O | -5.64 | 114.89 | 120.70 |
| 10 | W | 347 | PRO | CA-C-O | -5.64 | 115.34 | 121.77 |
| 19 | f | 165 | ASN | N-CA-CB | 5.64 | 120.39 | 111.43 |
| 7 | O | 639 | LEU | N-CA-C | 5.64 | 117.42 | 111.28 |
| 8 | P | 732 | LYS | CA-C-O | -5.64 | 114.58 | 120.55 |
| 2 | Z | 271 | GLN | OE1-CD-NE2 | 5.64 | 128.24 | 122.60 |
| 12 | u | 263 | TRP | N-CA-C | 5.64 | 122.81 | 110.80 |
| 14 | h | 269 | HIS | CA-C-N | 5.64 | 128.87 | 120.87 |
| 14 | h | 269 | HIS | C-N-CA | 5.64 | 128.87 | 120.87 |
| 16 | j | 197 | VAL | CB-CA-C | 5.64 | 121.73 | 111.30 |
| 19 | f | 107 | LYS | CA-C-N | 5.64 | 128.88 | 120.31 |
| 19 | f | 107 | LYS | C-N-CA | 5.64 | 128.88 | 120.31 |
| 19 | f | 719 | ALA | CA-C-O | -5.64 | 112.45 | 119.38 |
| 14 | a | 566 | ASN | CA-C-O | -5.64 | 113.14 | 119.79 |
| 2 | 1 | 232 | ILE | CB-CA-C | 5.63 | 117.77 | 111.80 |
| 2 | 1 | 872 | ASN | N-CA-C | -5.63 | 106.45 | 113.38 |
| 7 | M | 644 | LYS | N-CA-C | 5.63 | 117.42 | 111.28 |
| 7 | M | 1056 | LEU | O-C-N | 5.63 | 128.09 | 122.12 |
| 8 | N | 1217 | ARG | NE-CZ-NH2 | 5.63 | 124.27 | 119.20 |
| 7 | O | 892 | LYS | CA-C-O | 5.63 | 126.13 | 119.48 |
| 8 | P | 46 | ALA | CA-C-N | 5.63 | 131.22 | 122.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 46 | ALA | C-N-CA | 5.63 | 131.22 | 122.26 |
| 9 | S | 617 | LYS | N-CA-CB | 5.63 | 118.59 | 110.20 |
| 9 | T | 285 | TYR | N-CA-C | 5.63 | 117.50 | 111.36 |
| 1 | Y | 973 | ARG | O-C-N | -5.63 | 115.53 | 122.68 |
| 2 | Z | 818 | ASP | N-CA-C | -5.63 | 100.51 | 109.07 |
| 13 | x | 1442 | ALA | CA-C-O | 5.63 | 126.74 | 120.82 |
| 14 | h | 656 | ASP | N-CA-C | 5.63 | 118.62 | 111.69 |
| 15 | i | 508 | LEU | O-C-N | -5.63 | 115.41 | 120.71 |
| 20 | n | 375 | PHE | CA-CB-CG | -5.63 | 108.17 | 113.80 |
| 20 | n | 540 | HIS | CE1-NE2-CD2 | -5.63 | 103.36 | 109.00 |
| 21 | p | 29 | LYS | N-CA-CB | 5.63 | 118.40 | 110.12 |
| 15 | b | 565 | TYR | N-CA-C | -5.63 | 103.92 | 111.87 |
| 7 | O | 745 | ARG | NE-CZ-NH1 | -5.63 | 115.87 | 121.50 |
| 1 | Y | 297 | HIS | CA-C-N | 5.63 | 128.71 | 120.71 |
| 1 | Y | 297 | HIS | C-N-CA | 5.63 | 128.71 | 120.71 |
| 2 | Z | 587 | ALA | N-CA-C | -5.63 | 105.99 | 112.92 |
| 2 | 1 | 1339 | ALA | O-C-N | 5.63 | 128.37 | 122.23 |
| 7 | M | 252 | VAL | CA-C-O | -5.63 | 115.09 | 120.95 |
| 7 | M | 1657 | ASP | CB-CA-C | -5.63 | 104.73 | 113.57 |
| 8 | N | 675 | TYR | CA-C-N | 5.63 | 128.09 | 120.38 |
| 8 | N | 675 | TYR | C-N-CA | 5.63 | 128.09 | 120.38 |
| 7 | O | 1415 | ARG | NE-CZ-NH2 | -5.63 | 114.13 | 119.20 |
| 8 | P | 780 | HIS | N-CA-C | -5.63 | 106.30 | 112.72 |
| 9 | Q | 80 | PHE | N-CA-C | -5.63 | 98.80 | 110.80 |
| 9 | Q | 621 | HIS | CA-C-N | 5.63 | 127.76 | 120.44 |
| 9 | Q | 621 | HIS | C-N-CA | 5.63 | 127.76 | 120.44 |
| 9 | R | 829 | TYR | CA-C-N | 5.63 | 127.83 | 120.28 |
| 9 | R | 829 | TYR | C-N-CA | 5.63 | 127.83 | 120.28 |
| 14 | h | 684 | SER | N-CA-C | -5.63 | 105.72 | 112.59 |
| 16 | j | 610 | TRP | N-CA-C | -5.63 | 100.95 | 109.85 |
| 19 | m | 595 | ARG | NH1-CZ-NH2 | -5.63 | 111.98 | 119.30 |
| 20 | n | 135 | ALA | CA-C-O | -5.63 | 112.88 | 118.34 |
| 18 | e | 112 | TYR | N-CA-CB | 5.63 | 119.22 | 110.44 |
| 20 | g | 667 | LEU | CA-C-N | 5.63 | 127.76 | 120.44 |
| 20 | g | 667 | LEU | C-N-CA | 5.63 | 127.76 | 120.44 |
| 14 | a | 997 | ARG | NH1-CZ-NH2 | -5.63 | 111.98 | 119.30 |
| 7 | M | 175 | PHE | N-CA-C | 5.63 | 117.09 | 111.07 |
| 9 | T | 223 | ASN | CB-CG-OD1 | 5.63 | 132.06 | 120.80 |
| 9 | T | 775 | LEU | CA-C-N | 5.63 | 127.65 | 120.56 |
| 9 | T | 775 | LEU | C-N-CA | 5.63 | 127.65 | 120.56 |
| 2 | Z | 1387 | HIS | CE1-NE2-CD2 | -5.63 | 103.37 | 109.00 |
| 20 | g | 399 | ILE | CA-C-N | 5.63 | 132.05 | 122.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 399 | ILE | C-N-CA | 5.63 | 132.05 | 122.37 |
| 1 | 0 | 428 | PRO | N-CA-C | -5.63 | 108.22 | 114.92 |
| 1 | 0 | 430 | GLU | N-CA-C | -5.63 | 105.37 | 114.09 |
| 2 | 1 | 678 | LYS | N-CA-CB | 5.63 | 124.36 | 111.69 |
| 5 | B | 343 | PRO | N-CA-CB | 5.63 | 109.16 | 103.25 |
| 6 | I | 455 | GLU | O-C-N | -5.63 | 116.01 | 122.09 |
| 8 | P | 28 | ASP | CA-CB-CG | 5.63 | 118.23 | 112.60 |
| 9 | S | 766 | ASN | CA-C-O | 5.63 | 128.56 | 120.51 |
| 9 | T | 88 | LYS | N-CA-C | 5.63 | 118.35 | 111.82 |
| 1 | Y | 193 | TRP | CA-CB-CG | 5.63 | 124.30 | 113.60 |
| 15 | b | 679 | ASP | CA-C-O | 5.63 | 121.20 | 117.94 |
| 20 | g | 646 | PHE | CA-CB-CG | 5.63 | 119.43 | 113.80 |
| 20 | g | 845 | PHE | CA-CB-CG | -5.63 | 108.17 | 113.80 |
| 1 | 0 | 956 | ASN | CA-CB-CG | 5.63 | 118.23 | 112.60 |
| 5 | K | 385 | GLN | N-CA-C | -5.63 | 105.23 | 111.36 |
| 8 | N | 342 | ASP | CA-CB-CG | 5.63 | 118.23 | 112.60 |
| 7 | O | 1168 | ILE | CB-CA-C | 5.63 | 119.08 | 111.88 |
| 8 | P | 153 | ASP | O-C-N | 5.63 | 127.89 | 121.93 |
| 9 | Q | 121 | ILE | CA-C-N | 5.63 | 127.82 | 120.28 |
| 9 | Q | 121 | ILE | C-N-CA | 5.63 | 127.82 | 120.28 |
| 9 | Q | 419 | ASP | N-CA-CB | 5.63 | 120.87 | 111.53 |
| 9 | Q | 826 | ARG | NE-CZ-NH2 | -5.63 | 114.14 | 119.20 |
| 2 | Z | 389 | ASN | N-CA-C | -5.63 | 106.42 | 113.28 |
| 12 | v | 274 | LYS | CA-C-N | 5.63 | 127.75 | 120.44 |
| 12 | v | 274 | LYS | C-N-CA | 5.63 | 127.75 | 120.44 |
| 20 | n | 706 | LEU | O-C-N | -5.63 | 114.85 | 121.32 |
| 20 | g | 1091 | THR | N-CA-CB | 5.63 | 120.38 | 110.37 |
| 2 | Z | 503 | SER | CA-C-O | -5.62 | 113.16 | 118.33 |
| 12 | v | 222 | ASP | CA-C-N | 5.62 | 128.13 | 120.54 |
| 12 | v | 222 | ASP | C-N-CA | 5.62 | 128.13 | 120.54 |
| 15 | b | 469 | PHE | N-CA-CB | -5.62 | 103.42 | 110.90 |
| 18 | e | 109 | GLY | CA-C-N | 5.62 | 130.37 | 121.99 |
| 18 | e | 109 | GLY | C-N-CA | 5.62 | 130.37 | 121.99 |
| 2 | 1 | 1295 | SER | N-CA-C | 5.62 | 119.23 | 112.93 |
| 7 | M | 1138 | PHE | N-CA-C | 5.62 | 122.78 | 110.80 |
| 9 | T | 727 | TYR | CA-C-N | 5.62 | 127.81 | 120.28 |
| 9 | T | 727 | TYR | C-N-CA | 5.62 | 127.81 | 120.28 |
| 1 | Y | 1448 | MET | N-CA-CB | 5.62 | 118.39 | 110.12 |
| 16 | j | 443 | ASN | CA-CB-CG | 5.62 | 118.22 | 112.60 |
| 20 | g | 73 | GLN | OE1-CD-NE2 | 5.62 | 128.22 | 122.60 |
| 5 | B | 450 | PRO | CA-C-N | 5.62 | 127.81 | 120.28 |
| 5 | B | 450 | PRO | C-N-CA | 5.62 | 127.81 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | K | 465 | ILE | CA-C-O | -5.62 | 114.89 | 120.85 |
| 7 | M | 779 | PRO | CA-C-N | 5.62 | 127.85 | 120.60 |
| 7 | M | 779 | PRO | C-N-CA | 5.62 | 127.85 | 120.60 |
| 9 | Q | 133 | THR | CA-C-N | 5.62 | 127.75 | 120.44 |
| 9 | Q | 133 | THR | C-N-CA | 5.62 | 127.75 | 120.44 |
| 9 | R | 814 | MET | O-C-N | 5.62 | 127.88 | 122.03 |
| 12 | v | 335 | MET | N-CA-C | -5.62 | 103.11 | 110.53 |
| 17 | k | 13 | HIS | CE1-NE2-CD2 | -5.62 | 103.38 | 109.00 |
| 20 | n | 636 | ILE | CA-C-N | 5.62 | 132.28 | 121.54 |
| 20 | n | 636 | ILE | C-N-CA | 5.62 | 132.28 | 121.54 |
| 20 | g | 653 | VAL | N-CA-C | -5.62 | 97.65 | 109.34 |
| 6 | I | 346 | ASP | O-C-N | 5.62 | 127.86 | 122.07 |
| 8 | P | 385 | PHE | CA-C-O | -5.62 | 112.55 | 119.18 |
| 1 | Y | 112 | GLN | OE1-CD-NE2 | -5.62 | 116.98 | 122.60 |
| 2 | Z | 391 | LEU | N-CA-C | -5.62 | 106.47 | 113.55 |
| 14 | h | 437 | ASN | CA-C-O | 5.62 | 125.56 | 119.15 |
| 1 | 0 | 782 | ARG | N-CA-CB | 5.62 | 118.81 | 110.49 |
| 7 | M | 236 | ALA | CA-C-O | -5.62 | 114.56 | 120.63 |
| 8 | P | 901 | ILE | N-CA-C | 5.62 | 117.03 | 110.62 |
| 9 | Q | 607 | ARG | N-CA-C | -5.62 | 106.26 | 113.23 |
| 9 | R | 212 | PHE | N-CA-CB | 5.62 | 118.16 | 110.01 |
| 9 | R | 477 | TYR | N-CA-C | -5.62 | 106.27 | 113.01 |
| 9 | S | 441 | MET | O-C-N | -5.62 | 115.60 | 122.34 |
| 11 | V | 302 | ARG | CG-CD-NE | -5.62 | 99.64 | 112.00 |
| 11 | V | 350 | PHE | N-CA-C | -5.62 | 99.74 | 108.90 |
| 1 | Y | 1027 | HIS | CG-CD2-NE2 | 5.62 | 112.82 | 107.20 |
| 19 | f | 657 | ALA | CB-CA-C | -5.62 | 101.30 | 110.85 |
| 14 | a | 10 | ASN | OD1-CG-ND2 | 5.62 | 128.22 | 122.60 |
| 6 | C | 379 | LEU | CA-C-N | 5.62 | 127.74 | 120.44 |
| 6 | C | 379 | LEU | C-N-CA | 5.62 | 127.74 | 120.44 |
| 7 | O | 666 | SER | CA-C-N | 5.62 | 132.27 | 121.54 |
| 7 | O | 666 | SER | C-N-CA | 5.62 | 132.27 | 121.54 |
| 8 | P | 1633 | ARG | NE-CZ-NH2 | -5.62 | 114.14 | 119.20 |
| 15 | i | 597 | LYS | CA-C-O | -5.62 | 112.48 | 120.51 |
| 16 | j | 195 | GLU | CB-CG-CD | -5.62 | 103.05 | 112.60 |
| 2 | 1 | 192 | HIS | CB-CG-CD2 | -5.62 | 123.90 | 131.20 |
| 6 | I | 390 | ILE | CB-CA-C | -5.62 | 103.16 | 112.26 |
| 6 | I | 457 | ILE | CA-CB-CG1 | 5.62 | 119.95 | 110.40 |
| 7 | M | 505 | SER | N-CA-CB | 5.62 | 119.98 | 110.49 |
| 7 | M | 899 | PHE | N-CA-CB | 5.62 | 119.98 | 110.49 |
| 8 | P | 719 | ILE | CA-C-N | 5.62 | 128.37 | 120.28 |
| 8 | P | 719 | ILE | C-N-CA | 5.62 | 128.37 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1010 | GLU | CA-C-N | 5.62 | 128.37 | 120.28 |
| 8 | P | 1010 | GLU | C-N-CA | 5.62 | 128.37 | 120.28 |
| 12 | u | 113 | HIS | N-CA-C | -5.62 | 100.59 | 108.96 |
| 15 | i | 473 | LEU | N-CA-CB | 5.62 | 118.15 | 110.01 |
| 18 | e | 58 | ILE | N-CA-C | -5.62 | 100.25 | 108.11 |
| 7 | M | 460 | SER | N-CA-C | -5.61 | 98.38 | 108.48 |
| 8 | N | 928 | SER | N-CA-C | -5.61 | 105.35 | 113.21 |
| 7 | O | 23 | ASP | O-C-N | 5.61 | 130.06 | 122.59 |
| 7 | O | 431 | PHE | CA-CB-CG | 5.61 | 119.41 | 113.80 |
| 8 | P | 1352 | LEU | CA-C-N | 5.61 | 130.22 | 120.68 |
| 8 | P | 1352 | LEU | C-N-CA | 5.61 | 130.22 | 120.68 |
| 9 | R | 95 | PHE | CA-C-N | 5.61 | 127.74 | 120.44 |
| 9 | R | 95 | PHE | C-N-CA | 5.61 | 127.74 | 120.44 |
| 9 | S | 72 | LEU | N-CA-CB | 5.61 | 118.31 | 109.94 |
| 9 | S | 659 | SER | CA-C-N | 5.61 | 128.07 | 120.44 |
| 9 | S | 659 | SER | C-N-CA | 5.61 | 128.07 | 120.44 |
| 9 | T | 420 | LEU | N-CA-C | -5.61 | 101.89 | 110.14 |
| 10 | U | 352 | GLN | N-CA-C | -5.61 | 106.32 | 112.72 |
| 1 | Y | 1205 | SER | N-CA-CB | 5.61 | 119.71 | 110.39 |
| 2 | Z | 1226 | SER | N-CA-C | -5.61 | 106.42 | 113.72 |
| 14 | h | 372 | SER | N-CA-CB | 5.61 | 118.28 | 109.69 |
| 14 | h | 673 | CYS | CA-C-O | 5.61 | 126.28 | 119.49 |
| 14 | h | 938 | ARG | O-C-N | 5.61 | 127.85 | 122.07 |
| 20 | n | 397 | PRO | CB-CA-C | -5.61 | 104.20 | 111.39 |
| 21 | o | 36 | GLN | CA-C-O | 5.61 | 124.98 | 118.97 |
| 16 | c | 665 | ILE | CA-CB-CG2 | -5.61 | 100.96 | 110.50 |
| 19 | f | 700 | LYS | N-CA-C | 5.61 | 119.38 | 111.52 |
| 7 | O | 832 | PHE | N-CA-C | 5.61 | 118.16 | 111.71 |
| 7 | O | 1057 | GLU | CA-C-N | 5.61 | 129.58 | 120.60 |
| 7 | O | 1057 | GLU | C-N-CA | 5.61 | 129.58 | 120.60 |
| 8 | P | 1334 | ASP | N-CA-CB | 5.61 | 120.09 | 111.56 |
| 9 | R | 717 | LEU | N-CA-CB | 5.61 | 118.37 | 110.12 |
| 9 | T | 139 | PHE | CA-C-O | -5.61 | 114.60 | 120.55 |
| 11 | X | 293 | HIS | CE1-NE2-CD2 | -5.61 | 103.39 | 109.00 |
| 2 | Z | 1286 | HIS | CE1-NE2-CD2 | -5.61 | 103.39 | 109.00 |
| 21 | s | 75 | HIS | CB-CG-CD2 | -5.61 | 123.91 | 131.20 |
| 6 | C | 443 | VAL | CA-CB-CG1 | 5.61 | 119.94 | 110.40 |
| 7 | M | 35 | LEU | CA-C-O | -5.61 | 114.21 | 120.66 |
| 7 | M | 828 | PHE | CA-CB-CG | -5.61 | 108.19 | 113.80 |
| 7 | O | 1138 | PHE | CA-C-N | 5.61 | 129.85 | 121.77 |
| 7 | O | 1138 | PHE | C-N-CA | 5.61 | 129.85 | 121.77 |
| 7 | O | 1179 | THR | N-CA-CB | 5.61 | 119.97 | 110.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | T | 756 | LYS | N-CA-C | -5.61 | 106.29 | 113.02 |
| 1 | Y | 1408 | VAL | CA-C-N | 5.61 | 128.59 | 120.79 |
| 1 | Y | 1408 | VAL | C-N-CA | 5.61 | 128.59 | 120.79 |
| 21 | r | 48 | GLN | N-CA-C | 5.61 | 117.40 | 111.28 |
| 15 | b | 210 | ASN | N-CA-CB | 5.61 | 118.98 | 110.28 |
| 19 | f | 716 | ASP | CA-CB-CG | 5.61 | 118.21 | 112.60 |
| 8 | N | 1608 | HIS | CA-C-N | 5.61 | 125.45 | 119.28 |
| 8 | N | 1608 | HIS | C-N-CA | 5.61 | 125.45 | 119.28 |
| 7 | O | 483 | LEU | CA-C-N | 5.61 | 127.73 | 120.44 |
| 7 | O | 483 | LEU | C-N-CA | 5.61 | 127.73 | 120.44 |
| 8 | P | 1642 | ARG | NE-CZ-NH1 | 5.61 | 127.11 | 121.50 |
| 9 | R | 805 | SER | N-CA-CB | 5.61 | 118.37 | 110.12 |
| 1 | Y | 1262 | ILE | CA-C-O | 5.61 | 124.00 | 119.29 |
| 15 | i | 576 | PHE | CA-C-O | 5.61 | 125.61 | 118.54 |
| 18 | e | 77 | TYR | CB-CG-CD1 | 5.61 | 129.21 | 120.80 |
| 20 | g | 1019 | LEU | N-CA-CB | 5.61 | 118.46 | 110.16 |
| 5 | B | 390 | HIS | ND1-CE1-NE2 | 5.61 | 114.01 | 108.40 |
| 4 | D | 655 | PHE | CA-CB-CG | 5.61 | 119.41 | 113.80 |
| 5 | E | 447 | SER | O-C-N | 5.61 | 129.52 | 122.23 |
| 7 | M | 564 | ASP | CA-C-O | 5.61 | 127.24 | 121.07 |
| 8 | N | 49 | THR | N-CA-C | -5.61 | 104.07 | 112.54 |
| 8 | N | 455 | PHE | CB-CG-CD1 | 5.61 | 130.23 | 120.70 |
| 8 | N | 662 | THR | N-CA-C | -5.61 | 105.03 | 113.89 |
| 8 | N | 1335 | GLN | N-CA-C | 5.61 | 118.16 | 111.71 |
| 7 | O | 356 | ILE | CA-C-N | 5.61 | 126.85 | 119.84 |
| 7 | O | 356 | ILE | C-N-CA | 5.61 | 126.85 | 119.84 |
| 7 | O | 1151 | LEU | N-CA-CB | 5.61 | 118.10 | 109.91 |
| 9 | S | 563 | ASN | OD1-CG-ND2 | 5.61 | 128.21 | 122.60 |
| 1 | Y | 1149 | ALA | N-CA-C | 5.61 | 117.20 | 111.14 |
| 12 | u | 553 | ILE | CB-CA-C | -5.61 | 104.48 | 112.22 |
| 12 | u | 655 | LEU | CA-C-N | 5.61 | 127.79 | 120.28 |
| 12 | u | 655 | LEU | C-N-CA | 5.61 | 127.79 | 120.28 |
| 19 | m | 305 | ASN | CA-CB-CG | 5.61 | 118.21 | 112.60 |
| 16 | c | 649 | LYS | O-C-N | 5.61 | 130.05 | 122.59 |
| 20 | g | 690 | ARG | N-CA-C | -5.61 | 105.79 | 113.30 |
| 20 | g | 890 | GLN | CA-C-N | 5.61 | 128.47 | 122.97 |
| 20 | g | 890 | GLN | C-N-CA | 5.61 | 128.47 | 122.97 |
| 4 | D | 719 | GLU | CB-CG-CD | -5.61 | 103.07 | 112.60 |
| 4 | J | 646 | ASN | CA-CB-CG | -5.61 | 106.99 | 112.60 |
| 7 | O | 1527 | ARG | O-C-N | -5.61 | 116.30 | 122.07 |
| 8 | P | 1475 | SER | CA-C-O | 5.61 | 125.06 | 118.90 |
| 9 | S | 435 | TRP | CB-CG-CD2 | -5.61 | 118.95 | 126.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 196 | ASN | N-CA-C | -5.61 | 103.97 | 112.04 |
| 1 | Y | 1012 | ARG | N-CA-C | 5.61 | 117.97 | 110.35 |
| 1 | Y | 1402 | LEU | CA-C-N | 5.61 | 126.85 | 119.84 |
| 1 | Y | 1402 | LEU | C-N-CA | 5.61 | 126.85 | 119.84 |
| 14 | h | 13 | GLN | N-CA-CB | 5.61 | 118.88 | 110.53 |
| 15 | i | 170 | ASN | OD1-CG-ND2 | -5.61 | 117.00 | 122.60 |
| 16 | j | 523 | ASN | CA-C-N | 5.61 | 127.79 | 120.28 |
| 16 | j | 523 | ASN | C-N-CA | 5.61 | 127.79 | 120.28 |
| 20 | n | 579 | ILE | N-CA-C | -5.61 | 100.15 | 108.45 |
| 21 | s | 8 | THR | CA-CB-CG2 | -5.61 | 100.97 | 110.50 |
| 18 | e | 145 | LEU | CA-C-N | 5.61 | 127.73 | 120.44 |
| 18 | e | 145 | LEU | C-N-CA | 5.61 | 127.73 | 120.44 |
| 20 | g | 436 | SER | N-CA-C | -5.61 | 105.65 | 112.88 |
| 20 | g | 654 | VAL | CA-C-N | 5.61 | 131.27 | 121.52 |
| 20 | g | 654 | VAL | C-N-CA | 5.61 | 131.27 | 121.52 |
| 7 | M | 1411 | HIS | CE1-NE2-CD2 | -5.60 | 103.40 | 109.00 |
| 8 | P | 1227 | VAL | CB-CA-C | -5.60 | 104.80 | 111.97 |
| 9 | Q | 700 | ALA | N-CA-CB | 5.60 | 118.36 | 110.12 |
| 15 | i | 456 | SER | N-CA-C | -5.60 | 100.78 | 109.24 |
| 20 | g | 785 | HIS | ND1-CE1-NE2 | 5.60 | 114.00 | 108.40 |
| 5 | E | 455 | LYS | O-C-N | 5.60 | 129.16 | 122.27 |
| 8 | N | 588 | HIS | CE1-NE2-CD2 | -5.60 | 103.40 | 109.00 |
| 8 | P | 718 | PHE | CB-CG-CD1 | 5.60 | 130.22 | 120.70 |
| 8 | P | 1617 | ILE | CB-CG1-CD1 | 5.60 | 125.56 | 113.80 |
| 9 | Q | 216 | ALA | CA-C-N | 5.60 | 127.79 | 120.28 |
| 9 | Q | 216 | ALA | C-N-CA | 5.60 | 127.79 | 120.28 |
| 1 | Y | 1336 | ILE | CA-C-N | 5.60 | 128.83 | 120.31 |
| 1 | Y | 1336 | ILE | C-N-CA | 5.60 | 128.83 | 120.31 |
| 2 | Z | 605 | THR | CA-CB-OG1 | 5.60 | 118.00 | 109.60 |
| 2 | Z | 1183 | ILE | CA-C-O | -5.60 | 115.82 | 121.59 |
| 4 | y | 669 | LEU | O-C-N | 5.60 | 128.07 | 122.08 |
| 14 | h | 971 | ASN | CA-C-O | 5.60 | 127.31 | 121.15 |
| 15 | i | 484 | VAL | CA-C-N | 5.60 | 128.06 | 120.44 |
| 15 | i | 484 | VAL | C-N-CA | 5.60 | 128.06 | 120.44 |
| 19 | m | 181 | PHE | O-C-N | -5.60 | 114.78 | 122.46 |
| 19 | f | 61 | ASN | CA-C-O | 5.60 | 126.28 | 119.11 |
| 20 | g | 438 | SER | CA-C-N | 5.60 | 132.24 | 121.54 |
| 20 | g | 438 | SER | C-N-CA | 5.60 | 132.24 | 121.54 |
| 7 | M | 482 | PHE | CA-CB-CG | -5.60 | 108.20 | 113.80 |
| 2 | Z | 104 | ARG | NE-CZ-NH2 | -5.60 | 114.16 | 119.20 |
| 2 | Z | 489 | SER | CA-C-O | -5.60 | 115.28 | 121.33 |
| 14 | h | 751 | ARG | NE-CZ-NH2 | -5.60 | 114.16 | 119.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 148 | PHE | CB-CG-CD1 | 5.60 | 130.22 | 120.70 |
| 1 | 0 | 590 | GLY | CA-C-O | -5.60 | 113.31 | 120.03 |
| 2 | 1 | 214 | PHE | CA-CB-CG | 5.60 | 119.40 | 113.80 |
| 6 | I | 379 | LEU | CA-C-N | 5.60 | 127.72 | 120.44 |
| 6 | I | 379 | LEU | C-N-CA | 5.60 | 127.72 | 120.44 |
| 8 | N | 745 | HIS | ND1-CE1-NE2 | 5.60 | 114.00 | 108.40 |
| 7 | O | 473 | SER | N-CA-C | -5.60 | 105.04 | 112.94 |
| 8 | P | 1434 | ASN | O-C-N | -5.60 | 116.14 | 122.97 |
| 9 | T | 126 | GLU | O-C-N | 5.60 | 128.06 | 122.12 |
| 9 | T | 616 | GLU | CA-C-O | -5.60 | 114.58 | 120.63 |
| 11 | V | 369 | ALA | CA-C-N | 5.60 | 128.04 | 120.65 |
| 11 | V | 369 | ALA | C-N-CA | 5.60 | 128.04 | 120.65 |
| 2 | Z | 94 | ALA | CA-C-N | 5.60 | 127.78 | 120.28 |
| 2 | Z | 94 | ALA | C-N-CA | 5.60 | 127.78 | 120.28 |
| 12 | v | 700 | GLU | CA-C-N | 5.60 | 127.78 | 120.28 |
| 12 | v | 700 | GLU | C-N-CA | 5.60 | 127.78 | 120.28 |
| 19 | m | 416 | TYR | CA-C-N | 5.60 | 127.73 | 120.56 |
| 19 | m | 416 | TYR | C-N-CA | 5.60 | 127.73 | 120.56 |
| 20 | n | 343 | SER | N-CA-C | -5.60 | 98.87 | 110.80 |
| 16 | c | 764 | LEU | CB-CA-C | -5.60 | 98.96 | 110.38 |
| 20 | g | 603 | ILE | CB-CA-C | -5.60 | 104.49 | 112.22 |
| 14 | a | 298 | PHE | CA-CB-CG | -5.60 | 108.20 | 113.80 |
| 14 | a | 620 | HIS | CB-CG-CD2 | -5.60 | 123.92 | 131.20 |
| 2 | 1 | 582 | THR | N-CA-C | -5.60 | 100.42 | 109.82 |
| 8 | N | 1615 | ARG | CA-C-N | 5.60 | 129.89 | 122.95 |
| 8 | N | 1615 | ARG | C-N-CA | 5.60 | 129.89 | 122.95 |
| 7 | O | 1534 | GLY | O-C-N | -5.60 | 117.83 | 122.92 |
| 8 | P | 162 | HIS | ND1-CE1-NE2 | 5.60 | 114.00 | 108.40 |
| 9 | R | 500 | GLU | CA-C-N | 5.60 | 129.56 | 120.60 |
| 9 | R | 500 | GLU | C-N-CA | 5.60 | 129.56 | 120.60 |
| 16 | j | 621 | LEU | N-CA-C | 5.60 | 119.97 | 113.20 |
| 20 | n | 617 | THR | N-CA-C | 5.60 | 119.81 | 113.15 |
| 15 | b | 107 | TYR | N-CA-C | 5.60 | 117.38 | 111.28 |
| 15 | b | 162 | VAL | CA-C-N | 5.60 | 128.34 | 120.28 |
| 15 | b | 162 | VAL | C-N-CA | 5.60 | 128.34 | 120.28 |
| 16 | c | 489 | HIS | CB-CG-CD2 | -5.60 | 123.92 | 131.20 |
| 19 | f | 12 | PHE | CA-C-N | 5.60 | 128.24 | 120.29 |
| 19 | f | 12 | PHE | C-N-CA | 5.60 | 128.24 | 120.29 |
| 19 | f | 405 | GLU | CA-C-N | 5.60 | 132.23 | 121.54 |
| 19 | f | 405 | GLU | C-N-CA | 5.60 | 132.23 | 121.54 |
| 14 | a | 984 | TYR | CA-C-N | 5.60 | 128.10 | 120.77 |
| 14 | a | 984 | TYR | C-N-CA | 5.60 | 128.10 | 120.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 183 | SER | CA-C-N | 5.60 | 128.09 | 120.54 |
| 8 | N | 183 | SER | C-N-CA | 5.60 | 128.09 | 120.54 |
| 8 | P | 1433 | ILE | N-CA-C | -5.60 | 99.44 | 107.78 |
| 16 | j | 262 | LYS | CA-C-N | 5.60 | 128.24 | 120.29 |
| 16 | j | 262 | LYS | C-N-CA | 5.60 | 128.24 | 120.29 |
| 2 | 1 | 1002 | ILE | CA-CB-CG2 | -5.59 | 100.99 | 110.50 |
| 4 | A | 750 | THR | CA-CB-OG1 | 5.59 | 117.99 | 109.60 |
| 7 | M | 176 | GLN | N-CA-CB | 5.59 | 119.68 | 110.39 |
| 9 | T | 334 | TRP | CE2-CD2-CE3 | 5.59 | 124.39 | 118.80 |
| 12 | v | 648 | GLN | CA-C-N | 5.59 | 128.55 | 120.38 |
| 12 | v | 648 | GLN | C-N-CA | 5.59 | 128.55 | 120.38 |
| 4 | y | 649 | THR | CA-C-O | 5.59 | 126.48 | 120.55 |
| 14 | h | 666 | ASN | N-CA-CB | 5.59 | 119.52 | 110.40 |
| 15 | i | 84 | ALA | N-CA-C | -5.59 | 100.85 | 109.52 |
| 21 | o | 26 | THR | CA-CB-CG2 | 5.59 | 120.01 | 110.50 |
| 21 | o | 71 | HIS | CG-CD2-NE2 | 5.59 | 112.79 | 107.20 |
| 15 | b | 674 | ILE | CA-C-N | 5.59 | 132.23 | 121.54 |
| 15 | b | 674 | ILE | C-N-CA | 5.59 | 132.23 | 121.54 |
| 15 | b | 702 | ALA | CA-C-N | 5.59 | 132.22 | 121.54 |
| 15 | b | 702 | ALA | C-N-CA | 5.59 | 132.22 | 121.54 |
| 16 | c | 772 | LEU | CA-C-N | 5.59 | 126.83 | 119.84 |
| 16 | c | 772 | LEU | C-N-CA | 5.59 | 126.83 | 119.84 |
| 20 | g | 634 | VAL | N-CA-CB | -5.59 | 103.41 | 110.57 |
| 1 | 0 | 1189 | LYS | CA-C-N | 5.59 | 128.79 | 120.90 |
| 1 | 0 | 1189 | LYS | C-N-CA | 5.59 | 128.79 | 120.90 |
| 15 | b | 578 | ALA | N-CA-C | -5.59 | 105.81 | 113.30 |
| 16 | c | 391 | TYR | N-CA-C | -5.59 | 105.14 | 112.41 |
| 20 | g | 551 | ASN | CA-CB-CG | 5.59 | 118.19 | 112.60 |
| 2 | 1 | 948 | ARG | CA-C-N | 5.59 | 128.81 | 120.31 |
| 2 | 1 | 948 | ARG | C-N-CA | 5.59 | 128.81 | 120.31 |
| 5 | H | 334 | GLU | CA-C-N | 5.59 | 128.23 | 120.29 |
| 5 | H | 334 | GLU | C-N-CA | 5.59 | 128.23 | 120.29 |
| 7 | M | 302 | PHE | CA-C-O | 5.59 | 126.19 | 119.59 |
| 7 | M | 1101 | ILE | CA-CB-CG2 | -5.59 | 100.99 | 110.50 |
| 7 | M | 1238 | ASP | O-C-N | -5.59 | 116.36 | 123.24 |
| 8 | N | 85 | ASN | CA-CB-CG | -5.59 | 107.01 | 112.60 |
| 8 | N | 749 | ILE | CA-C-N | 5.59 | 127.71 | 120.44 |
| 8 | N | 749 | ILE | C-N-CA | 5.59 | 127.71 | 120.44 |
| 8 | N | 844 | TYR | CA-C-O | -5.59 | 114.95 | 120.82 |
| 7 | O | 541 | LEU | CA-C-N | 5.59 | 129.21 | 120.82 |
| 7 | O | 541 | LEU | C-N-CA | 5.59 | 129.21 | 120.82 |
| 7 | O | 1020 | SER | N-CA-C | 5.59 | 117.84 | 111.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1579 | ASN | CB-CA-C | -5.59 | 102.10 | 110.88 |
| 8 | P | 599 | THR | CA-CB-OG1 | 5.59 | 117.99 | 109.60 |
| 8 | P | 728 | ILE | CA-C-N | 5.59 | 132.34 | 122.67 |
| 8 | P | 728 | ILE | C-N-CA | 5.59 | 132.34 | 122.67 |
| 9 | T | 707 | HIS | CE1-NE2-CD2 | -5.59 | 103.41 | 109.00 |
| 1 | Y | 1377 | ASN | CA-CB-CG | 5.59 | 118.19 | 112.60 |
| 12 | v | 208 | PHE | N-CA-C | -5.59 | 99.41 | 108.52 |
| 14 | h | 697 | GLN | CB-CG-CD | -5.59 | 103.10 | 112.60 |
| 16 | j | 158 | MET | N-CA-CB | 5.59 | 121.55 | 111.37 |
| 16 | j | 234 | TRP | CD2-CE2-CZ2 | -5.59 | 116.81 | 122.40 |
| 1 | 0 | 1321 | ALA | N-CA-CB | 5.59 | 118.34 | 110.12 |
| 2 | 1 | 1247 | ASN | CB-CA-C | -5.59 | 101.35 | 110.85 |
| 7 | M | 1183 | TYR | CB-CG-CD1 | 5.59 | 129.19 | 120.80 |
| 8 | N | 846 | LYS | CA-C-N | 5.59 | 132.03 | 121.97 |
| 8 | N | 846 | LYS | C-N-CA | 5.59 | 132.03 | 121.97 |
| 8 | N | 1093 | ASN | OD1-CG-ND2 | 5.59 | 128.19 | 122.60 |
| 7 | O | 1162 | GLY | CA-C-N | 5.59 | 128.23 | 120.29 |
| 7 | O | 1162 | GLY | C-N-CA | 5.59 | 128.23 | 120.29 |
| 7 | O | 1188 | THR | CA-CB-OG1 | -5.59 | 101.21 | 109.60 |
| 9 | S | 796 | SER | CA-C-O | 5.59 | 127.37 | 121.33 |
| 9 | T | 218 | ILE | N-CA-CB | 5.59 | 118.97 | 110.58 |
| 13 | w | 1335 | SER | CA-C-O | 5.59 | 126.48 | 120.55 |
| 13 | w | 1353 | SER | CA-C-N | 5.59 | 127.71 | 120.44 |
| 13 | w | 1353 | SER | C-N-CA | 5.59 | 127.71 | 120.44 |
| 20 | n | 749 | LEU | N-CA-C | -5.59 | 106.35 | 112.72 |
| 19 | f | 382 | LYS | CA-C-N | 5.59 | 125.11 | 119.19 |
| 19 | f | 382 | LYS | C-N-CA | 5.59 | 125.11 | 119.19 |
| 20 | g | 867 | GLN | CA-C-N | 5.59 | 132.22 | 121.54 |
| 20 | g | 867 | GLN | C-N-CA | 5.59 | 132.22 | 121.54 |
| 6 | F | 309 | PRO | N-CA-C | 5.59 | 121.30 | 113.53 |
| 7 | M | 1494 | ASN | CA-C-N | 5.59 | 132.21 | 121.54 |
| 7 | M | 1494 | ASN | C-N-CA | 5.59 | 132.21 | 121.54 |
| 9 | R | 553 | ALA | CA-C-O | -5.59 | 114.92 | 121.07 |
| 16 | j | 774 | LEU | O-C-N | 5.59 | 130.18 | 123.36 |
| 21 | s | 24 | ILE | N-CA-C | 5.59 | 116.32 | 110.62 |
| 2 | 1 | 1360 | SER | CB-CA-C | -5.59 | 101.95 | 109.16 |
| 4 | J | 675 | GLN | CA-C-N | 5.59 | 128.35 | 120.42 |
| 4 | J | 675 | GLN | C-N-CA | 5.59 | 128.35 | 120.42 |
| 6 | L | 275 | GLN | CA-C-N | 5.59 | 128.22 | 120.29 |
| 6 | L | 275 | GLN | C-N-CA | 5.59 | 128.22 | 120.29 |
| 7 | M | 259 | PHE | CB-CG-CD2 | -5.59 | 111.20 | 120.70 |
| 8 | N | 747 | ILE | CA-C-O | -5.59 | 115.14 | 120.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 986 | SER | N-CA-CB | 5.59 | 119.93 | 110.49 |
| 9 | R | 630 | ARG | CA-C-O | -5.59 | 113.33 | 120.31 |
| 9 | R | 652 | ILE | CA-CB-CG2 | 5.59 | 120.00 | 110.50 |
| 9 | S | 469 | TYR | CA-C-N | 5.59 | 130.64 | 121.87 |
| 9 | S | 469 | TYR | C-N-CA | 5.59 | 130.64 | 121.87 |
| 9 | T | 644 | TYR | CA-C-O | -5.59 | 114.95 | 120.82 |
| 1 | Y | 680 | SER | CA-C-O | 5.59 | 126.47 | 120.55 |
| 2 | Z | 394 | LYS | CA-C-N | 5.59 | 128.77 | 120.95 |
| 2 | Z | 394 | LYS | C-N-CA | 5.59 | 128.77 | 120.95 |
| 2 | Z | 402 | ARG | CD-NE-CZ | 5.59 | 132.22 | 124.40 |
| 12 | u | 167 | ASN | N-CA-C | 5.59 | 117.50 | 110.24 |
| 13 | w | 1274 | ASN | CA-C-O | 5.59 | 126.69 | 120.82 |
| 20 | g | 1099 | TYR | CA-C-N | 5.59 | 127.38 | 120.34 |
| 20 | g | 1099 | TYR | C-N-CA | 5.59 | 127.38 | 120.34 |
| 14 | a | 202 | ASN | OD1-CG-ND2 | -5.59 | 117.01 | 122.60 |
| 4 | G | 688 | HIS | CA-C-N | 5.58 | 128.80 | 120.31 |
| 4 | G | 688 | HIS | C-N-CA | 5.58 | 128.80 | 120.31 |
| 7 | M | 1116 | VAL | N-CA-C | -5.58 | 100.29 | 108.11 |
| 11 | V | 267 | SER | N-CA-C | -5.58 | 104.28 | 113.50 |
| 2 | Z | 916 | PHE | N-CA-C | -5.58 | 95.36 | 111.00 |
| 16 | c | 162 | LYS | CA-CB-CG | 5.58 | 125.27 | 114.10 |
| 2 | 1 | 205 | LYS | CA-C-N | 5.58 | 130.87 | 123.00 |
| 2 | 1 | 205 | LYS | C-N-CA | 5.58 | 130.87 | 123.00 |
| 6 | C | 292 | HIS | CA-C-N | 5.58 | 127.70 | 120.44 |
| 6 | C | 292 | HIS | C-N-CA | 5.58 | 127.70 | 120.44 |
| 7 | M | 101 | ASN | CA-C-N | 5.58 | 126.30 | 119.99 |
| 7 | M | 101 | ASN | C-N-CA | 5.58 | 126.30 | 119.99 |
| 7 | M | 820 | GLN | O-C-N | 5.58 | 130.29 | 122.36 |
| 7 | M | 1658 | PRO | N-CA-CB | 5.58 | 109.47 | 103.33 |
| 8 | N | 730 | ILE | CB-CA-C | -5.58 | 105.45 | 111.59 |
| 8 | N | 1411 | SER | N-CA-CB | 5.58 | 118.33 | 110.12 |
| 9 | R | 122 | LEU | N-CA-C | 5.58 | 117.04 | 111.07 |
| 9 | R | 479 | LEU | CA-C-N | 5.58 | 127.76 | 120.28 |
| 9 | R | 479 | LEU | C-N-CA | 5.58 | 127.76 | 120.28 |
| 1 | Y | 365 | ARG | CA-C-O | 5.58 | 124.92 | 118.55 |
| 2 | Z | 1293 | LEU | CA-C-N | 5.58 | 127.76 | 120.28 |
| 2 | Z | 1293 | LEU | C-N-CA | 5.58 | 127.76 | 120.28 |
| 19 | m | 181 | PHE | CA-CB-CG | -5.58 | 108.22 | 113.80 |
| 20 | n | 1125 | SER | CA-C-O | -5.58 | 115.13 | 121.66 |
| 15 | b | 671 | LEU | N-CA-C | 5.58 | 117.44 | 111.36 |
| 1 | 0 | 1365 | ASN | N-CA-CB | 5.58 | 118.30 | 109.82 |
| 2 | 1 | 440 | ARG | N-CA-C | -5.58 | 105.24 | 113.61 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 1216 | TYR | N-CA-C | -5.58 | 105.07 | 113.89 |
| 2 | 1 | 1330 | GLU | N-CA-C | 5.58 | 117.36 | 111.28 |
| 7 | M | 1346 | ASN | CA-CB-CG | -5.58 | 107.02 | 112.60 |
| 9 | Q | 639 | ASP | N-CA-C | -5.58 | 105.28 | 111.36 |
| 9 | Q | 808 | ASN | CB-CA-C | -5.58 | 102.36 | 110.96 |
| 9 | R | 826 | ARG | CA-C-O | -5.58 | 114.63 | 120.55 |
| 1 | Y | 1384 | ILE | CA-CB-CG1 | 5.58 | 119.89 | 110.40 |
| 12 | u | 690 | ASP | CA-C-N | 5.58 | 127.76 | 120.28 |
| 12 | u | 690 | ASP | C-N-CA | 5.58 | 127.76 | 120.28 |
| 15 | i | 556 | ILE | CA-C-N | 5.58 | 128.08 | 120.54 |
| 15 | i | 556 | ILE | C-N-CA | 5.58 | 128.08 | 120.54 |
| 21 | s | 64 | ASN | O-C-N | 5.58 | 130.01 | 122.59 |
| 20 | g | 563 | PHE | CA-C-O | -5.58 | 112.79 | 119.15 |
| 14 | a | 608 | ASP | N-CA-C | -5.58 | 100.14 | 109.24 |
| 8 | N | 1336 | LEU | O-C-N | 5.58 | 128.03 | 122.12 |
| 8 | P | 318 | HIS | ND1-CE1-NE2 | 5.58 | 113.98 | 108.40 |
| 11 | X | 378 | ARG | N-CA-C | -5.58 | 104.44 | 111.92 |
| 1 | Y | 446 | LEU | N-CA-CB | 5.58 | 119.33 | 110.57 |
| 15 | i | 321 | ALA | CA-C-O | -5.58 | 114.91 | 121.44 |
| 1 | 0 | 179 | LEU | N-CA-C | -5.58 | 105.58 | 112.72 |
| 1 | 0 | 583 | TYR | CA-C-N | 5.58 | 126.13 | 119.94 |
| 1 | 0 | 583 | TYR | C-N-CA | 5.58 | 126.13 | 119.94 |
| 7 | M | 64 | PHE | O-C-N | -5.58 | 117.40 | 123.26 |
| 7 | M | 120 | ILE | CB-CA-C | 5.58 | 118.78 | 111.81 |
| 7 | M | 1143 | SER | N-CA-CB | 5.58 | 119.92 | 110.49 |
| 8 | N | 30 | SER | O-C-N | 5.58 | 128.94 | 122.19 |
| 7 | O | 1206 | ILE | CA-C-O | -5.58 | 114.12 | 120.65 |
| 7 | O | 1602 | VAL | CB-CA-C | -5.58 | 106.69 | 114.00 |
| 8 | P | 515 | ASN | CB-CA-C | 5.58 | 120.70 | 110.10 |
| 9 | R | 621 | HIS | CE1-NE2-CD2 | -5.58 | 103.42 | 109.00 |
| 1 | Y | 458 | GLU | CA-C-N | 5.58 | 129.17 | 120.75 |
| 1 | Y | 458 | GLU | C-N-CA | 5.58 | 129.17 | 120.75 |
| 2 | Z | 289 | ASN | CA-C-O | -5.58 | 111.32 | 120.80 |
| 12 | u | 266 | ARG | NE-CZ-NH2 | -5.58 | 114.18 | 119.20 |
| 14 | h | 390 | GLN | N-CA-C | -5.58 | 104.12 | 112.54 |
| 14 | h | 516 | PHE | N-CA-C | -5.58 | 103.02 | 111.56 |
| 14 | h | 647 | PHE | CA-C-N | 5.58 | 126.17 | 119.98 |
| 14 | h | 647 | PHE | C-N-CA | 5.58 | 126.17 | 119.98 |
| 14 | h | 692 | PHE | N-CA-CB | 5.58 | 118.77 | 110.29 |
| 20 | n | 111 | HIS | ND1-CE1-NE2 | 5.58 | 113.98 | 108.40 |
| 16 | c | 294 | ILE | O-C-N | -5.58 | 116.08 | 121.83 |
| 20 | g | 72 | LEU | N-CA-C | -5.58 | 106.31 | 113.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | a | 824 | PHE | CA-CB-CG | -5.58 | 108.22 | 113.80 |
| 2 | 1 | 1093 | GLU | CB-CA-C | 5.58 | 117.46 | 109.71 |
| 8 | N | 68 | HIS | CG-CD2-NE2 | 5.58 | 112.78 | 107.20 |
| 7 | O | 461 | LEU | N-CA-C | -5.58 | 103.02 | 110.55 |
| 8 | P | 204 | VAL | CA-C-N | 5.58 | 126.36 | 120.11 |
| 8 | P | 204 | VAL | C-N-CA | 5.58 | 126.36 | 120.11 |
| 19 | m | 102 | ARG | NE-CZ-NH1 | -5.58 | 115.92 | 121.50 |
| 14 | a | 312 | THR | N-CA-C | -5.58 | 100.59 | 109.07 |
| 1 | 0 | 136 | SER | N-CA-C | -5.58 | 100.24 | 108.99 |
| 1 | 0 | 959 | THR | N-CA-C | -5.58 | 105.08 | 113.89 |
| 5 | K | 299 | TRP | CZ3-CH2-CZ2 | -5.58 | 114.25 | 121.50 |
| 8 | N | 43 | PHE | CA-CB-CG | -5.58 | 108.22 | 113.80 |
| 8 | N | 893 | TYR | CA-C-N | 5.58 | 132.01 | 121.97 |
| 8 | N | 893 | TYR | C-N-CA | 5.58 | 132.01 | 121.97 |
| 7 | O | 162 | ILE | CA-C-N | 5.58 | 128.79 | 120.31 |
| 7 | O | 162 | ILE | C-N-CA | 5.58 | 128.79 | 120.31 |
| 7 | O | 1298 | LEU | CB-CA-C | -5.58 | 100.28 | 109.65 |
| 9 | S | 723 | ILE | N-CA-C | -5.58 | 105.19 | 113.39 |
| 9 | T | 708 | VAL | O-C-N | 5.58 | 127.28 | 121.87 |
| 11 | V | 378 | ARG | NE-CZ-NH2 | -5.58 | 114.18 | 119.20 |
| 1 | Y | 1315 | LEU | CA-C-N | 5.58 | 130.09 | 122.34 |
| 1 | Y | 1315 | LEU | C-N-CA | 5.58 | 130.09 | 122.34 |
| 14 | h | 1011 | ASP | N-CA-C | -5.58 | 98.92 | 110.80 |
| 20 | n | 1147 | THR | CA-C-N | 5.58 | 128.66 | 120.91 |
| 20 | n | 1147 | THR | C-N-CA | 5.58 | 128.66 | 120.91 |
| 14 | a | 584 | ASN | CA-C-O | -5.58 | 114.51 | 120.42 |
| 2 | 1 | 574 | THR | CA-C-N | 5.57 | 132.19 | 121.54 |
| 2 | 1 | 574 | THR | C-N-CA | 5.57 | 132.19 | 121.54 |
| 7 | M | 45 | ASN | CA-CB-CG | 5.57 | 118.17 | 112.60 |
| 7 | M | 787 | GLY | CA-C-N | 5.57 | 127.75 | 120.28 |
| 7 | M | 787 | GLY | C-N-CA | 5.57 | 127.75 | 120.28 |
| 8 | N | 405 | SER | N-CA-C | -5.57 | 99.84 | 108.42 |
| 9 | Q | 428 | VAL | N-CA-C | -5.57 | 105.97 | 111.77 |
| 1 | Y | 115 | ASP | CA-C-N | 5.57 | 130.03 | 120.72 |
| 1 | Y | 115 | ASP | C-N-CA | 5.57 | 130.03 | 120.72 |
| 14 | h | 924 | ARG | N-CA-C | -5.57 | 98.10 | 108.02 |
| 2 | 1 | 979 | GLN | N-CA-C | -5.57 | 105.74 | 112.54 |
| 5 | H | 290 | GLU | N-CA-C | 5.57 | 118.10 | 110.24 |
| 8 | N | 767 | ILE | N-CA-CB | -5.57 | 104.92 | 112.16 |
| 1 | Y | 849 | LEU | CA-C-O | -5.57 | 114.94 | 120.90 |
| 12 | v | 698 | ASN | N-CA-C | 5.57 | 117.03 | 111.07 |
| 4 | z | 645 | THR | CB-CA-C | -5.57 | 102.13 | 110.88 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 18 | l | 155 | LYS | N-CA-CB | 5.57 | 118.15 | 109.85 |
| 19 | f | 451 | SER | CA-C-O | 5.57 | 124.93 | 119.08 |
| 1 | 0 | 851 | GLU | N-CA-CB | 5.57 | 118.31 | 110.12 |
| 2 | 1 | 1130 | ARG | N-CA-C | -5.57 | 106.48 | 113.72 |
| 5 | H | 344 | SER | CA-C-N | 5.57 | 125.57 | 119.89 |
| 5 | H | 344 | SER | C-N-CA | 5.57 | 125.57 | 119.89 |
| 7 | M | 1240 | HIS | CE1-NE2-CD2 | -5.57 | 103.43 | 109.00 |
| 9 | R | 267 | ASP | CA-C-N | 5.57 | 132.00 | 121.97 |
| 9 | R | 267 | ASP | C-N-CA | 5.57 | 132.00 | 121.97 |
| 9 | T | 357 | LYS | N-CA-C | -5.57 | 100.27 | 108.79 |
| 18 | l | 34 | LYS | N-CA-CB | 5.57 | 119.91 | 110.49 |
| 18 | l | 190 | GLN | O-C-N | 5.57 | 130.13 | 122.72 |
| 19 | m | 600 | TRP | CD2-CE2-CZ2 | -5.57 | 116.83 | 122.40 |
| 18 | e | 312 | TRP | CB-CG-CD2 | 5.57 | 134.60 | 126.80 |
| 20 | g | 508 | ASN | N-CA-C | -5.57 | 100.60 | 109.07 |
| 1 | 0 | 156 | ILE | CA-CB-CG2 | -5.57 | 101.03 | 110.50 |
| 9 | T | 81 | GLU | N-CA-CB | 5.57 | 118.23 | 110.04 |
| 11 | V | 402 | ASN | CA-CB-CG | -5.57 | 107.03 | 112.60 |
| 15 | i | 688 | VAL | N-CA-C | -5.57 | 105.98 | 111.88 |
| 20 | n | 890 | GLN | CB-CG-CD | 5.57 | 122.07 | 112.60 |
| 15 | b | 155 | LEU | N-CA-C | -5.57 | 106.25 | 113.16 |
| 20 | g | 751 | TYR | N-CA-C | -5.57 | 105.21 | 112.23 |
| 7 | M | 606 | VAL | CA-C-O | -5.57 | 115.27 | 121.17 |
| 7 | M | 1671 | VAL | CA-C-N | 5.57 | 127.68 | 120.44 |
| 7 | M | 1671 | VAL | C-N-CA | 5.57 | 127.68 | 120.44 |
| 8 | P | 589 | GLU | O-C-N | -5.57 | 115.62 | 122.25 |
| 9 | R | 791 | GLU | N-CA-C | 5.57 | 118.30 | 110.23 |
| 11 | V | 354 | SER | N-CA-CB | 5.57 | 119.90 | 110.49 |
| 1 | Y | 1152 | TYR | N-CA-C | 5.57 | 117.79 | 111.11 |
| 12 | u | 160 | GLN | CA-C-O | 5.57 | 125.50 | 119.15 |
| 14 | h | 879 | PHE | CA-C-N | 5.57 | 132.17 | 121.54 |
| 14 | h | 879 | PHE | C-N-CA | 5.57 | 132.17 | 121.54 |
| 17 | d | 245 | LYS | N-CA-C | -5.57 | 101.41 | 109.59 |
| 14 | a | 988 | GLN | CA-C-O | -5.57 | 114.65 | 120.55 |
| 4 | J | 818 | ILE | CA-C-N | 5.57 | 128.77 | 120.31 |
| 4 | J | 818 | ILE | C-N-CA | 5.57 | 128.77 | 120.31 |
| 8 | N | 392 | ILE | CB-CG1-CD1 | 5.57 | 125.49 | 113.80 |
| 8 | N | 645 | SER | O-C-N | -5.57 | 116.26 | 122.55 |
| 8 | N | 1161 | PRO | N-CA-C | 5.57 | 120.33 | 111.26 |
| 8 | P | 839 | ILE | N-CA-C | -5.57 | 105.68 | 111.58 |
| 8 | P | 1182 | ASN | N-CA-CB | 5.57 | 118.30 | 110.12 |
| 9 | R | 236 | ASN | CB-CA-C | -5.57 | 101.55 | 110.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | S | 688 | LEU | N-CA-C | -5.57 | 103.84 | 110.41 |
| 1 | Y | 1232 | ARG | NE-CZ-NH1 | 5.57 | 127.07 | 121.50 |
| 16 | j | 325 | LEU | N-CA-C | -5.57 | 106.53 | 113.38 |
| 14 | a | 723 | PHE | O-C-N | 5.57 | 129.99 | 122.59 |
| 5 | B | 418 | GLN | N-CA-C | -5.56 | 106.45 | 113.18 |
| 7 | M | 1365 | ASN | N-CA-C | -5.56 | 99.36 | 108.76 |
| 7 | O | 532 | SER | CA-C-N | 5.56 | 131.40 | 122.83 |
| 7 | O | 532 | SER | C-N-CA | 5.56 | 131.40 | 122.83 |
| 1 | Y | 203 | VAL | CA-C-N | 5.56 | 130.79 | 123.11 |
| 1 | Y | 203 | VAL | C-N-CA | 5.56 | 130.79 | 123.11 |
| 12 | u | 256 | VAL | O-C-N | -5.56 | 116.10 | 121.83 |
| 15 | i | 78 | ASN | N-CA-C | -5.56 | 101.52 | 110.14 |
| 20 | n | 450 | ARG | N-CA-C | -5.56 | 105.70 | 112.88 |
| 20 | n | 469 | THR | N-CA-C | -5.56 | 102.23 | 110.46 |
| 20 | n | 1000 | SER | N-CA-C | -5.56 | 106.33 | 113.23 |
| 16 | c | 555 | GLU | O-C-N | -5.56 | 115.13 | 122.42 |
| 1 | 0 | 632 | TYR | CB-CG-CD2 | -5.56 | 112.45 | 120.80 |
| 6 | C | 330 | LEU | N-CA-CB | 5.56 | 118.30 | 110.12 |
| 4 | G | 817 | GLN | CB-CA-C | 5.56 | 120.12 | 110.72 |
| 8 | N | 900 | ILE | CA-C-N | 5.56 | 129.26 | 120.47 |
| 8 | N | 900 | ILE | C-N-CA | 5.56 | 129.26 | 120.47 |
| 9 | Q | 614 | ARG | CD-NE-CZ | -5.56 | 116.61 | 124.40 |
| 9 | R | 740 | GLU | N-CA-CB | 5.56 | 119.78 | 110.32 |
| 9 | R | 761 | SER | N-CA-C | -5.56 | 104.32 | 113.50 |
| 12 | u | 85 | ASP | N-CA-CB | 5.56 | 119.89 | 110.49 |
| 14 | h | 104 | GLN | O-C-N | -5.56 | 117.30 | 121.47 |
| 17 | k | 224 | SER | N-CA-C | 5.56 | 118.44 | 107.98 |
| 17 | d | 144 | HIS | N-CA-C | -5.56 | 99.66 | 108.73 |
| 19 | f | 430 | PRO | CA-C-O | -5.56 | 111.68 | 119.74 |
| 2 | 1 | 369 | THR | N-CA-C | -5.56 | 100.82 | 109.72 |
| 16 | j | 362 | SER | O-C-N | 5.56 | 128.73 | 122.22 |
| 2 | 1 | 157 | THR | N-CA-C | -5.56 | 100.85 | 109.24 |
| 4 | A | 753 | GLU | CB-CA-C | -5.56 | 101.07 | 110.19 |
| 5 | E | 300 | ASP | N-CA-CB | 5.56 | 118.50 | 110.77 |
| 4 | G | 714 | PHE | N-CA-C | -5.56 | 105.85 | 113.30 |
| 8 | N | 1562 | ASN | OD1-CG-ND2 | -5.56 | 117.04 | 122.60 |
| 7 | O | 823 | PRO | N-CD-CG | 5.56 | 111.54 | 103.20 |
| 7 | O | 1557 | PRO | CA-C-N | 5.56 | 131.11 | 122.49 |
| 7 | O | 1557 | PRO | C-N-CA | 5.56 | 131.11 | 122.49 |
| 7 | O | 1577 | LYS | CA-C-O | 5.56 | 128.46 | 120.51 |
| 12 | u | 138 | ARG | NE-CZ-NH2 | -5.56 | 114.20 | 119.20 |
| 14 | h | 657 | LEU | CA-C-N | 5.56 | 128.50 | 120.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 657 | LEU | C-N-CA | 5.56 | 128.50 | 120.38 |
| 19 | m | 670 | LYS | N-CA-C | 5.56 | 119.32 | 112.54 |
| 15 | b | 390 | TRP | CD2-CE2-CZ2 | -5.56 | 116.84 | 122.40 |
| 14 | a | 170 | SER | CA-C-N | 5.56 | 126.79 | 119.84 |
| 14 | a | 170 | SER | C-N-CA | 5.56 | 126.79 | 119.84 |
| 2 | 1 | 145 | ASN | CA-CB-CG | 5.56 | 118.16 | 112.60 |
| 2 | 1 | 211 | PRO | N-CA-C | -5.56 | 101.02 | 112.47 |
| 2 | 1 | 1098 | LEU | N-CA-C | -5.56 | 104.03 | 111.87 |
| 5 | B | 344 | SER | CA-C-O | -5.56 | 114.24 | 119.91 |
| 6 | F | 301 | HIS | ND1-CE1-NE2 | 5.56 | 113.96 | 108.40 |
| 7 | M | 166 | GLN | N-CA-C | -5.56 | 106.17 | 113.17 |
| 7 | O | 270 | THR | CA-CB-OG1 | 5.56 | 117.94 | 109.60 |
| 7 | O | 722 | ARG | NE-CZ-NH2 | -5.56 | 114.20 | 119.20 |
| 7 | O | 908 | GLY | CA-C-N | 5.56 | 128.28 | 120.28 |
| 7 | O | 908 | GLY | C-N-CA | 5.56 | 128.28 | 120.28 |
| 13 | w | 1357 | ASN | N-CA-C | 5.56 | 117.34 | 111.28 |
| 14 | h | 4 | LEU | O-C-N | 5.56 | 129.96 | 122.96 |
| 18 | l | 165 | LEU | N-CA-C | -5.56 | 105.28 | 113.61 |
| 20 | n | 264 | ASN | CA-C-N | 5.56 | 132.16 | 121.54 |
| 20 | n | 264 | ASN | C-N-CA | 5.56 | 132.16 | 121.54 |
| 15 | b | 277 | THR | O-C-N | -5.56 | 114.64 | 122.26 |
| 15 | b | 478 | ASP | CA-CB-CG | -5.56 | 107.04 | 112.60 |
| 20 | g | 272 | ASN | CA-C-N | 5.56 | 130.59 | 121.87 |
| 20 | g | 272 | ASN | C-N-CA | 5.56 | 130.59 | 121.87 |
| 5 | B | 511 | GLU | CB-CG-CD | 5.56 | 122.05 | 112.60 |
| 5 | E | 440 | PHE | CA-C-O | 5.56 | 126.36 | 119.97 |
| 4 | J | 651 | SER | CA-C-O | -5.56 | 113.58 | 119.97 |
| 7 | O | 251 | ASP | N-CA-C | -5.56 | 106.43 | 113.43 |
| 2 | Z | 850 | HIS | CB-CG-CD2 | -5.56 | 123.98 | 131.20 |
| 15 | i | 719 | SER | CB-CA-C | 5.56 | 120.14 | 111.70 |
| 2 | 1 | 235 | ILE | O-C-N | 5.55 | 128.72 | 122.67 |
| 7 | M | 1527 | ARG | N-CA-CB | 5.55 | 118.22 | 109.94 |
| 8 | N | 643 | GLU | N-CA-CB | 5.55 | 118.77 | 110.22 |
| 7 | O | 1526 | ILE | CA-C-N | 5.55 | 127.66 | 120.44 |
| 7 | O | 1526 | ILE | C-N-CA | 5.55 | 127.66 | 120.44 |
| 9 | Q | 812 | GLN | OE1-CD-NE2 | -5.55 | 117.05 | 122.60 |
| 9 | R | 673 | PRO | N-CA-CB | 5.55 | 108.14 | 103.25 |
| 9 | R | 823 | ARG | N-CA-C | -5.55 | 107.14 | 114.31 |
| 9 | S | 573 | HIS | CE1-NE2-CD2 | -5.55 | 103.44 | 109.00 |
| 1 | Y | 1094 | ARG | CA-C-N | 5.55 | 127.99 | 120.38 |
| 1 | Y | 1094 | ARG | C-N-CA | 5.55 | 127.99 | 120.38 |
| 14 | h | 650 | HIS | O-C-N | -5.55 | 116.23 | 122.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | i | 553 | ILE | CA-CB-CG1 | 5.55 | 119.84 | 110.40 |
| 18 | l | 208 | LEU | O-C-N | -5.55 | 114.93 | 121.32 |
| 18 | e | 18 | ASP | N-CA-C | -5.55 | 102.54 | 110.59 |
| 18 | e | 211 | HIS | CE1-NE2-CD2 | -5.55 | 103.44 | 109.00 |
| 5 | B | 409 | GLU | CA-C-N | 5.55 | 127.72 | 120.28 |
| 5 | B | 409 | GLU | C-N-CA | 5.55 | 127.72 | 120.28 |
| 4 | D | 753 | GLU | N-CA-C | -5.55 | 101.81 | 110.42 |
| 9 | S | 67 | THR | N-CA-C | -5.55 | 98.97 | 110.80 |
| 9 | S | 834 | ASN | CA-C-N | 5.55 | 131.70 | 121.70 |
| 9 | S | 834 | ASN | C-N-CA | 5.55 | 131.70 | 121.70 |
| 1 | Y | 422 | LYS | N-CA-C | -5.55 | 100.62 | 109.23 |
| 12 | u | 628 | MET | N-CA-C | 5.55 | 117.01 | 111.07 |
| 20 | n | 547 | PRO | N-CA-CB | 5.55 | 108.47 | 103.08 |
| 21 | s | 16 | ILE | CA-C-N | 5.55 | 130.61 | 121.39 |
| 21 | s | 16 | ILE | C-N-CA | 5.55 | 130.61 | 121.39 |
| 2 | 1 | 119 | LYS | N-CA-C | -5.55 | 105.11 | 112.94 |
| 4 | G | 702 | ARG | N-CA-C | -5.55 | 106.40 | 114.12 |
| 4 | G | 747 | THR | CA-C-N | 5.55 | 128.17 | 120.29 |
| 4 | G | 747 | THR | C-N-CA | 5.55 | 128.17 | 120.29 |
| 7 | M | 334 | GLN | N-CA-C | -5.55 | 107.51 | 114.56 |
| 8 | N | 362 | LEU | N-CA-C | -5.55 | 105.23 | 111.28 |
| 8 | N | 1051 | LYS | N-CA-C | 5.55 | 118.12 | 110.35 |
| 8 | N | 1314 | SER | CA-C-N | 5.55 | 128.36 | 120.53 |
| 8 | N | 1314 | SER | C-N-CA | 5.55 | 128.36 | 120.53 |
| 7 | O | 179 | ILE | N-CA-C | 5.55 | 116.28 | 110.62 |
| 7 | O | 754 | ASP | CB-CA-C | -5.55 | 101.93 | 110.81 |
| 7 | O | 1099 | TYR | CA-C-O | -5.55 | 114.97 | 120.80 |
| 9 | Q | 315 | LYS | CA-C-N | 5.55 | 132.14 | 121.54 |
| 9 | Q | 315 | LYS | C-N-CA | 5.55 | 132.14 | 121.54 |
| 1 | Y | 179 | LEU | CA-C-N | 5.55 | 132.15 | 121.54 |
| 1 | Y | 179 | LEU | C-N-CA | 5.55 | 132.15 | 121.54 |
| 4 | y | 767 | VAL | CA-C-N | 5.55 | 128.17 | 120.29 |
| 4 | y | 767 | VAL | C-N-CA | 5.55 | 128.17 | 120.29 |
| 16 | j | 413 | PRO | N-CA-C | 5.55 | 120.04 | 111.21 |
| 18 | e | 221 | ALA | CA-C-N | 5.55 | 125.48 | 119.76 |
| 18 | e | 221 | ALA | C-N-CA | 5.55 | 125.48 | 119.76 |
| 20 | g | 142 | PHE | N-CA-C | -5.55 | 100.53 | 109.58 |
| 2 | 1 | 107 | ASN | CA-C-N | 5.55 | 129.09 | 120.60 |
| 2 | 1 | 107 | ASN | C-N-CA | 5.55 | 129.09 | 120.60 |
| 7 | M | 19 | GLU | CA-C-N | 5.55 | 130.14 | 121.76 |
| 7 | M | 19 | GLU | C-N-CA | 5.55 | 130.14 | 121.76 |
| 7 | M | 1196 | SER | CA-C-N | 5.55 | 131.26 | 122.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 1196 | SER | C-N-CA | 5.55 | 131.26 | 122.60 |
| 8 | N | 894 | VAL | CA-CB-CG2 | -5.55 | 100.97 | 110.40 |
| 7 | O | 1434 | SER | CB-CA-C | 5.55 | 118.91 | 109.53 |
| 2 | Z | 1382 | TYR | N-CA-C | -5.55 | 98.98 | 110.80 |
| 20 | n | 340 | GLN | N-CA-C | -5.55 | 100.09 | 108.52 |
| 16 | c | 524 | ASP | N-CA-CB | 5.55 | 118.77 | 110.22 |
| 17 | d | 231 | CYS | N-CA-C | -5.55 | 99.38 | 108.76 |
| 2 | 1 | 748 | THR | N-CA-C | 5.55 | 117.90 | 110.35 |
| 4 | G | 794 | ILE | N-CA-C | -5.55 | 104.16 | 111.09 |
| 8 | N | 459 | ASP | CA-C-O | 5.55 | 127.02 | 120.58 |
| 8 | P | 61 | ASN | CB-CG-ND2 | 5.55 | 124.72 | 116.40 |
| 9 | S | 611 | LEU | N-CA-C | -5.55 | 100.14 | 108.96 |
| 11 | X | 401 | ASP | N-CA-C | 5.55 | 122.62 | 110.80 |
| 18 | e | 70 | ARG | NE-CZ-NH2 | 5.55 | 124.19 | 119.20 |
| 5 | E | 348 | ILE | CA-C-O | -5.55 | 117.06 | 119.94 |
| 8 | N | 450 | THR | N-CA-C | 5.55 | 122.61 | 110.80 |
| 8 | N | 912 | TRP | CZ3-CH2-CZ2 | -5.55 | 114.29 | 121.50 |
| 7 | O | 1117 | THR | CA-C-O | -5.55 | 115.50 | 121.38 |
| 7 | O | 1527 | ARG | CA-C-N | 5.55 | 128.04 | 120.77 |
| 7 | O | 1527 | ARG | C-N-CA | 5.55 | 128.04 | 120.77 |
| 8 | P | 291 | ASP | CA-CB-CG | 5.55 | 118.15 | 112.60 |
| 9 | T | 541 | TYR | N-CA-C | -5.55 | 104.08 | 111.24 |
| 1 | Y | 608 | ILE | N-CA-C | -5.55 | 99.65 | 107.75 |
| 1 | Y | 690 | ASN | N-CA-C | -5.55 | 106.64 | 113.41 |
| 4 | y | 722 | LEU | CA-C-O | -5.55 | 114.67 | 120.55 |
| 14 | h | 743 | ASN | CA-CB-CG | -5.55 | 107.05 | 112.60 |
| 16 | j | 252 | ASN | CA-C-N | 5.55 | 131.53 | 122.65 |
| 16 | j | 252 | ASN | C-N-CA | 5.55 | 131.53 | 122.65 |
| 16 | j | 391 | TYR | CB-CA-C | 5.55 | 120.09 | 110.72 |
| 17 | k | 238 | ASN | CA-C-N | 5.55 | 128.27 | 120.28 |
| 17 | k | 238 | ASN | C-N-CA | 5.55 | 128.27 | 120.28 |
| 20 | n | 923 | HIS | CG-CD2-NE2 | 5.55 | 112.75 | 107.20 |
| 15 | b | 158 | PHE | CA-CB-CG | 5.55 | 119.35 | 113.80 |
| 18 | e | 50 | SER | CB-CA-C | -5.55 | 101.75 | 110.79 |
| 1 | 0 | 943 | ASP | N-CA-C | -5.54 | 105.20 | 112.41 |
| 7 | M | 215 | SER | CA-C-O | -5.54 | 115.00 | 120.82 |
| 8 | P | 1163 | LEU | N-CA-CB | 5.54 | 118.98 | 110.61 |
| 10 | U | 326 | ARG | NE-CZ-NH2 | -5.54 | 114.21 | 119.20 |
| 1 | Y | 198 | ASP | N-CA-C | 5.54 | 117.32 | 111.28 |
| 19 | m | 382 | LYS | N-CA-C | -5.54 | 102.43 | 110.08 |
| 19 | f | 206 | ILE | N-CA-C | -5.54 | 107.33 | 112.43 |
| 1 | 0 | 1381 | SER | CA-C-N | 5.54 | 132.13 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 1381 | SER | C-N-CA | 5.54 | 132.13 | 121.54 |
| 4 | A | 713 | ASN | N-CA-C | -5.54 | 106.52 | 113.28 |
| 7 | M | 1479 | LEU | N-CA-C | -5.54 | 105.64 | 112.90 |
| 8 | N | 1250 | ILE | CB-CA-C | -5.54 | 105.81 | 112.19 |
| 9 | R | 96 | LEU | CA-C-O | 5.54 | 126.64 | 120.82 |
| 13 | x | 1442 | ALA | O-C-N | -5.54 | 116.36 | 122.07 |
| 15 | i | 536 | LYS | N-CA-CB | 5.54 | 118.38 | 110.67 |
| 19 | m | 450 | SER | CA-C-N | 5.54 | 132.13 | 121.54 |
| 19 | m | 450 | SER | C-N-CA | 5.54 | 132.13 | 121.54 |
| 20 | n | 969 | VAL | N-CA-CB | 5.54 | 120.11 | 110.96 |
| 15 | b | 107 | TYR | CA-C-N | 5.54 | 127.66 | 120.56 |
| 15 | b | 107 | TYR | C-N-CA | 5.54 | 127.66 | 120.56 |
| 20 | g | 235 | ASN | CA-CB-CG | 5.54 | 118.14 | 112.60 |
| 2 | 1 | 225 | ALA | CB-CA-C | -5.54 | 101.10 | 110.19 |
| 5 | E | 371 | GLN | OE1-CD-NE2 | 5.54 | 128.14 | 122.60 |
| 4 | J | 652 | ALA | O-C-N | 5.54 | 127.99 | 122.12 |
| 9 | S | 131 | GLY | O-C-N | -5.54 | 116.86 | 122.18 |
| 11 | X | 280 | ILE | CA-CB-CG1 | 5.54 | 119.82 | 110.40 |
| 2 | Z | 651 | PHE | N-CA-C | -5.54 | 105.34 | 111.71 |
| 12 | u | 91 | MET | CA-C-O | 5.54 | 127.25 | 120.60 |
| 12 | v | 168 | LYS | O-C-N | -5.54 | 115.22 | 121.43 |
| 15 | b | 300 | SER | N-CA-C | -5.54 | 105.87 | 113.30 |
| 16 | c | 479 | ALA | CB-CA-C | -5.54 | 101.59 | 110.79 |
| 14 | a | 155 | PRO | N-CA-CB | -5.54 | 97.43 | 103.25 |
| 1 | 0 | 1088 | PHE | O-C-N | -5.54 | 116.47 | 123.01 |
| 5 | K | 311 | PHE | CA-CB-CG | -5.54 | 108.26 | 113.80 |
| 2 | Z | 1057 | TYR | O-C-N | 5.54 | 128.07 | 122.09 |
| 2 | Z | 1163 | LEU | CA-C-N | 5.54 | 127.70 | 120.28 |
| 2 | Z | 1163 | LEU | C-N-CA | 5.54 | 127.70 | 120.28 |
| 21 | t | 73 | LYS | CB-CG-CD | 5.54 | 124.04 | 111.30 |
| 19 | f | 672 | VAL | N-CA-C | -5.54 | 106.91 | 112.17 |
| 20 | g | 936 | LYS | CA-C-N | 5.54 | 132.12 | 121.54 |
| 20 | g | 936 | LYS | C-N-CA | 5.54 | 132.12 | 121.54 |
| 7 | O | 188 | ARG | CA-C-N | 5.54 | 128.25 | 120.28 |
| 7 | O | 188 | ARG | C-N-CA | 5.54 | 128.25 | 120.28 |
| 7 | O | 1061 | ASN | N-CA-C | -5.54 | 105.30 | 113.61 |
| 7 | O | 1590 | LYS | N-CA-C | 5.54 | 117.00 | 111.07 |
| 8 | P | 1565 | ASN | CA-CB-CG | 5.54 | 118.14 | 112.60 |
| 9 | Q | 89 | ASP | O-C-N | 5.54 | 127.77 | 122.07 |
| 14 | h | 14 | TYR | CA-CB-CG | -5.54 | 103.93 | 113.90 |
| 14 | h | 923 | LEU | CA-C-O | -5.54 | 115.68 | 121.55 |
| 1 | 0 | 282 | ILE | N-CA-CB | 5.54 | 116.76 | 110.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 1080 | VAL | CB-CA-C | -5.54 | 104.61 | 111.70 |
| 7 | M | 137 | ASN | OD1-CG-ND2 | 5.54 | 128.14 | 122.60 |
| 7 | M | 951 | ARG | N-CA-C | -5.54 | 105.21 | 112.41 |
| 8 | P | 691 | SER | N-CA-CB | 5.54 | 119.85 | 110.49 |
| 9 | R | 72 | LEU | N-CA-CB | 5.54 | 118.04 | 110.01 |
| 9 | S | 442 | LEU | CB-CA-C | -5.54 | 100.04 | 109.51 |
| 9 | T | 158 | ASN | N-CA-CB | 5.54 | 118.10 | 110.07 |
| 1 | Y | 162 | HIS | CE1-NE2-CD2 | -5.54 | 103.46 | 109.00 |
| 2 | Z | 1215 | TYR | CB-CA-C | 5.54 | 119.50 | 109.37 |
| 19 | m | 171 | VAL | O-C-N | 5.54 | 129.76 | 122.12 |
| 21 | p | 38 | GLU | CA-C-O | -5.54 | 114.68 | 120.55 |
| 19 | f | 301 | TYR | N-CA-C | -5.54 | 105.34 | 111.71 |
| 1 | 0 | 642 | LEU | CA-C-N | 5.54 | 131.28 | 122.59 |
| 1 | 0 | 642 | LEU | C-N-CA | 5.54 | 131.28 | 122.59 |
| 8 | N | 1064 | GLU | O-C-N | -5.54 | 116.11 | 122.09 |
| 7 | O | 975 | SER | CA-C-N | 5.54 | 128.01 | 120.54 |
| 7 | O | 975 | SER | C-N-CA | 5.54 | 128.01 | 120.54 |
| 7 | O | 1340 | SER | CA-C-N | 5.54 | 129.97 | 120.72 |
| 7 | O | 1340 | SER | C-N-CA | 5.54 | 129.97 | 120.72 |
| 7 | O | 1591 | ASP | CB-CA-C | -5.54 | 101.60 | 110.79 |
| 9 | R | 777 | ILE | CA-C-N | 5.54 | 127.64 | 120.44 |
| 9 | R | 777 | ILE | C-N-CA | 5.54 | 127.64 | 120.44 |
| 9 | T | 826 | ARG | N-CA-C | 5.54 | 117.75 | 111.11 |
| 1 | Y | 921 | GLY | N-CA-C | -5.54 | 105.95 | 113.37 |
| 12 | u | 158 | ASN | CA-C-O | 5.54 | 127.94 | 121.46 |
| 12 | u | 298 | THR | N-CA-C | -5.54 | 102.29 | 110.48 |
| 15 | i | 550 | HIS | CA-C-N | 5.54 | 132.11 | 121.54 |
| 15 | i | 550 | HIS | C-N-CA | 5.54 | 132.11 | 121.54 |
| 16 | j | 330 | PRO | CB-CA-C | -5.54 | 102.43 | 111.56 |
| 20 | g | 248 | LEU | CA-C-N | 5.54 | 127.96 | 120.38 |
| 20 | g | 248 | LEU | C-N-CA | 5.54 | 127.96 | 120.38 |
| 1 | 0 | 365 | ARG | CD-NE-CZ | -5.53 | 116.65 | 124.40 |
| 2 | 1 | 1002 | ILE | CA-C-N | 5.53 | 127.69 | 120.28 |
| 2 | 1 | 1002 | ILE | C-N-CA | 5.53 | 127.69 | 120.28 |
| 5 | B | 346 | GLN | N-CA-CB | 5.53 | 119.84 | 110.49 |
| 6 | C | 397 | ALA | CA-C-N | 5.53 | 128.04 | 120.46 |
| 6 | C | 397 | ALA | C-N-CA | 5.53 | 128.04 | 120.46 |
| 5 | H | 408 | ILE | N-CA-C | 5.53 | 116.26 | 110.62 |
| 7 | M | 1123 | ASN | CA-CB-CG | 5.53 | 118.13 | 112.60 |
| 7 | M | 1526 | ILE | N-CA-C | -5.53 | 105.11 | 110.42 |
| 8 | N | 1448 | SER | CB-CA-C | -5.53 | 102.19 | 110.88 |
| 7 | O | 163 | ASN | CA-C-N | 5.53 | 127.69 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 163 | ASN | C-N-CA | 5.53 | 127.69 | 120.28 |
| 8 | P | 1429 | HIS | CA-C-N | 5.53 | 128.15 | 120.29 |
| 8 | P | 1429 | HIS | C-N-CA | 5.53 | 128.15 | 120.29 |
| 9 | R | 334 | TRP | CE2-CD2-CE3 | 5.53 | 124.33 | 118.80 |
| 1 | Y | 1211 | PHE | CA-CB-CG | 5.53 | 119.33 | 113.80 |
| 2 | Z | 751 | GLN | OE1-CD-NE2 | 5.53 | 128.13 | 122.60 |
| 2 | Z | 1190 | GLN | CA-C-N | 5.53 | 127.64 | 120.44 |
| 2 | Z | 1190 | GLN | C-N-CA | 5.53 | 127.64 | 120.44 |
| 12 | u | 634 | ILE | O-C-N | 5.53 | 127.33 | 121.91 |
| 13 | w | 1299 | VAL | CA-C-O | -5.53 | 114.91 | 121.05 |
| 14 | h | 694 | ASN | N-CA-C | -5.53 | 100.94 | 108.24 |
| 14 | h | 780 | HIS | N-CA-C | -5.53 | 99.59 | 108.55 |
| 20 | n | 649 | PHE | CA-C-O | 5.53 | 125.77 | 119.18 |
| 15 | b | 691 | VAL | CA-C-N | 5.53 | 129.74 | 121.77 |
| 15 | b | 691 | VAL | C-N-CA | 5.53 | 129.74 | 121.77 |
| 16 | c | 210 | ILE | CA-C-O | -5.53 | 114.68 | 120.27 |
| 19 | f | 253 | GLN | OE1-CD-NE2 | 5.53 | 128.13 | 122.60 |
| 20 | g | 552 | THR | N-CA-C | -5.53 | 106.38 | 113.02 |
| 14 | a | 553 | ILE | N-CA-C | -5.53 | 105.13 | 110.72 |
| 6 | I | 445 | GLU | CA-C-N | 5.53 | 127.69 | 120.28 |
| 6 | I | 445 | GLU | C-N-CA | 5.53 | 127.69 | 120.28 |
| 7 | M | 786 | THR | CA-CB-OG1 | 5.53 | 117.90 | 109.60 |
| 14 | h | 923 | LEU | O-C-N | 5.53 | 129.61 | 122.81 |
| 20 | n | 1081 | VAL | N-CA-C | 5.53 | 116.26 | 110.62 |
| 7 | M | 111 | GLN | N-CA-C | -5.53 | 104.11 | 111.24 |
| 7 | M | 662 | PRO | O-C-N | 5.53 | 128.29 | 122.93 |
| 7 | M | 1021 | HIS | CA-C-O | 5.53 | 126.82 | 120.90 |
| 8 | N | 1398 | VAL | CA-CB-CG1 | 5.53 | 119.80 | 110.40 |
| 7 | O | 743 | GLY | N-CA-C | -5.53 | 107.56 | 115.64 |
| 7 | O | 1671 | VAL | CA-C-N | 5.53 | 127.63 | 120.44 |
| 7 | O | 1671 | VAL | C-N-CA | 5.53 | 127.63 | 120.44 |
| 9 | R | 114 | ARG | CB-CA-C | 5.53 | 119.33 | 109.65 |
| 9 | T | 600 | ILE | N-CA-C | -5.53 | 96.94 | 108.88 |
| 2 | Z | 281 | VAL | CA-C-O | -5.53 | 114.72 | 121.13 |
| 2 | Z | 1346 | LEU | CA-C-O | 5.53 | 125.74 | 119.27 |
| 13 | x | 1108 | ASP | CA-C-O | -5.53 | 114.93 | 120.96 |
| 15 | i | 144 | VAL | CA-C-N | 5.53 | 127.69 | 120.28 |
| 15 | i | 144 | VAL | C-N-CA | 5.53 | 127.69 | 120.28 |
| 20 | n | 977 | ASN | CA-C-O | 5.53 | 126.96 | 120.43 |
| 18 | e | 54 | HIS | CG-CD2-NE2 | 5.53 | 112.73 | 107.20 |
| 19 | f | 149 | THR | CA-C-O | -5.53 | 115.00 | 120.70 |
| 19 | f | 315 | LEU | CA-C-N | 5.53 | 126.75 | 119.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | f | 315 | LEU | C-N-CA | 5.53 | 126.75 | 119.84 |
| 2 | 1 | 267 | GLU | CA-C-O | 5.53 | 125.22 | 119.14 |
| 2 | 1 | 1175 | ASN | OD1-CG-ND2 | 5.53 | 128.13 | 122.60 |
| 2 | 1 | 1176 | LEU | CA-C-N | 5.53 | 129.82 | 120.64 |
| 2 | 1 | 1176 | LEU | C-N-CA | 5.53 | 129.82 | 120.64 |
| 5 | K | 329 | HIS | CB-CG-CD2 | -5.53 | 124.01 | 131.20 |
| 8 | N | 17 | HIS | CB-CG-ND1 | -5.53 | 114.41 | 122.70 |
| 8 | N | 857 | LEU | N-CA-CB | 5.53 | 118.35 | 110.06 |
| 9 | T | 372 | LYS | N-CA-C | -5.53 | 104.78 | 113.02 |
| 21 | t | 50 | ASP | O-C-N | -5.53 | 116.26 | 122.12 |
| 2 | 1 | 871 | VAL | CA-CB-CG1 | -5.53 | 101.00 | 110.40 |
| 6 | C | 389 | ARG | N-CA-CB | 5.53 | 118.25 | 110.12 |
| 4 | G | 712 | ASP | CA-C-O | 5.53 | 126.19 | 119.11 |
| 7 | O | 1291 | SER | N-CA-CB | 5.53 | 118.03 | 110.01 |
| 9 | Q | 19 | ASN | CA-C-N | 5.53 | 127.96 | 120.44 |
| 9 | Q | 19 | ASN | C-N-CA | 5.53 | 127.96 | 120.44 |
| 9 | R | 722 | SER | N-CA-CB | 5.53 | 118.25 | 110.12 |
| 9 | S | 806 | LEU | CA-C-O | -5.53 | 113.27 | 119.79 |
| 1 | Y | 1438 | ASP | CA-C-N | 5.53 | 132.10 | 121.54 |
| 1 | Y | 1438 | ASP | C-N-CA | 5.53 | 132.10 | 121.54 |
| 16 | c | 213 | SER | O-C-N | 5.53 | 129.63 | 123.05 |
| 17 | d | 199 | THR | N-CA-C | -5.53 | 99.30 | 108.75 |
| 20 | g | 1027 | ASN | N-CA-C | -5.53 | 106.70 | 113.50 |
| 14 | a | 657 | LEU | CA-C-O | -5.53 | 114.69 | 120.55 |
| 8 | N | 1613 | ASN | CA-C-N | 5.53 | 127.62 | 120.44 |
| 8 | N | 1613 | ASN | C-N-CA | 5.53 | 127.62 | 120.44 |
| 7 | O | 1443 | ASN | N-CA-C | 5.53 | 119.52 | 112.34 |
| 8 | P | 196 | ASN | N-CA-C | -5.53 | 104.79 | 112.30 |
| 9 | R | 236 | ASN | O-C-N | 5.53 | 127.98 | 122.12 |
| 9 | R | 586 | PHE | N-CA-C | 5.53 | 120.13 | 113.17 |
| 4 | z | 771 | ASN | N-CA-C | -5.53 | 105.16 | 111.07 |
| 14 | h | 242 | HIS | CE1-NE2-CD2 | -5.53 | 103.47 | 109.00 |
| 15 | i | 371 | SER | CB-CA-C | -5.53 | 101.25 | 110.81 |
| 15 | i | 510 | HIS | CG-CD2-NE2 | 5.53 | 112.73 | 107.20 |
| 20 | n | 341 | ASP | N-CA-CB | 5.53 | 119.45 | 110.77 |
| 19 | f | 694 | VAL | CA-C-O | 5.53 | 125.38 | 119.91 |
| 14 | a | 12 | LEU | N-CA-C | -5.53 | 104.74 | 112.25 |
| 14 | a | 886 | LEU | O-C-N | -5.53 | 115.24 | 122.59 |
| 4 | G | 762 | LEU | O-C-N | -5.52 | 116.38 | 122.07 |
| 5 | H | 517 | GLN | CA-C-N | 5.52 | 127.62 | 120.44 |
| 5 | H | 517 | GLN | C-N-CA | 5.52 | 127.62 | 120.44 |
| 7 | M | 1423 | SER | CA-C-N | 5.52 | 127.95 | 120.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 1423 | SER | C-N-CA | 5.52 | 127.95 | 120.38 |
| 1 | Y | 1427 | TYR | CB-CG-CD2 | -5.52 | 112.51 | 120.80 |
| 15 | i | 639 | ARG | N-CA-CB | 5.52 | 119.03 | 110.80 |
| 16 | j | 235 | LYS | O-C-N | 5.52 | 128.45 | 122.15 |
| 19 | m | 375 | ALA | O-C-N | -5.52 | 116.46 | 122.92 |
| 1 | 0 | 1239 | ALA | N-CA-C | -5.52 | 106.04 | 112.89 |
| 6 | L | 292 | HIS | CE1-NE2-CD2 | -5.52 | 103.48 | 109.00 |
| 9 | Q | 18 | ALA | CA-C-N | 5.52 | 128.71 | 120.31 |
| 9 | Q | 18 | ALA | C-N-CA | 5.52 | 128.71 | 120.31 |
| 9 | S | 16 | LYS | N-CA-CB | 5.52 | 118.24 | 110.12 |
| 9 | S | 671 | ASP | N-CA-CB | 5.52 | 119.82 | 110.49 |
| 14 | h | 404 | VAL | O-C-N | -5.52 | 115.67 | 122.57 |
| 20 | n | 670 | THR | CA-C-N | 5.52 | 128.23 | 120.28 |
| 20 | n | 670 | THR | C-N-CA | 5.52 | 128.23 | 120.28 |
| 21 | r | 41 | ILE | CA-C-O | -5.52 | 115.32 | 121.17 |
| 14 | a | 703 | ASP | CA-CB-CG | -5.52 | 107.08 | 112.60 |
| 6 | C | 347 | THR | CA-C-N | 5.52 | 127.68 | 120.28 |
| 6 | C | 347 | THR | C-N-CA | 5.52 | 127.68 | 120.28 |
| 5 | H | 529 | LYS | CA-C-N | 5.52 | 128.13 | 120.29 |
| 5 | H | 529 | LYS | C-N-CA | 5.52 | 128.13 | 120.29 |
| 8 | N | 262 | SER | N-CA-C | -5.52 | 104.66 | 111.40 |
| 2 | Z | 543 | PRO | O-C-N | -5.52 | 115.19 | 122.64 |
| 20 | n | 827 | THR | CA-CB-OG1 | 5.52 | 117.88 | 109.60 |
| 5 | B | 305 | LYS | N-CA-CB | 5.52 | 120.86 | 112.47 |
| 4 | G | 691 | ASN | CA-CB-CG | 5.52 | 118.12 | 112.60 |
| 8 | N | 1010 | GLU | O-C-N | 5.52 | 129.93 | 122.59 |
| 7 | O | 1413 | LEU | N-CA-C | 5.52 | 118.06 | 111.71 |
| 8 | P | 1421 | ILE | CA-CB-CG2 | 5.52 | 119.88 | 110.50 |
| 9 | R | 114 | ARG | N-CA-C | -5.52 | 98.92 | 108.69 |
| 9 | T | 89 | ASP | O-C-N | -5.52 | 115.48 | 122.27 |
| 9 | T | 702 | ILE | N-CA-C | 5.52 | 116.25 | 110.62 |
| 1 | Y | 110 | HIS | CA-CB-CG | 5.52 | 119.32 | 113.80 |
| 1 | Y | 1240 | ASN | OD1-CG-ND2 | 5.52 | 128.12 | 122.60 |
| 1 | Y | 1332 | ASP | N-CA-CB | 5.52 | 119.82 | 110.49 |
| 4 | y | 693 | ILE | N-CA-C | 5.52 | 116.30 | 110.72 |
| 14 | h | 620 | HIS | CA-CB-CG | 5.52 | 119.32 | 113.80 |
| 19 | m | 180 | PHE | CA-C-O | -5.52 | 113.62 | 119.97 |
| 20 | n | 600 | PHE | N-CA-C | 5.52 | 116.98 | 111.07 |
| 20 | n | 1113 | ILE | CA-C-N | 5.52 | 127.95 | 120.44 |
| 20 | n | 1113 | ILE | C-N-CA | 5.52 | 127.95 | 120.44 |
| 2 | 1 | 153 | GLN | N-CA-C | -5.52 | 105.91 | 113.30 |
| 2 | 1 | 1378 | PRO | CA-C-O | -5.52 | 112.63 | 118.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | C | 281 | ASP | CA-C-O | 5.52 | 126.79 | 121.00 |
| 5 | E | 442 | THR | CA-C-N | 5.52 | 127.67 | 120.28 |
| 5 | E | 442 | THR | C-N-CA | 5.52 | 127.67 | 120.28 |
| 5 | H | 367 | GLU | N-CA-CB | 5.52 | 118.83 | 110.28 |
| 7 | O | 539 | ASN | CA-CB-CG | -5.52 | 107.08 | 112.60 |
| 9 | Q | 658 | ASN | CA-CB-CG | 5.52 | 118.12 | 112.60 |
| 9 | T | 431 | SER | O-C-N | -5.52 | 116.75 | 123.10 |
| 9 | T | 766 | ASN | CA-CB-CG | -5.52 | 107.08 | 112.60 |
| 10 | U | 319 | LYS | CA-C-N | 5.52 | 132.08 | 121.54 |
| 10 | U | 319 | LYS | C-N-CA | 5.52 | 132.08 | 121.54 |
| 10 | W | 328 | LEU | CA-C-O | 5.52 | 125.81 | 119.35 |
| 1 | Y | 987 | ALA | CA-C-N | 5.52 | 128.22 | 120.28 |
| 1 | Y | 987 | ALA | C-N-CA | 5.52 | 128.22 | 120.28 |
| 2 | Z | 504 | PRO | N-CA-C | -5.52 | 106.96 | 113.86 |
| 14 | h | 819 | TYR | CA-CB-CG | -5.52 | 103.97 | 113.90 |
| 15 | i | 363 | TYR | CB-CA-C | -5.52 | 101.23 | 110.56 |
| 15 | b | 330 | ASP | N-CA-C | -5.52 | 106.71 | 113.50 |
| 20 | g | 992 | LYS | CB-CA-C | -5.52 | 101.83 | 110.94 |
| 7 | M | 60 | ASP | CA-CB-CG | 5.52 | 118.12 | 112.60 |
| 8 | N | 364 | THR | CA-C-O | 5.52 | 126.45 | 120.55 |
| 9 | R | 250 | ASN | N-CA-CB | 5.52 | 118.23 | 110.12 |
| 1 | Y | 1240 | ASN | N-CA-C | -5.52 | 106.55 | 113.28 |
| 15 | i | 591 | LEU | CA-C-O | -5.52 | 114.70 | 120.55 |
| 20 | n | 477 | PHE | N-CA-CB | 5.52 | 119.25 | 110.65 |
| 15 | b | 531 | LEU | CA-C-O | -5.52 | 114.05 | 120.34 |
| 16 | c | 611 | SER | O-C-N | 5.52 | 129.15 | 122.20 |
| 19 | f | 614 | PRO | N-CA-CB | 5.52 | 109.04 | 103.25 |
| 8 | N | 1250 | ILE | CA-C-O | 5.51 | 125.65 | 120.14 |
| 8 | P | 1176 | PRO | O-C-N | -5.51 | 115.50 | 122.17 |
| 8 | P | 1536 | TRP | N-CA-C | 5.51 | 118.31 | 110.10 |
| 1 | Y | 651 | LYS | N-CA-C | -5.51 | 102.36 | 110.52 |
| 2 | Z | 1225 | VAL | N-CA-C | -5.51 | 107.61 | 112.90 |
| 12 | v | 311 | GLN | N-CA-CB | 5.51 | 120.29 | 111.91 |
| 15 | i | 267 | ARG | NE-CZ-NH1 | 5.51 | 127.02 | 121.50 |
| 21 | t | 17 | THR | O-C-N | 5.51 | 129.52 | 123.01 |
| 8 | N | 336 | GLN | N-CA-C | -5.51 | 105.17 | 112.94 |
| 7 | O | 60 | ASP | CB-CA-C | 5.51 | 118.28 | 109.02 |
| 7 | O | 566 | THR | CA-C-N | 5.51 | 128.12 | 120.29 |
| 7 | O | 566 | THR | C-N-CA | 5.51 | 128.12 | 120.29 |
| 8 | P | 1519 | CYS | CA-C-O | -5.51 | 115.03 | 120.82 |
| 9 | Q | 621 | HIS | CG-CD2-NE2 | 5.51 | 112.71 | 107.20 |
| 2 | Z | 282 | ASN | CA-CB-CG | 5.51 | 118.11 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 13 | x | 1397 | LYS | CB-CA-C | -5.51 | 102.22 | 110.88 |
| 14 | h | 893 | HIS | CE1-NE2-CD2 | -5.51 | 103.49 | 109.00 |
| 21 | p | 50 | ASP | O-C-N | -5.51 | 116.28 | 122.12 |
| 16 | c | 272 | ILE | CA-C-N | 5.51 | 128.01 | 120.46 |
| 16 | c | 272 | ILE | C-N-CA | 5.51 | 128.01 | 120.46 |
| 1 | 0 | 188 | ASN | N-CA-C | -5.51 | 106.14 | 112.92 |
| 1 | 0 | 1062 | LYS | CA-C-N | 5.51 | 131.60 | 122.73 |
| 1 | 0 | 1062 | LYS | C-N-CA | 5.51 | 131.60 | 122.73 |
| 2 | 1 | 180 | LEU | O-C-N | -5.51 | 116.86 | 123.31 |
| 8 | N | 494 | PRO | N-CA-CB | 5.51 | 108.47 | 103.34 |
| 8 | P | 1125 | GLU | N-CA-C | -5.51 | 104.22 | 112.54 |
| 8 | P | 1235 | LYS | N-CA-C | -5.51 | 104.67 | 111.40 |
| 9 | Q | 762 | ASN | CA-C-O | 5.51 | 127.45 | 121.06 |
| 11 | X | 393 | GLU | CA-C-N | 5.51 | 128.69 | 120.31 |
| 11 | X | 393 | GLU | C-N-CA | 5.51 | 128.69 | 120.31 |
| 1 | Y | 159 | GLU | CA-C-O | 5.51 | 126.16 | 119.38 |
| 19 | f | 291 | ASN | O-C-N | 5.51 | 127.96 | 122.12 |
| 14 | a | 815 | PHE | N-CA-CB | 5.51 | 119.62 | 110.91 |
| 4 | A | 720 | ALA | N-CA-CB | 5.51 | 118.78 | 110.30 |
| 8 | P | 949 | LEU | N-CA-CB | 5.51 | 118.91 | 110.70 |
| 8 | P | 1466 | TYR | N-CA-C | 5.51 | 118.05 | 111.71 |
| 9 | R | 514 | LYS | CB-CA-C | -5.51 | 99.46 | 110.42 |
| 9 | S | 826 | ARG | N-CA-C | -5.51 | 106.06 | 112.89 |
| 15 | i | 287 | ASP | CA-CB-CG | -5.51 | 107.09 | 112.60 |
| 15 | i | 427 | LYS | N-CA-C | -5.51 | 106.46 | 114.12 |
| 18 | l | 226 | ARG | NH1-CZ-NH2 | -5.51 | 112.14 | 119.30 |
| 19 | m | 421 | LYS | N-CA-C | 5.51 | 117.28 | 111.28 |
| 15 | b | 521 | TRP | CB-CG-CD2 | 5.51 | 134.51 | 126.80 |
| 20 | g | 500 | GLN | N-CA-C | -5.51 | 105.60 | 112.93 |
| 14 | a | 663 | LEU | N-CA-C | 5.51 | 117.28 | 111.28 |
| 2 | 1 | 104 | ARG | CA-C-N | 5.51 | 131.46 | 122.65 |
| 2 | 1 | 104 | ARG | C-N-CA | 5.51 | 131.46 | 122.65 |
| 7 | O | 1489 | ILE | CA-C-O | -5.51 | 115.22 | 120.95 |
| 8 | P | 651 | TYR | CA-C-N | 5.51 | 129.08 | 120.82 |
| 8 | P | 651 | TYR | C-N-CA | 5.51 | 129.08 | 120.82 |
| 9 | Q | 571 | LEU | N-CA-CB | 5.51 | 118.22 | 110.12 |
| 1 | Y | 659 | PHE | CA-CB-CG | 5.51 | 119.31 | 113.80 |
| 12 | u | 99 | ASN | CA-CB-CG | 5.51 | 118.11 | 112.60 |
| 12 | v | 417 | ILE | N-CA-C | -5.51 | 107.49 | 112.12 |
| 14 | h | 734 | HIS | CG-CD2-NE2 | 5.51 | 112.71 | 107.20 |
| 15 | b | 349 | TYR | CA-C-N | 5.51 | 132.06 | 121.54 |
| 15 | b | 349 | TYR | C-N-CA | 5.51 | 132.06 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | f | 378 | ASP | CA-CB-CG | 5.51 | 118.11 | 112.60 |
| 14 | a | 138 | LEU | N-CA-C | 5.51 | 120.11 | 112.90 |
| 1 | 0 | 687 | CYS | N-CA-C | -5.51 | 106.41 | 114.39 |
| 2 | 1 | 1203 | SER | CA-C-O | 5.51 | 125.87 | 119.32 |
| 2 | 1 | 1360 | SER | N-CA-C | -5.51 | 107.81 | 114.75 |
| 7 | M | 1519 | LYS | CA-C-O | -5.51 | 113.88 | 120.10 |
| 8 | N | 983 | ASN | CA-CB-CG | -5.51 | 107.09 | 112.60 |
| 7 | O | 314 | VAL | N-CA-C | -5.51 | 107.11 | 112.29 |
| 7 | O | 860 | ASN | O-C-N | -5.51 | 116.23 | 122.23 |
| 8 | P | 802 | LEU | N-CA-C | 5.51 | 117.28 | 111.28 |
| 8 | P | 1514 | VAL | CA-C-N | 5.51 | 127.64 | 120.26 |
| 8 | P | 1514 | VAL | C-N-CA | 5.51 | 127.64 | 120.26 |
| 1 | Y | 780 | LEU | CA-C-N | 5.51 | 130.76 | 122.67 |
| 1 | Y | 780 | LEU | C-N-CA | 5.51 | 130.76 | 122.67 |
| 1 | Y | 1257 | GLN | CA-CB-CG | -5.51 | 103.09 | 114.10 |
| 12 | u | 66 | ASP | N-CA-CB | 5.51 | 119.80 | 110.49 |
| 12 | u | 369 | GLN | N-CA-CB | 5.51 | 120.54 | 111.62 |
| 19 | m | 311 | ASP | CA-CB-CG | 5.51 | 118.11 | 112.60 |
| 19 | f | 417 | ILE | CA-C-O | -5.51 | 115.01 | 120.85 |
| 19 | f | 645 | ASP | N-CA-C | -5.51 | 102.37 | 110.52 |
| 2 | 1 | 275 | THR | N-CA-C | -5.50 | 100.70 | 109.07 |
| 6 | I | 438 | ALA | CA-C-O | 5.50 | 128.38 | 120.51 |
| 8 | N | 859 | ILE | N-CA-C | -5.50 | 105.75 | 111.58 |
| 12 | v | 337 | TRP | CB-CG-CD2 | -5.50 | 119.09 | 126.80 |
| 14 | h | 533 | LEU | CA-C-N | 5.50 | 128.21 | 120.28 |
| 14 | h | 533 | LEU | C-N-CA | 5.50 | 128.21 | 120.28 |
| 16 | j | 510 | LEU | N-CA-CB | -5.50 | 102.03 | 110.12 |
| 16 | c | 218 | LYS | N-CA-C | -5.50 | 106.56 | 113.28 |
| 18 | e | 95 | GLY | CA-C-O | 5.50 | 125.95 | 119.45 |
| 19 | f | 261 | ARG | CA-C-N | 5.50 | 127.66 | 120.28 |
| 19 | f | 261 | ARG | C-N-CA | 5.50 | 127.66 | 120.28 |
| 2 | 1 | 413 | SER | N-CA-C | -5.50 | 101.01 | 109.76 |
| 5 | H | 374 | ILE | N-CA-CB | 5.50 | 118.84 | 110.58 |
| 6 | L | 320 | SER | N-CA-C | 5.50 | 117.28 | 111.28 |
| 7 | O | 260 | MET | CB-CA-C | -5.50 | 102.24 | 110.88 |
| 8 | P | 459 | ASP | CB-CA-C | -5.50 | 102.58 | 111.28 |
| 8 | P | 1079 | VAL | O-C-N | -5.50 | 114.52 | 122.12 |
| 9 | T | 827 | GLU | N-CA-C | 5.50 | 118.20 | 111.82 |
| 10 | U | 280 | PHE | CD1-CG-CD2 | -5.50 | 110.34 | 118.60 |
| 12 | u | 437 | LEU | CD1-CG-CD2 | 5.50 | 122.91 | 110.80 |
| 14 | h | 353 | VAL | CA-C-O | 5.50 | 126.93 | 120.71 |
| 16 | j | 504 | GLU | N-CA-C | -5.50 | 104.20 | 111.96 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | b | 537 | GLU | N-CA-CB | 5.50 | 118.21 | 110.12 |
| 7 | O | 273 | VAL | CA-C-O | -5.50 | 115.23 | 120.95 |
| 8 | P | 1234 | LEU | N-CA-C | -5.50 | 106.41 | 114.39 |
| 1 | Y | 163 | GLU | O-C-N | 5.50 | 127.95 | 122.12 |
| 14 | h | 857 | GLN | N-CA-CB | 5.50 | 120.27 | 111.91 |
| 16 | j | 652 | ARG | N-CA-C | -5.50 | 105.88 | 112.59 |
| 19 | m | 123 | MET | N-CA-CB | 5.50 | 118.77 | 110.30 |
| 21 | r | 45 | VAL | CA-C-N | 5.50 | 127.65 | 120.28 |
| 21 | r | 45 | VAL | C-N-CA | 5.50 | 127.65 | 120.28 |
| 5 | K | 301 | PRO | N-CA-CB | 5.50 | 108.58 | 103.41 |
| 7 | M | 1411 | HIS | CG-CD2-NE2 | 5.50 | 112.70 | 107.20 |
| 9 | R | 330 | GLY | N-CA-C | -5.50 | 107.18 | 115.32 |
| 11 | V | 362 | SER | CA-C-N | 5.50 | 125.02 | 119.19 |
| 11 | V | 362 | SER | C-N-CA | 5.50 | 125.02 | 119.19 |
| 19 | m | 357 | SER | CA-C-O | -5.50 | 115.03 | 120.70 |
| 19 | f | 289 | HIS | CE1-NE2-CD2 | -5.50 | 103.50 | 109.00 |
| 1 | 0 | 780 | LEU | O-C-N | 5.50 | 127.81 | 122.09 |
| 1 | 0 | 1242 | PHE | N-CA-CB | 5.50 | 118.83 | 109.10 |
| 1 | 0 | 1428 | TYR | N-CA-C | -5.50 | 104.69 | 111.40 |
| 6 | C | 449 | LEU | CA-C-N | 5.50 | 128.10 | 120.29 |
| 6 | C | 449 | LEU | C-N-CA | 5.50 | 128.10 | 120.29 |
| 6 | L | 276 | GLU | CB-CA-C | -5.50 | 101.50 | 110.85 |
| 7 | M | 706 | VAL | CA-C-N | 5.50 | 127.91 | 120.65 |
| 7 | M | 706 | VAL | C-N-CA | 5.50 | 127.91 | 120.65 |
| 7 | O | 925 | HIS | N-CA-CB | 5.50 | 117.98 | 110.01 |
| 7 | O | 1460 | LEU | CA-C-N | 5.50 | 127.65 | 120.28 |
| 7 | O | 1460 | LEU | C-N-CA | 5.50 | 127.65 | 120.28 |
| 9 | Q | 264 | LYS | N-CA-C | -5.50 | 105.20 | 111.14 |
| 2 | Z | 963 | THR | N-CA-CB | 5.50 | 118.20 | 110.12 |
| 12 | v | 689 | ILE | N-CA-C | 5.50 | 116.23 | 110.62 |
| 14 | h | 193 | HIS | ND1-CE1-NE2 | 5.50 | 113.90 | 108.40 |
| 17 | k | 282 | LYS | N-CA-CB | 5.50 | 119.14 | 110.56 |
| 20 | n | 692 | GLU | CA-C-O | 5.50 | 124.74 | 119.08 |
| 19 | f | 143 | LYS | CA-C-O | -5.50 | 114.83 | 120.99 |
| 6 | I | 436 | LEU | CA-C-N | 5.50 | 128.63 | 120.17 |
| 6 | I | 436 | LEU | C-N-CA | 5.50 | 128.63 | 120.17 |
| 4 | J | 666 | ASP | CA-CB-CG | -5.50 | 107.10 | 112.60 |
| 6 | L | 341 | ASP | O-C-N | 5.50 | 129.28 | 122.19 |
| 7 | M | 21 | ASP | CA-CB-CG | 5.50 | 118.10 | 112.60 |
| 8 | P | 354 | GLU | CA-CB-CG | -5.50 | 103.11 | 114.10 |
| 9 | R | 572 | CYS | N-CA-CB | 5.50 | 117.98 | 110.01 |
| 1 | Y | 778 | THR | O-C-N | -5.50 | 116.31 | 122.03 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 948 | ASP | CA-C-O | -5.50 | 115.67 | 121.88 |
| 1 | Y | 1286 | ASP | CA-C-O | 5.50 | 126.45 | 120.95 |
| 2 | Z | 378 | LEU | N-CA-C | -5.50 | 101.00 | 109.52 |
| 2 | Z | 1015 | VAL | O-C-N | 5.50 | 127.80 | 122.25 |
| 2 | Z | 1135 | ALA | N-CA-C | 5.50 | 118.03 | 111.71 |
| 12 | u | 412 | SER | CA-C-N | 5.50 | 129.69 | 121.72 |
| 12 | u | 412 | SER | C-N-CA | 5.50 | 129.69 | 121.72 |
| 13 | w | 1395 | LEU | CA-C-N | 5.50 | 127.64 | 120.28 |
| 13 | w | 1395 | LEU | C-N-CA | 5.50 | 127.64 | 120.28 |
| 17 | k | 130 | PHE | N-CA-CB | 5.50 | 118.61 | 109.60 |
| 20 | n | 510 | ASN | O-C-N | -5.50 | 115.00 | 121.32 |
| 15 | b | 359 | GLY | N-CA-C | 5.50 | 120.72 | 114.67 |
| 7 | M | 1011 | SER | N-CA-C | 5.50 | 118.19 | 111.82 |
| 7 | M | 1594 | GLY | N-CA-C | -5.50 | 100.16 | 113.18 |
| 10 | W | 340 | ILE | N-CA-C | -5.50 | 98.12 | 106.42 |
| 1 | 0 | 221 | PRO | N-CA-C | -5.49 | 107.48 | 114.35 |
| 8 | N | 826 | SER | CA-C-O | -5.49 | 112.63 | 120.16 |
| 7 | O | 914 | ASP | CA-CB-CG | -5.49 | 107.11 | 112.60 |
| 7 | O | 1488 | ILE | CA-C-N | 5.49 | 127.99 | 120.46 |
| 7 | O | 1488 | ILE | C-N-CA | 5.49 | 127.99 | 120.46 |
| 7 | O | 1584 | ASN | CA-C-O | 5.49 | 123.68 | 118.63 |
| 8 | P | 809 | PRO | O-C-N | 5.49 | 128.26 | 122.93 |
| 9 | Q | 162 | LEU | CA-C-N | 5.49 | 127.99 | 120.46 |
| 9 | Q | 162 | LEU | C-N-CA | 5.49 | 127.99 | 120.46 |
| 9 | Q | 212 | PHE | N-CA-CB | 5.49 | 117.98 | 110.01 |
| 9 | Q | 664 | THR | O-C-N | 5.49 | 129.21 | 122.34 |
| 17 | k | 212 | TRP | CD2-CE2-CZ2 | -5.49 | 116.91 | 122.40 |
| 21 | p | 20 | LEU | CA-C-N | 5.49 | 127.95 | 120.54 |
| 21 | p | 20 | LEU | C-N-CA | 5.49 | 127.95 | 120.54 |
| 15 | b | 270 | LEU | CA-C-N | 5.49 | 126.96 | 120.09 |
| 15 | b | 270 | LEU | C-N-CA | 5.49 | 126.96 | 120.09 |
| 17 | d | 176 | GLY | N-CA-C | -5.49 | 102.01 | 111.57 |
| 14 | a | 359 | THR | N-CA-C | -5.49 | 104.12 | 111.87 |
| 7 | M | 262 | ASP | CA-CB-CG | 5.49 | 118.09 | 112.60 |
| 7 | O | 889 | ILE | O-C-N | -5.49 | 116.32 | 121.87 |
| 1 | Y | 696 | ARG | N-CA-C | -5.49 | 106.62 | 113.38 |
| 16 | c | 406 | HIS | N-CA-C | -5.49 | 105.19 | 111.07 |
| 18 | e | 242 | ILE | N-CA-CB | 5.49 | 117.39 | 112.06 |
| 2 | 1 | 656 | HIS | ND1-CE1-NE2 | 5.49 | 113.89 | 108.40 |
| 6 | C | 280 | LEU | N-CA-C | -5.49 | 105.84 | 112.54 |
| 7 | M | 1060 | LEU | O-C-N | -5.49 | 116.76 | 122.96 |
| 7 | M | 1332 | PHE | N-CA-CB | 5.49 | 117.97 | 110.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 590 | LEU | N-CA-C | -5.49 | 99.43 | 108.49 |
| 8 | P | 1075 | ILE | N-CA-C | 5.49 | 119.80 | 111.89 |
| 8 | P | 1399 | ASN | CA-C-N | 5.49 | 125.42 | 119.76 |
| 8 | P | 1399 | ASN | C-N-CA | 5.49 | 125.42 | 119.76 |
| 9 | S | 574 | GLU | CA-C-N | 5.49 | 127.64 | 120.28 |
| 9 | S | 574 | GLU | C-N-CA | 5.49 | 127.64 | 120.28 |
| 14 | h | 320 | PRO | CB-CA-C | 5.49 | 118.61 | 111.64 |
| 14 | h | 483 | LEU | N-CA-C | -5.49 | 102.36 | 110.48 |
| 14 | h | 726 | SER | CA-C-N | 5.49 | 127.58 | 120.44 |
| 14 | h | 726 | SER | C-N-CA | 5.49 | 127.58 | 120.44 |
| 1 | 0 | 1331 | ARG | CA-C-O | 5.49 | 126.77 | 120.84 |
| 2 | 1 | 952 | ASP | CA-CB-CG | -5.49 | 107.11 | 112.60 |
| 4 | J | 709 | ASN | OD1-CG-ND2 | -5.49 | 117.11 | 122.60 |
| 8 | N | 1033 | PHE | CA-C-O | -5.49 | 115.05 | 120.70 |
| 8 | P | 390 | ILE | CA-C-O | -5.49 | 114.93 | 119.76 |
| 9 | T | 798 | THR | CA-C-N | 5.49 | 128.18 | 120.28 |
| 9 | T | 798 | THR | C-N-CA | 5.49 | 128.18 | 120.28 |
| 14 | h | 840 | PHE | O-C-N | 5.49 | 129.02 | 122.27 |
| 14 | h | 925 | LEU | N-CA-C | -5.49 | 99.11 | 110.80 |
| 17 | k | 107 | TRP | CG-CD2-CE3 | -5.49 | 128.41 | 133.90 |
| 15 | b | 544 | ASN | N-CA-C | 5.49 | 117.34 | 111.36 |
| 20 | g | 412 | GLU | CA-C-O | 5.49 | 125.18 | 119.14 |
| 20 | g | 1011 | ASP | N-CA-CB | 5.49 | 118.11 | 110.04 |
| 2 | 1 | 1138 | ASN | CA-CB-CG | 5.49 | 118.09 | 112.60 |
| 4 | A | 723 | SER | CB-CA-C | -5.49 | 99.50 | 110.42 |
| 6 | C | 395 | GLU | O-C-N | -5.49 | 115.89 | 122.15 |
| 1 | Y | 1307 | LEU | N-CA-C | -5.49 | 99.37 | 108.75 |
| 20 | n | 678 | TYR | CA-C-N | 5.49 | 129.03 | 120.75 |
| 20 | n | 678 | TYR | C-N-CA | 5.49 | 129.03 | 120.75 |
| 1 | 0 | 1170 | ARG | N-CA-C | -5.49 | 105.28 | 112.41 |
| 2 | 1 | 1270 | ILE | N-CA-C | -5.49 | 105.50 | 110.82 |
| 4 | J | 670 | VAL | N-CA-CB | 5.49 | 121.32 | 110.95 |
| 8 | N | 799 | ALA | CA-C-N | 5.49 | 127.63 | 120.28 |
| 8 | N | 799 | ALA | C-N-CA | 5.49 | 127.63 | 120.28 |
| 8 | N | 1530 | LYS | CA-C-N | 5.49 | 127.63 | 120.28 |
| 8 | N | 1530 | LYS | C-N-CA | 5.49 | 127.63 | 120.28 |
| 8 | P | 912 | TRP | CD2-CE2-CZ2 | -5.49 | 116.91 | 122.40 |
| 9 | Q | 414 | LEU | N-CA-C | -5.49 | 104.71 | 111.40 |
| 14 | h | 92 | THR | N-CA-C | -5.49 | 99.96 | 108.90 |
| 14 | h | 99 | ASN | CA-C-N | 5.49 | 129.03 | 120.75 |
| 14 | h | 99 | ASN | C-N-CA | 5.49 | 129.03 | 120.75 |
| 20 | n | 229 | PHE | CA-CB-CG | -5.49 | 108.31 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 17 | d | 79 | VAL | N-CA-C | -5.49 | 98.56 | 107.28 |
| 19 | f | 391 | HIS | N-CA-CB | 5.49 | 118.18 | 110.12 |
| 20 | g | 475 | LEU | CA-C-N | 5.49 | 130.73 | 122.99 |
| 20 | g | 475 | LEU | C-N-CA | 5.49 | 130.73 | 122.99 |
| 2 | 1 | 183 | TRP | O-C-N | -5.48 | 116.80 | 122.94 |
| 11 | V | 287 | HIS | ND1-CE1-NE2 | 5.48 | 113.88 | 108.40 |
| 16 | j | 267 | ARG | CA-C-N | 5.48 | 128.41 | 120.79 |
| 16 | j | 267 | ARG | C-N-CA | 5.48 | 128.41 | 120.79 |
| 15 | b | 557 | ALA | CB-CA-C | -5.48 | 98.75 | 110.32 |
| 15 | b | 736 | ASN | CA-CB-CG | 5.48 | 118.08 | 112.60 |
| 20 | g | 692 | GLU | N-CA-CB | 5.48 | 120.25 | 111.20 |
| 20 | g | 761 | ASN | CA-CB-CG | 5.48 | 118.08 | 112.60 |
| 20 | g | 1144 | LYS | N-CA-C | -5.48 | 101.08 | 109.41 |
| 2 | 1 | 1250 | SER | CA-CB-OG | 5.48 | 122.07 | 111.10 |
| 6 | I | 397 | ALA | N-CA-C | 5.48 | 116.94 | 111.07 |
| 6 | L | 393 | ASP | CA-CB-CG | 5.48 | 118.08 | 112.60 |
| 8 | P | 159 | SER | CA-C-N | 5.48 | 129.26 | 121.42 |
| 8 | P | 159 | SER | C-N-CA | 5.48 | 129.26 | 121.42 |
| 8 | P | 1211 | ILE | CA-C-N | 5.48 | 128.18 | 120.28 |
| 8 | P | 1211 | ILE | C-N-CA | 5.48 | 128.18 | 120.28 |
| 9 | Q | 25 | LEU | CB-CA-C | -5.48 | 101.53 | 110.85 |
| 1 | Y | 151 | GLN | N-CA-CB | -5.48 | 106.49 | 111.59 |
| 2 | Z | 404 | PHE | CA-CB-CG | 5.48 | 119.28 | 113.80 |
| 16 | j | 297 | TYR | CB-CG-CD2 | -5.48 | 112.58 | 120.80 |
| 17 | d | 26 | THR | N-CA-C | -5.48 | 99.96 | 108.90 |
| 1 | 0 | 437 | VAL | N-CA-CB | 5.48 | 118.97 | 111.41 |
| 4 | G | 800 | HIS | CB-CG-ND1 | 5.48 | 130.92 | 122.70 |
| 5 | K | 389 | LYS | CA-C-N | 5.48 | 131.72 | 122.79 |
| 5 | K | 389 | LYS | C-N-CA | 5.48 | 131.72 | 122.79 |
| 7 | O | 615 | LEU | O-C-N | -5.48 | 116.17 | 122.09 |
| 8 | P | 178 | GLN | OE1-CD-NE2 | 5.48 | 128.08 | 122.60 |
| 9 | Q | 600 | ILE | CA-C-N | 5.48 | 125.48 | 119.89 |
| 9 | Q | 600 | ILE | C-N-CA | 5.48 | 125.48 | 119.89 |
| 9 | R | 645 | GLN | OE1-CD-NE2 | 5.48 | 128.08 | 122.60 |
| 2 | Z | 232 | ILE | CB-CA-C | 5.48 | 117.61 | 111.80 |
| 13 | x | 1310 | VAL | O-C-N | 5.48 | 127.19 | 121.87 |
| 15 | i | 372 | ALA | CA-C-N | 5.48 | 129.95 | 120.58 |
| 15 | i | 372 | ALA | C-N-CA | 5.48 | 129.95 | 120.58 |
| 19 | m | 678 | LEU | N-CA-C | -5.48 | 99.13 | 110.80 |
| 21 | o | 60 | ILE | O-C-N | -5.48 | 117.34 | 123.26 |
| 21 | p | 40 | ASP | O-C-N | 5.48 | 127.93 | 122.12 |
| 16 | c | 436 | LYS | O-C-N | -5.48 | 114.90 | 122.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | a | 326 | SER | N-CA-C | 5.48 | 122.47 | 110.80 |
| 7 | M | 304 | THR | N-CA-C | -5.48 | 105.89 | 113.18 |
| 8 | N | 1288 | PHE | N-CA-C | 5.48 | 117.96 | 111.33 |
| 7 | O | 980 | ASP | N-CA-CB | 5.48 | 118.28 | 110.06 |
| 9 | Q | 788 | ILE | CB-CA-C | -5.48 | 104.37 | 111.88 |
| 1 | Y | 1464 | ASP | CA-CB-CG | 5.48 | 118.08 | 112.60 |
| 16 | j | 402 | LEU | N-CA-C | -5.48 | 105.72 | 112.90 |
| 20 | n | 542 | ASN | N-CA-C | -5.48 | 106.37 | 113.16 |
| 21 | p | 10 | ILE | CA-C-O | 5.48 | 126.09 | 120.39 |
| 15 | b | 584 | GLN | N-CA-C | -5.48 | 102.37 | 110.48 |
| 16 | c | 144 | PHE | CA-CB-CG | 5.48 | 119.28 | 113.80 |
| 2 | 1 | 375 | GLY | CA-C-N | 5.48 | 126.69 | 119.84 |
| 2 | 1 | 375 | GLY | C-N-CA | 5.48 | 126.69 | 119.84 |
| 4 | J | 714 | PHE | N-CA-C | -5.48 | 106.27 | 113.17 |
| 8 | N | 694 | ILE | N-CA-C | 5.48 | 116.25 | 110.72 |
| 8 | P | 440 | ILE | O-C-N | -5.48 | 114.86 | 121.10 |
| 9 | S | 374 | TYR | CA-C-O | -5.48 | 111.49 | 120.80 |
| 9 | S | 612 | HIS | CA-C-N | 5.48 | 129.93 | 121.71 |
| 9 | S | 612 | HIS | C-N-CA | 5.48 | 129.93 | 121.71 |
| 9 | S | 692 | MET | CA-CB-CG | 5.48 | 125.06 | 114.10 |
| 10 | U | 269 | HIS | ND1-CE1-NE2 | 5.48 | 113.88 | 108.40 |
| 2 | Z | 1297 | ILE | CA-C-O | 5.48 | 126.64 | 119.85 |
| 12 | v | 559 | GLU | CA-C-N | 5.48 | 127.56 | 120.44 |
| 12 | v | 559 | GLU | C-N-CA | 5.48 | 127.56 | 120.44 |
| 4 | z | 667 | GLN | CA-C-O | -5.48 | 115.07 | 120.82 |
| 14 | h | 350 | ASN | CA-C-N | 5.48 | 130.21 | 121.66 |
| 14 | h | 350 | ASN | C-N-CA | 5.48 | 130.21 | 121.66 |
| 14 | h | 803 | HIS | CA-C-O | -5.48 | 115.55 | 121.36 |
| 19 | m | 381 | ASP | N-CA-C | 5.48 | 117.25 | 111.28 |
| 16 | c | 518 | LEU | N-CA-C | -5.48 | 105.39 | 113.61 |
| 20 | g | 867 | GLN | N-CA-C | -5.48 | 102.03 | 109.54 |
| 5 | E | 398 | ILE | CA-CB-CG1 | 5.48 | 119.71 | 110.40 |
| 5 | H | 528 | GLU | CA-C-N | 5.48 | 128.63 | 120.31 |
| 5 | H | 528 | GLU | C-N-CA | 5.48 | 128.63 | 120.31 |
| 7 | M | 784 | ILE | CA-C-N | 5.48 | 128.16 | 120.28 |
| 7 | M | 784 | ILE | C-N-CA | 5.48 | 128.16 | 120.28 |
| 8 | P | 914 | ASP | N-CA-CB | 5.48 | 120.80 | 111.66 |
| 2 | Z | 1003 | ASN | CA-CB-CG | 5.48 | 118.08 | 112.60 |
| 17 | d | 286 | GLU | N-CA-CB | 5.48 | 119.74 | 110.49 |
| 20 | g | 111 | HIS | CE1-NE2-CD2 | -5.48 | 103.52 | 109.00 |
| 1 | 0 | 193 | TRP | CA-C-N | 5.47 | 128.62 | 120.95 |
| 1 | 0 | 193 | TRP | C-N-CA | 5.47 | 128.62 | 120.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 382 | ILE | O-C-N | 5.47 | 129.13 | 123.05 |
| 1 | 0 | 585 | ILE | CA-CB-CG1 | 5.47 | 119.71 | 110.40 |
| 7 | M | 1527 | ARG | NE-CZ-NH1 | 5.47 | 126.97 | 121.50 |
| 8 | N | 153 | ASP | N-CA-C | -5.47 | 106.53 | 113.43 |
| 8 | N | 1463 | SER | CA-C-N | 5.47 | 132.14 | 121.41 |
| 8 | N | 1463 | SER | C-N-CA | 5.47 | 132.14 | 121.41 |
| 7 | O | 1161 | LEU | N-CA-C | 5.47 | 118.00 | 111.71 |
| 11 | X | 372 | GLU | N-CA-C | 5.47 | 118.38 | 110.28 |
| 14 | h | 116 | GLN | N-CA-C | -5.47 | 99.39 | 108.75 |
| 14 | h | 788 | ASP | CA-CB-CG | 5.47 | 118.07 | 112.60 |
| 19 | m | 30 | GLN | N-CA-CB | -5.47 | 101.79 | 110.28 |
| 20 | n | 835 | PHE | CB-CG-CD1 | -5.47 | 111.39 | 120.70 |
| 21 | o | 24 | ILE | N-CA-C | 5.47 | 115.67 | 110.42 |
| 21 | t | 25 | LEU | CA-C-N | 5.47 | 127.89 | 120.44 |
| 21 | t | 25 | LEU | C-N-CA | 5.47 | 127.89 | 120.44 |
| 15 | b | 494 | THR | N-CA-CB | 5.47 | 119.74 | 110.49 |
| 20 | g | 270 | LEU | N-CA-C | -5.47 | 100.75 | 109.07 |
| 5 | K | 513 | LEU | CA-C-N | 5.47 | 128.06 | 120.29 |
| 5 | K | 513 | LEU | C-N-CA | 5.47 | 128.06 | 120.29 |
| 7 | M | 1274 | ASP | N-CA-C | -5.47 | 105.65 | 112.93 |
| 8 | P | 280 | ALA | CA-C-O | -5.47 | 115.59 | 121.56 |
| 9 | T | 565 | GLY | CA-C-N | 5.47 | 124.99 | 119.19 |
| 9 | T | 565 | GLY | C-N-CA | 5.47 | 124.99 | 119.19 |
| 1 | Y | 444 | VAL | CA-C-O | 5.47 | 127.06 | 120.66 |
| 14 | h | 803 | HIS | CB-CG-ND1 | 5.47 | 130.91 | 122.70 |
| 16 | j | 536 | GLN | CA-C-N | 5.47 | 128.16 | 120.28 |
| 16 | j | 536 | GLN | C-N-CA | 5.47 | 128.16 | 120.28 |
| 19 | f | 339 | SER | CA-C-N | 5.47 | 131.37 | 122.67 |
| 19 | f | 339 | SER | C-N-CA | 5.47 | 131.37 | 122.67 |
| 19 | f | 352 | LEU | N-CA-C | -5.47 | 105.34 | 112.23 |
| 1 | 0 | 257 | PHE | CA-CB-CG | -5.47 | 108.33 | 113.80 |
| 1 | 0 | 591 | LYS | N-CA-C | -5.47 | 101.15 | 108.86 |
| 2 | 1 | 1258 | GLN | N-CA-CB | 5.47 | 118.23 | 110.13 |
| 7 | M | 840 | ILE | CA-C-N | 5.47 | 128.16 | 120.28 |
| 7 | M | 840 | ILE | C-N-CA | 5.47 | 128.16 | 120.28 |
| 7 | O | 672 | TRP | CD2-CE3-CZ3 | 5.47 | 125.71 | 118.60 |
| 9 | R | 74 | ALA | CB-CA-C | -5.47 | 102.29 | 110.88 |
| 15 | i | 466 | LEU | CB-CA-C | -5.47 | 101.60 | 110.79 |
| 17 | k | 13 | HIS | CA-C-O | -5.47 | 113.12 | 119.14 |
| 4 | J | 645 | THR | CA-C-N | 5.47 | 128.06 | 120.29 |
| 4 | J | 645 | THR | C-N-CA | 5.47 | 128.06 | 120.29 |
| 7 | M | 870 | LYS | CA-C-N | 5.47 | 127.54 | 120.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 870 | LYS | C-N-CA | 5.47 | 127.54 | 120.70 |
| 7 | O | 767 | ILE | CA-CB-CG1 | 5.47 | 119.70 | 110.40 |
| 9 | R | 348 | GLU | CA-C-N | 5.47 | 127.61 | 120.28 |
| 9 | R | 348 | GLU | C-N-CA | 5.47 | 127.61 | 120.28 |
| 9 | T | 122 | LEU | N-CA-C | 5.47 | 116.92 | 111.07 |
| 2 | Z | 607 | ASN | N-CA-C | -5.47 | 105.72 | 112.72 |
| 2 | Z | 627 | ASN | CA-C-O | -5.47 | 112.67 | 120.16 |
| 2 | Z | 769 | HIS | ND1-CE1-NE2 | 5.47 | 113.87 | 108.40 |
| 14 | h | 330 | SER | N-CA-C | -5.47 | 100.86 | 109.50 |
| 18 | l | 146 | ARG | NE-CZ-NH2 | -5.47 | 114.28 | 119.20 |
| 19 | f | 144 | TRP | CG-CD2-CE3 | 5.47 | 139.37 | 133.90 |
| 14 | a | 456 | ALA | N-CA-CB | 5.47 | 119.73 | 110.49 |
| 2 | 1 | 428 | THR | CA-CB-CG2 | -5.47 | 101.20 | 110.50 |
| 2 | 1 | 854 | THR | CA-CB-OG1 | 5.47 | 117.80 | 109.60 |
| 2 | 1 | 1200 | LEU | CA-C-N | 5.47 | 126.67 | 119.84 |
| 2 | 1 | 1200 | LEU | C-N-CA | 5.47 | 126.67 | 119.84 |
| 7 | M | 1088 | ARG | NE-CZ-NH2 | 5.47 | 124.12 | 119.20 |
| 8 | N | 1033 | PHE | N-CA-C | 5.47 | 117.04 | 111.14 |
| 7 | O | 771 | ARG | N-CA-C | 5.47 | 117.94 | 111.33 |
| 7 | O | 1239 | PHE | CA-CB-CG | -5.47 | 108.33 | 113.80 |
| 9 | R | 551 | ARG | CA-C-N | 5.47 | 128.24 | 120.53 |
| 9 | R | 551 | ARG | C-N-CA | 5.47 | 128.24 | 120.53 |
| 9 | S | 595 | ARG | N-CA-C | 5.47 | 117.24 | 111.28 |
| 11 | V | 294 | ILE | CA-CB-CG1 | 5.47 | 119.69 | 110.40 |
| 12 | v | 530 | ASP | N-CA-C | 5.47 | 116.92 | 111.07 |
| 16 | j | 356 | LYS | N-CA-CB | 5.47 | 118.75 | 110.28 |
| 19 | m | 521 | LYS | N-CA-CB | 5.47 | 121.69 | 113.65 |
| 20 | n | 599 | LYS | CG-CD-CE | 5.47 | 123.87 | 111.30 |
| 1 | 0 | 702 | PHE | N-CA-C | -5.46 | 106.74 | 113.41 |
| 2 | 1 | 656 | HIS | CG-CD2-NE2 | 5.46 | 112.66 | 107.20 |
| 5 | B | 470 | ALA | N-CA-CB | 5.46 | 117.93 | 110.01 |
| 5 | H | 386 | LEU | N-CA-C | -5.46 | 104.73 | 111.40 |
| 4 | J | 700 | ILE | N-CA-C | -5.46 | 106.98 | 112.17 |
| 7 | O | 173 | ALA | O-C-N | -5.46 | 116.41 | 122.09 |
| 9 | T | 570 | GLU | CA-C-N | 5.46 | 127.55 | 120.44 |
| 9 | T | 570 | GLU | C-N-CA | 5.46 | 127.55 | 120.44 |
| 12 | v | 90 | VAL | N-CA-CB | 5.46 | 121.32 | 111.21 |
| 15 | i | 623 | THR | N-CA-C | -5.46 | 105.98 | 113.30 |
| 21 | o | 69 | VAL | CA-CB-CG1 | -5.46 | 101.11 | 110.40 |
| 14 | a | 632 | GLN | N-CA-C | 5.46 | 117.24 | 111.28 |
| 15 | i | 426 | ALA | N-CA-C | -5.46 | 106.49 | 112.72 |
| 20 | n | 806 | GLU | CB-CA-C | -5.46 | 102.27 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | f | 703 | LEU | N-CA-C | -5.46 | 105.62 | 114.09 |
| 6 | F | 456 | ARG | CD-NE-CZ | -5.46 | 116.75 | 124.40 |
| 7 | O | 1411 | HIS | CA-CB-CG | 5.46 | 119.26 | 113.80 |
| 9 | T | 143 | ASN | CA-C-N | 5.46 | 127.86 | 120.38 |
| 9 | T | 143 | ASN | C-N-CA | 5.46 | 127.86 | 120.38 |
| 10 | U | 322 | LEU | O-C-N | -5.46 | 115.94 | 122.27 |
| 13 | w | 1113 | LEU | N-CA-C | -5.46 | 95.71 | 111.00 |
| 4 | y | 656 | GLU | O-C-N | 5.46 | 127.91 | 122.12 |
| 14 | h | 240 | ASN | CA-CB-CG | -5.46 | 107.14 | 112.60 |
| 15 | i | 515 | THR | N-CA-C | 5.46 | 118.24 | 110.10 |
| 21 | s | 24 | ILE | CA-C-O | -5.46 | 115.27 | 120.95 |
| 18 | e | 74 | SER | N-CA-CB | 5.46 | 119.27 | 110.86 |
| 20 | g | 854 | HIS | ND1-CE1-NE2 | 5.46 | 113.86 | 108.40 |
| 20 | g | 987 | LEU | N-CA-C | 5.46 | 117.31 | 111.36 |
| 14 | a | 480 | ASN | OD1-CG-ND2 | 5.46 | 128.06 | 122.60 |
| 1 | 0 | 514 | SER | CA-C-N | 5.46 | 131.80 | 121.97 |
| 1 | 0 | 514 | SER | C-N-CA | 5.46 | 131.80 | 121.97 |
| 7 | O | 131 | TYR | N-CA-C | -5.46 | 104.97 | 111.69 |
| 9 | Q | 431 | SER | CB-CA-C | -5.46 | 99.88 | 109.71 |
| 12 | u | 366 | LEU | CA-C-N | 5.46 | 126.67 | 119.84 |
| 12 | u | 366 | LEU | C-N-CA | 5.46 | 126.67 | 119.84 |
| 6 | C | 447 | PHE | CB-CG-CD2 | -5.46 | 111.42 | 120.70 |
| 4 | J | 659 | THR | N-CA-CB | 5.46 | 117.92 | 110.01 |
| 8 | N | 1036 | ASP | CA-C-O | -5.46 | 114.34 | 119.80 |
| 8 | P | 144 | ILE | CA-C-N | 5.46 | 128.17 | 120.42 |
| 8 | P | 144 | ILE | C-N-CA | 5.46 | 128.17 | 120.42 |
| 2 | Z | 843 | TYR | CA-C-N | 5.46 | 127.59 | 120.28 |
| 2 | Z | 843 | TYR | C-N-CA | 5.46 | 127.59 | 120.28 |
| 13 | w | 1272 | ILE | CB-CA-C | -5.46 | 104.77 | 112.14 |
| 18 | l | 27 | CYS | CA-C-O | -5.46 | 114.74 | 120.80 |
| 19 | m | 507 | ASP | CA-C-N | 5.46 | 128.14 | 120.28 |
| 19 | m | 507 | ASP | C-N-CA | 5.46 | 128.14 | 120.28 |
| 20 | n | 1034 | LYS | CA-C-N | 5.46 | 127.59 | 120.28 |
| 20 | n | 1034 | LYS | C-N-CA | 5.46 | 127.59 | 120.28 |
| 17 | d | 279 | THR | CB-CA-C | 5.46 | 119.22 | 110.16 |
| 20 | g | 445 | ASP | CA-CB-CG | 5.46 | 118.06 | 112.60 |
| 4 | G | 693 | ILE | CA-C-O | 5.46 | 125.43 | 120.30 |
| 8 | P | 102 | PHE | N-CA-C | -5.46 | 104.20 | 111.24 |
| 9 | Q | 486 | GLY | N-CA-C | -5.46 | 106.13 | 115.08 |
| 9 | R | 111 | PHE | N-CA-CB | 5.46 | 119.71 | 110.49 |
| 9 | R | 599 | ARG | N-CA-C | 5.46 | 118.44 | 109.76 |
| 9 | R | 615 | ASP | CA-CB-CG | 5.46 | 118.06 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | T | 605 | GLU | CB-CG-CD | -5.46 | 103.33 | 112.60 |
| 9 | T | 616 | GLU | CA-C-N | 5.46 | 127.53 | 120.44 |
| 9 | T | 616 | GLU | C-N-CA | 5.46 | 127.53 | 120.44 |
| 12 | v | 29 | SER | CA-C-N | 5.46 | 131.07 | 122.78 |
| 12 | v | 29 | SER | C-N-CA | 5.46 | 131.07 | 122.78 |
| 19 | m | 470 | LEU | CA-C-N | 5.46 | 126.51 | 120.45 |
| 19 | m | 470 | LEU | C-N-CA | 5.46 | 126.51 | 120.45 |
| 20 | n | 959 | ASN | CA-C-O | 5.46 | 126.20 | 120.42 |
| 20 | g | 877 | GLU | CA-CB-CG | -5.46 | 103.19 | 114.10 |
| 4 | A | 789 | GLU | N-CA-C | -5.46 | 106.63 | 113.72 |
| 7 | O | 925 | HIS | CE1-NE2-CD2 | -5.46 | 103.55 | 109.00 |
| 9 | Q | 156 | MET | CB-CA-C | -5.46 | 101.73 | 110.79 |
| 2 | Z | 288 | TYR | CB-CG-CD1 | -5.46 | 112.62 | 120.80 |
| 12 | v | 145 | LEU | N-CA-CB | -5.46 | 101.52 | 110.68 |
| 13 | x | 1338 | GLN | CA-C-N | 5.46 | 129.41 | 120.63 |
| 13 | x | 1338 | GLN | C-N-CA | 5.46 | 129.41 | 120.63 |
| 16 | c | 521 | SER | N-CA-C | -5.46 | 100.44 | 108.79 |
| 2 | 1 | 180 | LEU | CA-C-O | 5.45 | 126.37 | 120.32 |
| 8 | N | 729 | HIS | CG-CD2-NE2 | 5.45 | 112.65 | 107.20 |
| 8 | P | 937 | SER | CA-C-O | -5.45 | 115.35 | 121.40 |
| 8 | P | 1122 | PHE | CB-CG-CD1 | 5.45 | 129.97 | 120.70 |
| 8 | P | 1551 | THR | CA-C-N | 5.45 | 127.85 | 120.65 |
| 8 | P | 1551 | THR | C-N-CA | 5.45 | 127.85 | 120.65 |
| 9 | R | 76 | SER | N-CA-C | 5.45 | 122.42 | 110.80 |
| 10 | U | 277 | LEU | N-CA-CB | 5.45 | 118.92 | 110.80 |
| 1 | Y | 227 | ALA | CA-C-N | 5.45 | 127.93 | 120.35 |
| 1 | Y | 227 | ALA | C-N-CA | 5.45 | 127.93 | 120.35 |
| 2 | Z | 170 | ASN | N-CA-C | 5.45 | 118.77 | 111.24 |
| 2 | Z | 1179 | ASN | CA-CB-CG | 5.45 | 118.05 | 112.60 |
| 12 | u | 555 | GLU | CA-C-N | 5.45 | 127.59 | 120.28 |
| 12 | u | 555 | GLU | C-N-CA | 5.45 | 127.59 | 120.28 |
| 12 | v | 181 | ASP | N-CA-CB | 5.45 | 120.27 | 111.65 |
| 4 | z | 765 | LEU | CA-C-N | 5.45 | 127.93 | 120.46 |
| 4 | z | 765 | LEU | C-N-CA | 5.45 | 127.93 | 120.46 |
| 21 | o | 8 | THR | CA-C-O | -5.45 | 114.30 | 120.46 |
| 14 | a | 383 | ASN | O-C-N | -5.45 | 115.76 | 122.25 |
| 7 | M | 235 | PRO | CA-C-N | 5.45 | 127.85 | 120.38 |
| 7 | M | 235 | PRO | C-N-CA | 5.45 | 127.85 | 120.38 |
| 7 | M | 1458 | LEU | N-CA-C | -5.45 | 99.19 | 110.80 |
| 9 | R | 608 | GLN | CA-CB-CG | 5.45 | 125.00 | 114.10 |
| 4 | y | 807 | LEU | CA-C-N | 5.45 | 127.86 | 120.44 |
| 4 | y | 807 | LEU | C-N-CA | 5.45 | 127.86 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | m | 653 | TYR | CA-C-N | 5.45 | 130.68 | 121.14 |
| 19 | m | 653 | TYR | C-N-CA | 5.45 | 130.68 | 121.14 |
| 15 | b | 216 | ASP | N-CA-CB | 5.45 | 119.70 | 110.49 |
| 20 | g | 512 | ILE | CA-C-N | 5.45 | 130.12 | 121.18 |
| 20 | g | 512 | ILE | C-N-CA | 5.45 | 130.12 | 121.18 |
| 14 | a | 903 | ASN | OD1-CG-ND2 | 5.45 | 128.05 | 122.60 |
| 1 | 0 | 275 | SER | CA-C-O | 5.45 | 127.71 | 121.28 |
| 2 | 1 | 278 | THR | CA-CB-OG1 | 5.45 | 117.78 | 109.60 |
| 7 | M | 609 | LEU | CA-C-O | -5.45 | 114.64 | 120.42 |
| 8 | N | 366 | SER | CA-C-O | -5.45 | 115.10 | 120.82 |
| 7 | O | 223 | LEU | CA-C-O | -5.45 | 114.47 | 120.36 |
| 8 | P | 903 | LEU | CA-C-N | 5.45 | 127.58 | 120.28 |
| 8 | P | 903 | LEU | C-N-CA | 5.45 | 127.58 | 120.28 |
| 9 | S | 265 | SER | O-C-N | 5.45 | 129.79 | 122.49 |
| 9 | T | 557 | LEU | N-CA-C | -5.45 | 108.41 | 114.62 |
| 12 | u | 692 | LYS | O-C-N | 5.45 | 127.68 | 122.07 |
| 12 | v | 42 | ILE | CA-C-N | 5.45 | 129.18 | 122.37 |
| 12 | v | 42 | ILE | C-N-CA | 5.45 | 129.18 | 122.37 |
| 15 | b | 458 | ARG | N-CA-C | -5.45 | 99.19 | 110.80 |
| 18 | e | 159 | ILE | CA-C-O | -5.45 | 112.65 | 119.95 |
| 20 | g | 830 | SER | N-CA-C | -5.45 | 100.45 | 108.79 |
| 2 | 1 | 676 | LYS | CA-C-N | 5.45 | 126.65 | 119.84 |
| 2 | 1 | 676 | LYS | C-N-CA | 5.45 | 126.65 | 119.84 |
| 2 | 1 | 983 | TYR | CB-CG-CD1 | 5.45 | 128.97 | 120.80 |
| 7 | M | 553 | ILE | CA-C-O | -5.45 | 115.58 | 121.19 |
| 8 | P | 446 | ALA | CA-C-N | 5.45 | 131.64 | 122.87 |
| 8 | P | 446 | ALA | C-N-CA | 5.45 | 131.64 | 122.87 |
| 9 | R | 724 | ARG | CA-C-N | 5.45 | 127.58 | 120.28 |
| 9 | R | 724 | ARG | C-N-CA | 5.45 | 127.58 | 120.28 |
| 2 | Z | 363 | VAL | N-CA-C | -5.45 | 100.73 | 108.58 |
| 12 | u | 184 | ASP | CA-C-N | 5.45 | 131.50 | 121.85 |
| 12 | u | 184 | ASP | C-N-CA | 5.45 | 131.50 | 121.85 |
| 12 | u | 281 | VAL | CA-CB-CG1 | -5.45 | 101.14 | 110.40 |
| 12 | u | 535 | PHE | CA-C-N | 5.45 | 127.58 | 120.28 |
| 12 | u | 535 | PHE | C-N-CA | 5.45 | 127.58 | 120.28 |
| 19 | m | 76 | HIS | CA-C-N | 5.45 | 128.59 | 120.31 |
| 19 | m | 76 | HIS | C-N-CA | 5.45 | 128.59 | 120.31 |
| 20 | n | 122 | VAL | N-CA-CB | 5.45 | 118.84 | 111.21 |
| 21 | r | 30 | ASP | CA-C-N | 5.45 | 127.58 | 120.28 |
| 21 | r | 30 | ASP | C-N-CA | 5.45 | 127.58 | 120.28 |
| 20 | g | 890 | GLN | OE1-CD-NE2 | -5.45 | 117.15 | 122.60 |
| 14 | a | 26 | LEU | N-CA-C | -5.45 | 99.55 | 108.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 849 | LEU | CA-C-O | 5.45 | 126.32 | 120.55 |
| 4 | A | 702 | ARG | N-CA-CB | 5.45 | 118.94 | 110.44 |
| 7 | O | 1445 | VAL | N-CA-C | 5.45 | 116.17 | 110.62 |
| 8 | P | 1509 | GLN | CA-C-O | -5.45 | 112.70 | 119.18 |
| 9 | T | 509 | GLY | N-CA-C | 5.45 | 119.27 | 112.73 |
| 2 | Z | 545 | TYR | CA-C-O | 5.45 | 127.82 | 120.47 |
| 16 | c | 489 | HIS | CA-C-N | 5.45 | 128.59 | 120.31 |
| 16 | c | 489 | HIS | C-N-CA | 5.45 | 128.59 | 120.31 |
| 20 | g | 491 | VAL | O-C-N | 5.45 | 128.95 | 123.07 |
| 6 | F | 282 | GLN | CB-CG-CD | -5.45 | 103.34 | 112.60 |
| 8 | N | 571 | ASN | CA-CB-CG | -5.45 | 107.16 | 112.60 |
| 7 | O | 930 | VAL | CA-C-N | 5.45 | 132.09 | 121.41 |
| 7 | O | 930 | VAL | C-N-CA | 5.45 | 132.09 | 121.41 |
| 9 | S | 329 | ASN | N-CA-CB | 5.45 | 119.69 | 110.49 |
| 19 | f | 546 | LEU | N-CA-CB | 5.45 | 119.89 | 111.39 |
| 8 | P | 560 | ASN | OD1-CG-ND2 | 5.44 | 128.04 | 122.60 |
| 9 | Q | 771 | ILE | CA-C-N | 5.44 | 126.65 | 119.84 |
| 9 | Q | 771 | ILE | C-N-CA | 5.44 | 126.65 | 119.84 |
| 15 | i | 661 | HIS | ND1-CE1-NE2 | 5.44 | 113.84 | 108.40 |
| 18 | e | 338 | GLU | N-CA-C | -5.44 | 99.20 | 110.80 |
| 14 | a | 316 | GLN | CA-C-N | 5.44 | 131.55 | 122.73 |
| 14 | a | 316 | GLN | C-N-CA | 5.44 | 131.55 | 122.73 |
| 2 | 1 | 1083 | TYR | N-CA-CB | 5.44 | 118.12 | 110.12 |
| 5 | E | 410 | LYS | CA-C-O | 5.44 | 126.53 | 120.82 |
| 7 | O | 1148 | LEU | N-CA-CB | 5.44 | 117.90 | 110.01 |
| 7 | O | 1463 | LEU | O-C-N | -5.44 | 114.95 | 122.46 |
| 7 | O | 1598 | PHE | O-C-N | 5.44 | 129.83 | 122.59 |
| 8 | P | 14 | THR | N-CA-C | -5.44 | 97.26 | 108.53 |
| 8 | P | 638 | ILE | CA-C-N | 5.44 | 131.94 | 121.54 |
| 8 | P | 638 | ILE | C-N-CA | 5.44 | 131.94 | 121.54 |
| 9 | Q | 478 | TYR | N-CA-CB | -5.44 | 101.84 | 110.22 |
| 2 | Z | 768 | ILE | CA-CB-CG1 | 5.44 | 119.65 | 110.40 |
| 2 | Z | 1316 | VAL | N-CA-C | -5.44 | 100.55 | 108.17 |
| 12 | v | 117 | ASP | CA-CB-CG | 5.44 | 118.04 | 112.60 |
| 14 | h | 921 | THR | CA-CB-OG1 | 5.44 | 117.76 | 109.60 |
| 18 | l | 192 | ILE | O-C-N | -5.44 | 116.73 | 122.83 |
| 16 | c | 598 | ILE | N-CA-C | -5.44 | 105.07 | 111.00 |
| 20 | g | 295 | TRP | CB-CG-CD1 | -5.44 | 118.73 | 126.90 |
| 20 | g | 425 | VAL | CA-CB-CG1 | 5.44 | 119.65 | 110.40 |
| 1 | 0 | 140 | ASN | N-CA-C | -5.44 | 99.21 | 110.80 |
| 1 | 0 | 161 | LEU | O-C-N | 5.44 | 127.89 | 122.12 |
| 1 | 0 | 526 | ILE | N-CA-C | -5.44 | 99.97 | 108.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 953 | ASN | N-CA-C | -5.44 | 95.77 | 111.00 |
| 9 | S | 468 | SER | O-C-N | 5.44 | 128.78 | 122.09 |
| 2 | Z | 140 | ARG | NE-CZ-NH2 | 5.44 | 124.10 | 119.20 |
| 12 | u | 147 | GLU | CA-C-O | -5.44 | 112.70 | 119.28 |
| 19 | m | 180 | PHE | CA-CB-CG | 5.44 | 119.24 | 113.80 |
| 20 | g | 253 | LYS | CA-CB-CG | -5.44 | 103.22 | 114.10 |
| 14 | a | 972 | LYS | N-CA-C | -5.44 | 106.37 | 114.64 |
| 7 | O | 82 | ASN | CA-CB-CG | 5.44 | 118.04 | 112.60 |
| 21 | q | 25 | LEU | CA-C-N | 5.44 | 127.51 | 120.44 |
| 21 | q | 25 | LEU | C-N-CA | 5.44 | 127.51 | 120.44 |
| 14 | a | 384 | LYS | CA-C-N | 5.44 | 130.06 | 120.87 |
| 14 | a | 384 | LYS | C-N-CA | 5.44 | 130.06 | 120.87 |
| 1 | 0 | 257 | PHE | N-CA-C | -5.44 | 99.23 | 108.26 |
| 2 | 1 | 559 | ALA | N-CA-C | -5.44 | 101.02 | 109.72 |
| 5 | H | 382 | LYS | N-CA-CB | 5.44 | 117.89 | 110.01 |
| 8 | N | 929 | MET | CA-C-O | 5.44 | 126.31 | 120.38 |
| 7 | O | 1104 | ASN | CA-C-N | 5.44 | 127.57 | 120.28 |
| 7 | O | 1104 | ASN | C-N-CA | 5.44 | 127.57 | 120.28 |
| 8 | P | 59 | ARG | O-C-N | 5.44 | 129.82 | 122.59 |
| 8 | P | 618 | LEU | CA-C-O | -5.44 | 112.73 | 120.51 |
| 8 | P | 1025 | ASN | N-CA-C | -5.44 | 104.86 | 112.25 |
| 9 | R | 151 | HIS | CA-C-O | 5.44 | 125.12 | 119.14 |
| 9 | T | 820 | ILE | N-CA-C | -5.44 | 106.18 | 112.98 |
| 1 | Y | 853 | PHE | CA-C-O | -5.44 | 113.95 | 120.10 |
| 12 | v | 377 | SER | CA-C-O | -5.44 | 114.95 | 120.71 |
| 4 | z | 819 | ASN | O-C-N | -5.44 | 115.14 | 122.43 |
| 14 | h | 94 | ASN | O-C-N | -5.44 | 116.87 | 123.29 |
| 14 | h | 548 | GLU | CA-C-N | 5.44 | 127.57 | 120.28 |
| 14 | h | 548 | GLU | C-N-CA | 5.44 | 127.57 | 120.28 |
| 17 | d | 84 | GLU | CA-C-O | 5.44 | 127.72 | 121.47 |
| 2 | 1 | 679 | SER | N-CA-C | -5.44 | 99.22 | 110.80 |
| 5 | H | 507 | ASN | N-CA-C | -5.44 | 106.84 | 112.93 |
| 5 | K | 449 | ASP | CB-CA-C | -5.44 | 100.93 | 109.52 |
| 9 | Q | 225 | SER | N-CA-CB | 5.44 | 118.11 | 110.12 |
| 2 | Z | 1346 | LEU | O-C-N | -5.44 | 115.01 | 122.46 |
| 14 | h | 807 | ILE | CB-CA-C | -5.44 | 104.75 | 110.62 |
| 5 | B | 436 | MET | N-CA-CB | 5.43 | 117.95 | 110.07 |
| 6 | I | 327 | LYS | N-CA-CB | 5.43 | 117.89 | 110.01 |
| 7 | M | 162 | ILE | N-CA-C | 5.43 | 115.64 | 110.42 |
| 7 | M | 270 | THR | CA-CB-OG1 | 5.43 | 117.75 | 109.60 |
| 9 | S | 801 | GLN | CA-C-N | 5.43 | 127.50 | 120.44 |
| 9 | S | 801 | GLN | C-N-CA | 5.43 | 127.50 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | W | 307 | ILE | CA-C-O | -5.43 | 114.65 | 120.85 |
| 2 | Z | 651 | PHE | N-CA-CB | 5.43 | 118.59 | 110.22 |
| 12 | u | 257 | SER | CB-CA-C | -5.43 | 101.77 | 110.79 |
| 19 | f | 232 | ASN | N-CA-CB | 5.43 | 121.10 | 110.88 |
| 1 | 0 | 1096 | GLN | OE1-CD-NE2 | -5.43 | 117.17 | 122.60 |
| 1 | 0 | 1470 | ASP | CA-C-N | 5.43 | 127.35 | 120.72 |
| 1 | 0 | 1470 | ASP | C-N-CA | 5.43 | 127.35 | 120.72 |
| 6 | C | 293 | HIS | CE1-NE2-CD2 | -5.43 | 103.57 | 109.00 |
| 4 | D | 703 | GLN | N-CA-C | -5.43 | 105.36 | 111.28 |
| 5 | H | 537 | TYR | CB-CG-CD2 | -5.43 | 112.65 | 120.80 |
| 7 | M | 1505 | HIS | N-CA-C | -5.43 | 107.20 | 113.88 |
| 8 | N | 1636 | PHE | CA-C-N | 5.43 | 127.90 | 120.46 |
| 8 | N | 1636 | PHE | C-N-CA | 5.43 | 127.90 | 120.46 |
| 7 | O | 1284 | SER | N-CA-C | 5.43 | 117.20 | 111.28 |
| 9 | Q | 127 | GLN | N-CA-C | 5.43 | 117.20 | 111.28 |
| 9 | R | 74 | ALA | N-CA-C | 5.43 | 116.88 | 111.07 |
| 9 | R | 219 | VAL | N-CA-C | 5.43 | 116.16 | 110.62 |
| 11 | X | 277 | PRO | N-CA-C | 5.43 | 119.75 | 111.11 |
| 2 | Z | 1292 | ILE | CA-C-N | 5.43 | 127.56 | 120.28 |
| 2 | Z | 1292 | ILE | C-N-CA | 5.43 | 127.56 | 120.28 |
| 12 | u | 582 | GLU | CA-C-O | 5.43 | 125.34 | 119.15 |
| 14 | h | 709 | VAL | CA-C-O | -5.43 | 115.30 | 120.95 |
| 14 | h | 719 | PHE | O-C-N | 5.43 | 129.55 | 122.87 |
| 20 | n | 331 | LEU | CA-C-N | 5.43 | 128.57 | 120.31 |
| 20 | n | 331 | LEU | C-N-CA | 5.43 | 128.57 | 120.31 |
| 15 | b | 395 | VAL | N-CA-CB | 5.43 | 120.19 | 111.23 |
| 15 | b | 478 | ASP | N-CA-C | -5.43 | 99.58 | 108.76 |
| 19 | f | 451 | SER | N-CA-C | -5.43 | 104.24 | 112.99 |
| 6 | F | 292 | HIS | CA-CB-CG | 5.43 | 119.23 | 113.80 |
| 8 | N | 953 | TYR | N-CA-CB | -5.43 | 101.98 | 109.91 |
| 1 | Y | 697 | SER | CA-C-N | 5.43 | 128.57 | 120.31 |
| 1 | Y | 697 | SER | C-N-CA | 5.43 | 128.57 | 120.31 |
| 14 | h | 897 | SER | N-CA-CB | 5.43 | 119.67 | 110.49 |
| 15 | i | 684 | ASP | CA-C-N | 5.43 | 131.91 | 121.54 |
| 15 | i | 684 | ASP | C-N-CA | 5.43 | 131.91 | 121.54 |
| 20 | n | 75 | ASP | CA-CB-CG | -5.43 | 107.17 | 112.60 |
| 5 | K | 511 | GLU | CA-C-O | -5.43 | 114.80 | 120.55 |
| 7 | M | 709 | PHE | CB-CG-CD2 | -5.43 | 111.47 | 120.70 |
| 11 | X | 366 | ALA | CA-C-N | 5.43 | 130.64 | 121.14 |
| 11 | X | 366 | ALA | C-N-CA | 5.43 | 130.64 | 121.14 |
| 1 | Y | 923 | ASP | CA-CB-CG | 5.43 | 118.03 | 112.60 |
| 12 | u | 227 | LEU | CA-C-O | -5.43 | 115.12 | 120.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 16 | j | 375 | LEU | N-CA-C | -5.43 | 96.35 | 107.70 |
| 20 | n | 566 | ASN | CA-CB-CG | 5.43 | 118.03 | 112.60 |
| 21 | s | 45 | VAL | N-CA-CB | 5.43 | 116.90 | 110.55 |
| 16 | c | 143 | ARG | CB-CA-C | 5.43 | 119.14 | 111.86 |
| 7 | M | 771 | ARG | CD-NE-CZ | -5.43 | 116.80 | 124.40 |
| 20 | n | 372 | SER | N-CA-CB | 5.43 | 119.29 | 110.77 |
| 1 | 0 | 429 | GLU | CA-C-O | -5.43 | 112.86 | 119.32 |
| 1 | 0 | 896 | MET | O-C-N | 5.43 | 127.87 | 122.12 |
| 1 | 0 | 1152 | TYR | CB-CG-CD1 | -5.43 | 112.66 | 120.80 |
| 1 | 0 | 1378 | VAL | CA-C-N | 5.43 | 131.90 | 121.54 |
| 1 | 0 | 1378 | VAL | C-N-CA | 5.43 | 131.90 | 121.54 |
| 4 | D | 716 | THR | N-CA-C | 5.43 | 117.20 | 111.28 |
| 6 | L | 281 | ASP | CA-C-N | 5.43 | 129.78 | 120.72 |
| 6 | L | 281 | ASP | C-N-CA | 5.43 | 129.78 | 120.72 |
| 7 | M | 699 | VAL | CA-CB-CG2 | -5.43 | 101.17 | 110.40 |
| 8 | N | 687 | LYS | CA-C-O | 5.43 | 127.12 | 121.15 |
| 8 | N | 996 | THR | CA-CB-OG1 | -5.43 | 101.46 | 109.60 |
| 8 | P | 1282 | ASN | CB-CG-ND2 | 5.43 | 124.54 | 116.40 |
| 9 | T | 734 | GLU | N-CA-C | -5.43 | 106.16 | 112.89 |
| 1 | Y | 260 | HIS | CE1-NE2-CD2 | -5.43 | 103.57 | 109.00 |
| 1 | Y | 459 | ALA | N-CA-CB | 5.43 | 118.02 | 110.04 |
| 2 | Z | 114 | PRO | O-C-N | 5.43 | 129.25 | 123.01 |
| 2 | Z | 253 | VAL | N-CA-C | -5.43 | 100.51 | 108.11 |
| 2 | Z | 302 | ILE | CA-C-O | -5.43 | 116.14 | 121.67 |
| 17 | k | 79 | VAL | N-CA-C | -5.43 | 98.65 | 107.28 |
| 19 | f | 609 | SER | CB-CA-C | -5.43 | 99.88 | 109.70 |
| 20 | g | 105 | VAL | N-CA-C | -5.43 | 98.09 | 106.72 |
| 20 | g | 542 | ASN | CA-CB-CG | 5.43 | 118.03 | 112.60 |
| 20 | g | 910 | ASP | N-CA-C | -5.43 | 99.25 | 108.26 |
| 1 | 0 | 212 | GLN | OE1-CD-NE2 | 5.42 | 128.03 | 122.60 |
| 7 | O | 331 | ILE | CA-C-O | -5.42 | 114.84 | 121.13 |
| 7 | O | 1411 | HIS | CE1-NE2-CD2 | -5.42 | 103.58 | 109.00 |
| 9 | T | 405 | ASP | CA-C-N | 5.42 | 126.62 | 119.84 |
| 9 | T | 405 | ASP | C-N-CA | 5.42 | 126.62 | 119.84 |
| 1 | Y | 940 | VAL | CA-C-N | 5.42 | 127.55 | 120.28 |
| 1 | Y | 940 | VAL | C-N-CA | 5.42 | 127.55 | 120.28 |
| 1 | Y | 1420 | GLY | O-C-N | 5.42 | 128.63 | 122.55 |
| 2 | Z | 340 | GLU | O-C-N | 5.42 | 129.81 | 122.59 |
| 4 | y | 713 | ASN | O-C-N | 5.42 | 127.66 | 122.07 |
| 21 | p | 50 | ASP | CA-C-N | 5.42 | 127.50 | 120.56 |
| 21 | p | 50 | ASP | C-N-CA | 5.42 | 127.50 | 120.56 |
| 15 | b | 287 | ASP | O-C-N | -5.42 | 115.85 | 122.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 18 | e | 177 | ARG | NE-CZ-NH1 | 5.42 | 126.92 | 121.50 |
| 8 | N | 444 | ASN | N-CA-CB | -5.42 | 102.34 | 110.91 |
| 8 | N | 1503 | VAL | CB-CA-C | -5.42 | 104.74 | 112.22 |
| 8 | P | 1344 | PHE | CA-CB-CG | 5.42 | 119.22 | 113.80 |
| 1 | Y | 1368 | SER | N-CA-CB | 5.42 | 118.19 | 110.06 |
| 18 | e | 244 | LYS | CA-C-N | 5.42 | 131.06 | 122.33 |
| 18 | e | 244 | LYS | C-N-CA | 5.42 | 131.06 | 122.33 |
| 19 | f | 539 | LEU | O-C-N | 5.42 | 129.85 | 122.37 |
| 4 | A | 762 | LEU | N-CA-C | 5.42 | 116.87 | 111.07 |
| 7 | O | 1423 | SER | N-CA-C | 5.42 | 117.94 | 111.71 |
| 9 | Q | 421 | SER | N-CA-CB | 5.42 | 119.65 | 110.49 |
| 9 | R | 273 | VAL | N-CA-C | -5.42 | 105.09 | 111.00 |
| 9 | T | 339 | TYR | CA-C-N | 5.42 | 128.55 | 120.31 |
| 9 | T | 339 | TYR | C-N-CA | 5.42 | 128.55 | 120.31 |
| 15 | i | 469 | PHE | N-CA-CB | 5.42 | 118.16 | 110.13 |
| 19 | m | 285 | ASP | CA-C-N | 5.42 | 127.49 | 120.44 |
| 19 | m | 285 | ASP | C-N-CA | 5.42 | 127.49 | 120.44 |
| 21 | o | 55 | ASN | CA-CB-CG | -5.42 | 107.18 | 112.60 |
| 15 | b | 403 | HIS | CA-CB-CG | -5.42 | 108.38 | 113.80 |
| 15 | b | 718 | LYS | CA-C-O | 5.42 | 126.35 | 120.12 |
| 19 | f | 312 | GLU | CA-C-N | 5.42 | 130.41 | 122.77 |
| 19 | f | 312 | GLU | C-N-CA | 5.42 | 130.41 | 122.77 |
| 14 | a | 121 | VAL | N-CA-CB | 5.42 | 120.36 | 111.58 |
| 14 | a | 445 | ASN | CA-C-N | 5.42 | 127.54 | 120.28 |
| 14 | a | 445 | ASN | C-N-CA | 5.42 | 127.54 | 120.28 |
| 1 | 0 | 630 | THR | CB-CA-C | 5.42 | 118.13 | 109.02 |
| 2 | 1 | 859 | THR | O-C-N | 5.42 | 129.29 | 122.19 |
| 5 | H | 454 | GLY | CA-C-N | 5.42 | 128.29 | 120.38 |
| 5 | H | 454 | GLY | C-N-CA | 5.42 | 128.29 | 120.38 |
| 7 | M | 1019 | ILE | CA-C-N | 5.42 | 128.32 | 120.79 |
| 7 | M | 1019 | ILE | C-N-CA | 5.42 | 128.32 | 120.79 |
| 7 | O | 1313 | ILE | CA-CB-CG1 | 5.42 | 119.61 | 110.40 |
| 8 | P | 302 | LEU | N-CA-CB | 5.42 | 118.68 | 110.28 |
| 9 | R | 234 | ILE | N-CA-C | -5.42 | 107.84 | 113.10 |
| 12 | v | 273 | GLN | N-CA-CB | 5.42 | 117.97 | 110.17 |
| 21 | p | 59 | VAL | N-CA-C | -5.42 | 100.31 | 108.12 |
| 15 | b | 608 | PRO | N-CD-CG | 5.42 | 111.33 | 103.20 |
| 1 | 0 | 179 | LEU | CA-C-N | 5.42 | 131.89 | 121.54 |
| 1 | 0 | 179 | LEU | C-N-CA | 5.42 | 131.89 | 121.54 |
| 1 | 0 | 1027 | HIS | N-CA-C | -5.42 | 106.14 | 114.16 |
| 1 | 0 | 1448 | MET | CG-SD-CE | -5.42 | 88.98 | 100.90 |
| 5 | B | 374 | ILE | CA-CB-CG2 | 5.42 | 119.71 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | J | 796 | ILE | CA-C-O | -5.42 | 114.40 | 120.25 |
| 8 | N | 64 | SER | N-CA-CB | 5.42 | 119.92 | 110.65 |
| 7 | O | 1363 | ILE | CA-C-O | 5.42 | 123.67 | 118.90 |
| 8 | P | 902 | GLU | CA-C-N | 5.42 | 128.32 | 120.79 |
| 8 | P | 902 | GLU | C-N-CA | 5.42 | 128.32 | 120.79 |
| 9 | R | 26 | LEU | CA-C-N | 5.42 | 127.54 | 120.28 |
| 9 | R | 26 | LEU | C-N-CA | 5.42 | 127.54 | 120.28 |
| 9 | T | 435 | TRP | O-C-N | 5.42 | 127.86 | 122.12 |
| 11 | V | 383 | GLY | N-CA-C | -5.42 | 103.05 | 111.12 |
| 1 | Y | 778 | THR | CA-C-N | 5.42 | 127.54 | 120.28 |
| 1 | Y | 778 | THR | C-N-CA | 5.42 | 127.54 | 120.28 |
| 12 | v | 652 | GLN | N-CA-C | -5.42 | 105.03 | 111.69 |
| 12 | v | 695 | LYS | O-C-N | 5.42 | 127.86 | 122.12 |
| 13 | w | 1361 | GLU | CA-C-O | -5.42 | 114.81 | 120.55 |
| 15 | i | 385 | ASP | N-CA-C | -5.42 | 100.41 | 109.24 |
| 19 | m | 668 | HIS | CB-CG-ND1 | 5.42 | 130.83 | 122.70 |
| 15 | b | 661 | HIS | CA-CB-CG | 5.42 | 119.22 | 113.80 |
| 16 | c | 412 | LEU | CA-C-N | 5.42 | 126.61 | 119.84 |
| 16 | c | 412 | LEU | C-N-CA | 5.42 | 126.61 | 119.84 |
| 14 | a | 16 | GLU | N-CA-C | -5.42 | 106.68 | 113.72 |
| 14 | a | 151 | HIS | CB-CG-CD2 | -5.42 | 124.16 | 131.20 |
| 2 | 1 | 138 | PHE | CB-CA-C | -5.42 | 98.40 | 109.94 |
| 5 | B | 302 | ASN | CB-CG-ND2 | 5.42 | 124.53 | 116.40 |
| 7 | M | 881 | THR | N-CA-C | 5.42 | 117.61 | 111.11 |
| 7 | O | 1376 | THR | O-C-N | 5.42 | 128.93 | 122.27 |
| 9 | T | 715 | MET | CG-SD-CE | -5.42 | 88.98 | 100.90 |
| 9 | T | 741 | LEU | N-CA-C | 5.42 | 118.10 | 111.82 |
| 14 | h | 150 | PHE | CA-CB-CG | -5.42 | 108.38 | 113.80 |
| 15 | i | 629 | VAL | O-C-N | 5.42 | 127.22 | 121.91 |
| 15 | i | 674 | ILE | CA-C-N | 5.42 | 131.88 | 121.54 |
| 15 | i | 674 | ILE | C-N-CA | 5.42 | 131.88 | 121.54 |
| 16 | j | 272 | ILE | N-CA-CB | 5.42 | 117.91 | 110.54 |
| 19 | m | 223 | ILE | N-CA-C | -5.42 | 107.47 | 112.83 |
| 1 | 0 | 1481 | ASN | OD1-CG-ND2 | 5.42 | 128.01 | 122.60 |
| 4 | A | 715 | GLU | CB-CA-C | -5.42 | 101.64 | 110.85 |
| 6 | C | 317 | LYS | N-CA-C | 5.42 | 117.18 | 111.28 |
| 7 | M | 1171 | SER | CA-C-O | 5.42 | 125.01 | 119.05 |
| 9 | S | 616 | GLU | CA-C-O | -5.42 | 112.94 | 119.27 |
| 9 | T | 569 | VAL | CA-C-N | 5.42 | 127.98 | 120.29 |
| 9 | T | 569 | VAL | C-N-CA | 5.42 | 127.98 | 120.29 |
| 2 | Z | 788 | SER | CA-C-N | 5.42 | 127.54 | 120.28 |
| 2 | Z | 788 | SER | C-N-CA | 5.42 | 127.54 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 16 | j | 490 | SER | CA-C-N | 5.42 | 127.98 | 120.29 |
| 16 | j | 490 | SER | C-N-CA | 5.42 | 127.98 | 120.29 |
| 19 | m | 536 | ARG | CB-CA-C | -5.42 | 102.38 | 110.88 |
| 21 | r | 55 | ASN | OD1-CG-ND2 | -5.42 | 117.19 | 122.60 |
| 15 | b | 424 | CYS | N-CA-C | -5.42 | 99.27 | 110.80 |
| 14 | a | 878 | HIS | ND1-CE1-NE2 | 5.42 | 113.81 | 108.40 |
| 1 | 0 | 231 | LEU | N-CA-C | -5.41 | 99.59 | 108.41 |
| 5 | H | 299 | TRP | CE3-CZ3-CH2 | -5.41 | 114.06 | 121.10 |
| 7 | M | 935 | GLN | CA-C-N | 5.41 | 127.38 | 120.56 |
| 7 | M | 935 | GLN | C-N-CA | 5.41 | 127.38 | 120.56 |
| 8 | N | 770 | HIS | CG-CD2-NE2 | 5.41 | 112.61 | 107.20 |
| 8 | P | 185 | LEU | O-C-N | 5.41 | 127.86 | 122.12 |
| 9 | R | 659 | SER | CA-C-N | 5.41 | 128.08 | 120.28 |
| 9 | R | 659 | SER | C-N-CA | 5.41 | 128.08 | 120.28 |
| 1 | Y | 681 | THR | N-CA-C | 5.41 | 117.18 | 111.28 |
| 16 | c | 189 | TYR | N-CA-C | -5.41 | 105.28 | 111.07 |
| 19 | f | 289 | HIS | CB-CG-ND1 | 5.41 | 130.82 | 122.70 |
| 14 | a | 1011 | ASP | CA-C-N | 5.41 | 128.92 | 120.75 |
| 14 | a | 1011 | ASP | C-N-CA | 5.41 | 128.92 | 120.75 |
| 7 | M | 1137 | ASN | CB-CA-C | -5.41 | 99.82 | 110.10 |
| 7 | M | 1279 | CYS | CA-C-N | 5.41 | 127.38 | 120.56 |
| 7 | M | 1279 | CYS | C-N-CA | 5.41 | 127.38 | 120.56 |
| 7 | O | 1120 | THR | CA-C-O | 5.41 | 126.64 | 120.80 |
| 8 | P | 672 | VAL | CA-C-N | 5.41 | 127.48 | 120.44 |
| 8 | P | 672 | VAL | C-N-CA | 5.41 | 127.48 | 120.44 |
| 10 | W | 314 | VAL | N-CA-C | 5.41 | 116.06 | 109.30 |
| 15 | i | 527 | VAL | CA-CB-CG1 | -5.41 | 101.20 | 110.40 |
| 21 | p | 74 | GLY | N-CA-C | -5.41 | 107.64 | 115.27 |
| 1 | 0 | 1479 | ILE | CA-C-N | 5.41 | 131.88 | 121.54 |
| 1 | 0 | 1479 | ILE | C-N-CA | 5.41 | 131.88 | 121.54 |
| 2 | 1 | 1109 | LEU | CA-C-O | -5.41 | 113.13 | 119.24 |
| 7 | M | 1450 | GLY | CA-C-O | -5.41 | 114.84 | 120.90 |
| 7 | O | 278 | ILE | CA-C-N | 5.41 | 127.84 | 120.54 |
| 7 | O | 278 | ILE | C-N-CA | 5.41 | 127.84 | 120.54 |
| 9 | Q | 319 | SER | CA-C-O | -5.41 | 115.49 | 121.33 |
| 9 | T | 573 | HIS | CA-C-N | 5.41 | 127.47 | 120.44 |
| 9 | T | 573 | HIS | C-N-CA | 5.41 | 127.47 | 120.44 |
| 9 | T | 592 | LYS | CA-C-O | -5.41 | 115.63 | 121.36 |
| 1 | Y | 1155 | ARG | NE-CZ-NH2 | -5.41 | 114.33 | 119.20 |
| 2 | Z | 627 | ASN | N-CA-CB | 5.41 | 120.00 | 110.37 |
| 2 | Z | 854 | THR | CA-CB-OG1 | 5.41 | 117.72 | 109.60 |
| 14 | h | 978 | ALA | CA-C-O | -5.41 | 114.68 | 120.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | i | 561 | ARG | O-C-N | -5.41 | 113.75 | 122.41 |
| 16 | j | 615 | ASN | CA-CB-CG | -5.41 | 107.19 | 112.60 |
| 19 | m | 717 | LEU | N-CA-C | -5.41 | 106.52 | 113.23 |
| 20 | n | 720 | GLN | N-CA-C | -5.41 | 106.72 | 113.38 |
| 21 | s | 19 | LYS | CA-C-N | 5.41 | 127.97 | 120.29 |
| 21 | s | 19 | LYS | C-N-CA | 5.41 | 127.97 | 120.29 |
| 16 | c | 599 | LEU | CA-C-N | 5.41 | 129.88 | 120.68 |
| 16 | c | 599 | LEU | C-N-CA | 5.41 | 129.88 | 120.68 |
| 14 | a | 1016 | GLN | O-C-N | -5.41 | 116.98 | 123.31 |
| 2 | 1 | 253 | VAL | O-C-N | -5.41 | 117.50 | 123.18 |
| 7 | M | 57 | GLU | N-CA-C | -5.41 | 100.21 | 109.24 |
| 8 | N | 1389 | LEU | CA-C-N | 5.41 | 127.53 | 120.28 |
| 8 | N | 1389 | LEU | C-N-CA | 5.41 | 127.53 | 120.28 |
| 7 | O | 563 | SER | N-CA-CB | 5.41 | 118.07 | 110.12 |
| 8 | P | 1188 | THR | N-CA-CB | 5.41 | 117.85 | 110.01 |
| 9 | S | 634 | ASP | CA-C-N | 5.41 | 128.94 | 121.26 |
| 9 | S | 634 | ASP | C-N-CA | 5.41 | 128.94 | 121.26 |
| 9 | T | 417 | ARG | N-CA-CB | 5.41 | 119.63 | 110.49 |
| 1 | Y | 846 | ILE | N-CA-C | -5.41 | 98.09 | 109.34 |
| 14 | h | 507 | PHE | CA-CB-CG | -5.41 | 108.39 | 113.80 |
| 14 | h | 749 | TYR | N-CA-C | -5.41 | 100.90 | 108.96 |
| 14 | h | 752 | HIS | CE1-NE2-CD2 | -5.41 | 103.59 | 109.00 |
| 15 | i | 455 | PHE | CA-CB-CG | -5.41 | 108.39 | 113.80 |
| 20 | n | 1059 | GLN | N-CA-C | 5.41 | 117.25 | 111.36 |
| 16 | c | 224 | MET | CA-C-N | 5.41 | 129.86 | 121.26 |
| 16 | c | 224 | MET | C-N-CA | 5.41 | 129.86 | 121.26 |
| 16 | c | 566 | ASP | N-CA-CB | 5.41 | 119.77 | 110.68 |
| 19 | f | 520 | GLY | CA-C-N | 5.41 | 131.87 | 121.54 |
| 19 | f | 520 | GLY | C-N-CA | 5.41 | 131.87 | 121.54 |
| 20 | g | 621 | TYR | N-CA-CB | 5.41 | 120.03 | 111.43 |
| 14 | a | 561 | GLN | N-CA-CB | -5.41 | 103.15 | 110.67 |
| 6 | F | 389 | ARG | N-CA-CB | 5.41 | 117.91 | 110.07 |
| 8 | N | 1043 | LEU | N-CA-C | -5.41 | 104.28 | 112.99 |
| 7 | O | 1555 | VAL | N-CA-C | -5.41 | 107.46 | 112.43 |
| 9 | Q | 643 | LEU | N-CA-C | -5.41 | 106.53 | 113.23 |
| 9 | S | 615 | ASP | N-CA-C | -5.41 | 99.28 | 110.80 |
| 4 | z | 641 | VAL | O-C-N | 5.41 | 127.11 | 121.87 |
| 14 | h | 564 | ILE | CA-C-O | 5.41 | 126.31 | 120.47 |
| 14 | h | 759 | MET | CA-CB-CG | 5.41 | 124.92 | 114.10 |
| 20 | n | 587 | LEU | CA-C-O | 5.41 | 126.03 | 119.38 |
| 20 | n | 736 | ASP | CA-C-N | 5.41 | 128.53 | 120.31 |
| 20 | n | 736 | ASP | C-N-CA | 5.41 | 128.53 | 120.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | f | 686 | GLU | CA-C-O | 5.41 | 128.24 | 120.51 |
| 14 | a | 558 | LEU | CA-C-O | -5.41 | 114.79 | 121.06 |
| 14 | a | 828 | LEU | N-CA-CB | 5.41 | 117.81 | 109.91 |
| 1 | 0 | 956 | ASN | CB-CG-ND2 | -5.41 | 108.29 | 116.40 |
| 1 | 0 | 1312 | ALA | N-CA-CB | 5.41 | 119.63 | 110.49 |
| 5 | B | 439 | GLN | OE1-CD-NE2 | -5.41 | 117.19 | 122.60 |
| 4 | D | 798 | ASN | CA-CB-CG | -5.41 | 107.19 | 112.60 |
| 9 | Q | 120 | ASN | CA-C-N | 5.41 | 127.37 | 120.56 |
| 9 | Q | 120 | ASN | C-N-CA | 5.41 | 127.37 | 120.56 |
| 9 | R | 241 | ILE | N-CA-C | -5.41 | 107.48 | 112.83 |
| 2 | Z | 173 | TRP | N-CA-CB | 5.41 | 119.04 | 110.55 |
| 12 | v | 230 | SER | CA-C-N | 5.41 | 127.97 | 120.29 |
| 12 | v | 230 | SER | C-N-CA | 5.41 | 127.97 | 120.29 |
| 15 | i | 385 | ASP | CA-C-O | 5.41 | 126.32 | 120.43 |
| 15 | b | 338 | VAL | CB-CA-C | 5.41 | 119.68 | 112.22 |
| 15 | b | 457 | TYR | N-CA-C | -5.41 | 99.79 | 108.55 |
| 15 | b | 550 | HIS | ND1-CE1-NE2 | 5.41 | 113.81 | 108.40 |
| 5 | K | 313 | TYR | CA-C-N | 5.40 | 129.42 | 120.94 |
| 5 | K | 313 | TYR | C-N-CA | 5.40 | 129.42 | 120.94 |
| 7 | M | 750 | TRP | CA-C-N | 5.40 | 125.02 | 119.56 |
| 7 | M | 750 | TRP | C-N-CA | 5.40 | 125.02 | 119.56 |
| 7 | O | 330 | SER | N-CA-CB | 5.40 | 119.95 | 111.20 |
| 8 | P | 301 | ALA | N-CA-C | -5.40 | 106.82 | 113.41 |
| 9 | T | 313 | LEU | CB-CA-C | -5.40 | 103.91 | 111.85 |
| 9 | T | 500 | GLU | CA-C-N | 5.40 | 127.47 | 120.44 |
| 9 | T | 500 | GLU | C-N-CA | 5.40 | 127.47 | 120.44 |
| 9 | T | 513 | LEU | CA-C-N | -5.40 | 111.22 | 121.54 |
| 9 | T | 513 | LEU | C-N-CA | -5.40 | 111.22 | 121.54 |
| 1 | Y | 1369 | ASN | CA-CB-CG | -5.40 | 107.20 | 112.60 |
| 2 | Z | 214 | PHE | CA-C-O | -5.40 | 115.15 | 120.82 |
| 15 | i | 261 | ALA | N-CA-C | 5.40 | 116.98 | 111.14 |
| 20 | g | 944 | LEU | CA-C-O | -5.40 | 112.73 | 119.38 |
| 1 | 0 | 1212 | GLU | CA-C-N | 5.40 | 127.52 | 120.28 |
| 1 | 0 | 1212 | GLU | C-N-CA | 5.40 | 127.52 | 120.28 |
| 1 | 0 | 1271 | ILE | CA-C-N | 5.40 | 128.06 | 120.28 |
| 1 | 0 | 1271 | ILE | C-N-CA | 5.40 | 128.06 | 120.28 |
| 2 | 1 | 503 | SER | N-CA-C | 5.40 | 120.10 | 112.75 |
| 2 | 1 | 1056 | HIS | CE1-NE2-CD2 | -5.40 | 103.60 | 109.00 |
| 7 | M | 288 | TRP | CG-CD2-CE3 | -5.40 | 128.50 | 133.90 |
| 7 | M | 757 | PHE | CB-CA-C | -5.40 | 102.36 | 110.90 |
| 7 | M | 1295 | ALA | N-CA-C | 5.40 | 116.85 | 111.07 |
| 8 | N | 1227 | VAL | N-CA-C | 5.40 | 115.61 | 110.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 142 | ILE | CA-C-N | 5.40 | 129.78 | 121.19 |
| 8 | P | 142 | ILE | C-N-CA | 5.40 | 129.78 | 121.19 |
| 2 | Z | 799 | ILE | N-CA-C | -5.40 | 105.26 | 110.72 |
| 14 | h | 389 | LEU | N-CA-CB | 5.40 | 118.85 | 110.80 |
| 18 | l | 327 | LYS | CA-C-N | 5.40 | 128.66 | 120.77 |
| 18 | l | 327 | LYS | C-N-CA | 5.40 | 128.66 | 120.77 |
| 19 | m | 289 | HIS | CB-CG-CD2 | -5.40 | 124.18 | 131.20 |
| 20 | n | 130 | ASP | CA-C-O | 5.40 | 124.84 | 118.90 |
| 20 | n | 181 | ILE | N-CA-CB | 5.40 | 120.14 | 111.23 |
| 20 | n | 246 | LYS | CA-C-N | 5.40 | 131.86 | 121.54 |
| 20 | n | 246 | LYS | C-N-CA | 5.40 | 131.86 | 121.54 |
| 21 | o | 10 | ILE | CB-CA-C | -5.40 | 103.97 | 110.99 |
| 16 | c | 563 | SER | N-CA-CB | 5.40 | 119.62 | 110.49 |
| 7 | M | 356 | ILE | N-CA-C | -5.40 | 104.00 | 109.02 |
| 7 | M | 1004 | ASP | CA-CB-CG | 5.40 | 118.00 | 112.60 |
| 7 | M | 1552 | PHE | N-CA-C | -5.40 | 104.66 | 113.19 |
| 7 | O | 63 | THR | CA-CB-OG1 | 5.40 | 117.70 | 109.60 |
| 7 | O | 125 | HIS | O-C-N | -5.40 | 115.62 | 122.43 |
| 9 | T | 161 | ILE | CA-C-O | -5.40 | 115.44 | 121.17 |
| 9 | T | 733 | GLN | N-CA-CB | 5.40 | 119.84 | 110.44 |
| 15 | i | 219 | PRO | O-C-N | 5.40 | 131.36 | 121.10 |
| 19 | m | 49 | LEU | CA-C-N | 5.40 | 127.52 | 120.28 |
| 19 | m | 49 | LEU | C-N-CA | 5.40 | 127.52 | 120.28 |
| 16 | c | 138 | ILE | N-CA-CB | 5.40 | 118.68 | 110.58 |
| 8 | N | 595 | ILE | N-CA-CB | 5.40 | 117.88 | 110.54 |
| 8 | N | 1230 | VAL | CA-C-N | 5.40 | 127.96 | 120.29 |
| 8 | N | 1230 | VAL | C-N-CA | 5.40 | 127.96 | 120.29 |
| 1 | 0 | 239 | GLU | O-C-N | -5.40 | 117.10 | 123.25 |
| 6 | C | 329 | ASP | CA-C-N | 5.40 | 127.51 | 120.28 |
| 6 | C | 329 | ASP | C-N-CA | 5.40 | 127.51 | 120.28 |
| 7 | M | 628 | LYS | N-CA-C | 5.40 | 116.84 | 111.07 |
| 8 | N | 804 | GLN | CG-CD-NE2 | -5.40 | 108.30 | 116.40 |
| 7 | O | 80 | GLU | O-C-N | 5.40 | 127.84 | 122.12 |
| 9 | Q | 292 | LYS | O-C-N | -5.40 | 115.06 | 122.46 |
| 9 | S | 98 | PRO | CB-CA-C | -5.40 | 104.45 | 112.55 |
| 9 | T | 73 | LEU | N-CA-C | 5.40 | 117.16 | 111.28 |
| 10 | U | 283 | ILE | N-CA-C | 5.40 | 115.08 | 106.88 |
| 2 | Z | 1096 | ASN | O-C-N | 5.40 | 127.86 | 122.03 |
| 13 | w | 1339 | PHE | N-CA-C | 5.40 | 118.97 | 112.38 |
| 14 | h | 697 | GLN | CA-C-O | -5.40 | 115.13 | 120.90 |
| 17 | k | 205 | ASP | CA-C-N | 5.40 | 128.43 | 120.82 |
| 17 | k | 205 | ASP | C-N-CA | 5.40 | 128.43 | 120.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | n | 306 | LYS | N-CA-CB | 5.40 | 117.98 | 109.83 |
| 16 | c | 552 | TYR | O-C-N | -5.40 | 116.48 | 122.09 |
| 19 | f | 518 | ILE | N-CA-C | -5.40 | 107.72 | 112.90 |
| 14 | a | 454 | LYS | CA-C-N | 5.40 | 128.51 | 120.90 |
| 14 | a | 454 | LYS | C-N-CA | 5.40 | 128.51 | 120.90 |
| 6 | I | 304 | LEU | CA-C-N | 5.40 | 128.08 | 120.42 |
| 6 | I | 304 | LEU | C-N-CA | 5.40 | 128.08 | 120.42 |
| 7 | M | 511 | ILE | CA-CB-CG2 | -5.40 | 101.33 | 110.50 |
| 7 | M | 672 | TRP | O-C-N | 5.40 | 127.70 | 122.09 |
| 7 | O | 192 | ILE | O-C-N | 5.40 | 127.10 | 121.87 |
| 9 | S | 431 | SER | CA-C-N | 5.40 | 129.15 | 120.30 |
| 9 | S | 431 | SER | C-N-CA | 5.40 | 129.15 | 120.30 |
| 9 | T | 641 | ILE | N-CA-CB | 5.40 | 116.50 | 110.51 |
| 1 | Y | 380 | TYR | O-C-N | -5.40 | 116.60 | 123.24 |
| 14 | h | 242 | HIS | ND1-CE1-NE2 | 5.40 | 113.80 | 108.40 |
| 21 | p | 72 | GLU | N-CA-C | -5.40 | 101.37 | 109.95 |
| 1 | 0 | 359 | LEU | N-CA-C | -5.39 | 100.91 | 109.59 |
| 8 | P | 720 | ARG | N-CA-C | 5.39 | 117.91 | 111.71 |
| 9 | R | 418 | CYS | CA-C-N | 5.39 | 131.84 | 121.54 |
| 9 | R | 418 | CYS | C-N-CA | 5.39 | 131.84 | 121.54 |
| 9 | T | 816 | TYR | N-CA-C | -5.39 | 105.43 | 112.23 |
| 1 | Y | 115 | ASP | N-CA-C | 5.39 | 117.16 | 111.28 |
| 12 | u | 282 | GLN | CA-C-O | -5.39 | 115.44 | 121.81 |
| 13 | w | 1388 | GLU | CB-CA-C | -5.39 | 101.84 | 110.79 |
| 14 | h | 153 | GLN | N-CA-CB | 5.39 | 121.55 | 111.52 |
| 19 | m | 137 | LYS | N-CA-C | -5.39 | 99.31 | 110.80 |
| 15 | b | 317 | PHE | CA-C-N | 5.39 | 127.14 | 120.34 |
| 15 | b | 317 | PHE | C-N-CA | 5.39 | 127.14 | 120.34 |
| 19 | f | 169 | LEU | N-CA-CB | 5.39 | 119.17 | 110.65 |
| 1 | 0 | 1416 | PHE | O-C-N | -5.39 | 115.83 | 122.25 |
| 2 | 1 | 637 | LEU | CA-C-O | 5.39 | 126.17 | 119.97 |
| 7 | M | 76 | SER | CA-C-N | 5.39 | 127.77 | 120.38 |
| 7 | M | 76 | SER | C-N-CA | 5.39 | 127.77 | 120.38 |
| 7 | O | 161 | GLN | N-CA-CB | 5.39 | 117.83 | 110.01 |
| 7 | O | 564 | ASP | CB-CG-OD2 | -5.39 | 106.00 | 118.40 |
| 8 | P | 1490 | ARG | CA-C-N | 5.39 | 127.51 | 120.28 |
| 8 | P | 1490 | ARG | C-N-CA | 5.39 | 127.51 | 120.28 |
| 9 | Q | 766 | ASN | N-CA-C | -5.39 | 106.18 | 114.16 |
| 12 | u | 39 | GLN | CA-C-N | 5.39 | 129.84 | 122.34 |
| 12 | u | 39 | GLN | C-N-CA | 5.39 | 129.84 | 122.34 |
| 14 | h | 511 | ARG | NH1-CZ-NH2 | -5.39 | 112.29 | 119.30 |
| 2 | 1 | 227 | LEU | CA-C-O | 5.39 | 126.67 | 120.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | H | 535 | LYS | N-CA-C | -5.39 | 105.40 | 112.41 |
| 7 | M | 706 | VAL | N-CA-C | -5.39 | 107.11 | 111.91 |
| 7 | M | 1443 | ASN | N-CA-C | 5.39 | 119.35 | 112.34 |
| 2 | Z | 992 | ASP | CA-C-N | 5.39 | 125.69 | 119.92 |
| 2 | Z | 992 | ASP | C-N-CA | 5.39 | 125.69 | 119.92 |
| 14 | h | 1011 | ASP | N-CA-CB | 5.39 | 119.60 | 110.49 |
| 20 | n | 1045 | ILE | N-CA-C | -5.39 | 105.28 | 110.72 |
| 16 | c | 571 | ALA | CA-C-O | 5.39 | 125.60 | 119.18 |
| 1 | 0 | 1358 | GLU | CA-C-N | 5.39 | 130.59 | 123.05 |
| 1 | 0 | 1358 | GLU | C-N-CA | 5.39 | 130.59 | 123.05 |
| 2 | 1 | 760 | SER | CA-C-O | 5.39 | 126.13 | 120.42 |
| 7 | M | 1218 | ASN | OD1-CG-ND2 | -5.39 | 117.21 | 122.60 |
| 9 | Q | 121 | ILE | O-C-N | 5.39 | 127.19 | 121.91 |
| 11 | V | 393 | GLU | N-CA-C | 5.39 | 117.23 | 111.36 |
| 11 | X | 376 | ILE | CA-CB-CG1 | 5.39 | 119.56 | 110.40 |
| 1 | Y | 1208 | SER | CB-CA-C | -5.39 | 103.77 | 112.07 |
| 12 | u | 589 | ASP | CA-C-N | 5.39 | 127.45 | 120.44 |
| 12 | u | 589 | ASP | C-N-CA | 5.39 | 127.45 | 120.44 |
| 19 | m | 334 | ARG | NE-CZ-NH1 | 5.39 | 126.89 | 121.50 |
| 15 | b | 64 | LYS | N-CA-CB | 5.39 | 119.23 | 110.17 |
| 18 | e | 8 | HIS | N-CA-CB | 5.39 | 119.91 | 111.56 |
| 20 | g | 747 | LYS | CB-CA-C | 5.39 | 119.83 | 110.94 |
| 20 | g | 869 | ASP | N-CA-CB | 5.39 | 118.64 | 110.28 |
| 20 | g | 1117 | ILE | CA-C-O | 5.39 | 126.56 | 120.85 |
| 7 | M | 564 | ASP | O-C-N | -5.39 | 116.31 | 122.08 |
| 7 | M | 1296 | LEU | O-C-N | 5.39 | 127.62 | 122.07 |
| 7 | O | 1334 | THR | O-C-N | 5.39 | 129.57 | 122.30 |
| 9 | S | 588 | VAL | N-CA-C | -5.39 | 106.59 | 113.22 |
| 1 | Y | 1476 | GLU | CB-CG-CD | -5.39 | 103.44 | 112.60 |
| 2 | Z | 1230 | ASP | N-CA-C | -5.39 | 100.24 | 109.24 |
| 15 | i | 204 | PHE | N-CA-C | -5.39 | 105.10 | 110.97 |
| 19 | f | 398 | ILE | N-CA-C | 5.39 | 116.16 | 110.72 |
| 1 | 0 | 1478 | LYS | N-CA-C | -5.39 | 100.53 | 108.99 |
| 2 | 1 | 108 | THR | CA-C-N | 5.39 | 125.68 | 119.92 |
| 2 | 1 | 108 | THR | C-N-CA | 5.39 | 125.68 | 119.92 |
| 4 | A | 698 | GLN | CA-C-N | 5.39 | 127.77 | 120.44 |
| 4 | A | 698 | GLN | C-N-CA | 5.39 | 127.77 | 120.44 |
| 6 | C | 294 | LEU | N-CA-C | -5.39 | 106.21 | 112.89 |
| 6 | F | 292 | HIS | CE1-NE2-CD2 | -5.39 | 103.61 | 109.00 |
| 6 | L | 300 | ASP | N-CA-C | -5.39 | 105.74 | 114.09 |
| 7 | M | 201 | VAL | O-C-N | -5.39 | 116.14 | 122.07 |
| 7 | O | 321 | GLN | N-CA-C | 5.39 | 116.83 | 111.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1232 | HIS | CA-CB-CG | -5.39 | 108.41 | 113.80 |
| 1 | Y | 281 | ARG | CA-C-N | 5.39 | 129.32 | 122.37 |
| 1 | Y | 281 | ARG | C-N-CA | 5.39 | 129.32 | 122.37 |
| 1 | Y | 657 | GLU | N-CA-C | -5.39 | 107.72 | 114.56 |
| 1 | Y | 775 | LEU | N-CA-CB | 5.39 | 119.33 | 110.39 |
| 13 | w | 1358 | HIS | CA-C-N | 5.39 | 127.44 | 120.44 |
| 13 | w | 1358 | HIS | C-N-CA | 5.39 | 127.44 | 120.44 |
| 21 | s | 65 | PHE | O-C-N | -5.39 | 117.59 | 123.52 |
| 20 | g | 687 | LYS | N-CA-CB | 5.39 | 118.46 | 110.49 |
| 20 | g | 868 | HIS | CB-CG-ND1 | 5.39 | 130.78 | 122.70 |
| 1 | 0 | 1236 | LEU | O-C-N | 5.38 | 128.97 | 122.35 |
| 8 | N | 844 | TYR | O-C-N | 5.38 | 127.61 | 122.07 |
| 8 | N | 1349 | TYR | CB-CA-C | 5.38 | 119.73 | 110.79 |
| 7 | O | 160 | GLN | OE1-CD-NE2 | 5.38 | 127.98 | 122.60 |
| 9 | T | 247 | GLY | CA-C-N | 5.38 | 127.50 | 120.28 |
| 9 | T | 247 | GLY | C-N-CA | 5.38 | 127.50 | 120.28 |
| 1 | Y | 1441 | ASN | N-CA-CB | 5.38 | 118.04 | 110.12 |
| 12 | u | 702 | LEU | O-C-N | 5.38 | 127.83 | 122.12 |
| 4 | z | 699 | TYR | O-C-N | 5.38 | 129.89 | 122.46 |
| 15 | i | 618 | ASN | N-CA-C | -5.38 | 105.49 | 111.36 |
| 16 | j | 572 | ILE | CB-CA-C | 5.38 | 120.98 | 112.26 |
| 17 | k | 174 | VAL | N-CA-C | -5.38 | 100.72 | 108.42 |
| 17 | d | 60 | ASP | O-C-N | -5.38 | 117.11 | 123.41 |
| 20 | g | 148 | GLU | CA-CB-CG | 5.38 | 124.87 | 114.10 |
| 1 | 0 | 1482 | ASP | CA-CB-CG | -5.38 | 107.22 | 112.60 |
| 2 | 1 | 765 | PHE | N-CA-C | -5.38 | 105.52 | 112.68 |
| 7 | M | 42 | LEU | CA-C-N | 5.38 | 129.96 | 121.56 |
| 7 | M | 42 | LEU | C-N-CA | 5.38 | 129.96 | 121.56 |
| 7 | M | 1219 | VAL | N-CA-C | -5.38 | 97.25 | 108.88 |
| 8 | N | 1034 | ILE | CA-C-N | 5.38 | 133.07 | 122.73 |
| 8 | N | 1034 | ILE | C-N-CA | 5.38 | 133.07 | 122.73 |
| 8 | N | 1468 | VAL | O-C-N | 5.38 | 127.31 | 121.87 |
| 18 | e | 344 | VAL | CA-CB-CG1 | 5.38 | 119.55 | 110.40 |
| 20 | g | 724 | ASP | O-C-N | 5.38 | 127.61 | 122.07 |
| 8 | N | 799 | ALA | N-CA-C | 5.38 | 117.90 | 111.71 |
| 8 | N | 871 | SER | CA-C-N | 5.38 | 129.21 | 120.60 |
| 8 | N | 871 | SER | C-N-CA | 5.38 | 129.21 | 120.60 |
| 8 | N | 1465 | LEU | N-CA-C | -5.38 | 106.77 | 113.55 |
| 7 | O | 1089 | ASN | N-CA-C | -5.38 | 103.29 | 110.07 |
| 8 | P | 1525 | PHE | CA-C-N | 5.38 | 126.06 | 120.03 |
| 8 | P | 1525 | PHE | C-N-CA | 5.38 | 126.06 | 120.03 |
| 9 | R | 477 | TYR | N-CA-CB | 5.38 | 119.81 | 110.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | S | 298 | LEU | N-CA-CB | 5.38 | 119.58 | 110.49 |
| 9 | S | 657 | VAL | CA-C-N | 5.38 | 127.49 | 120.28 |
| 9 | S | 657 | VAL | C-N-CA | 5.38 | 127.49 | 120.28 |
| 11 | V | 375 | THR | CA-C-O | 5.38 | 128.21 | 120.51 |
| 12 | v | 710 | THR | CA-C-N | 5.38 | 129.71 | 120.72 |
| 12 | v | 710 | THR | C-N-CA | 5.38 | 129.71 | 120.72 |
| 14 | h | 836 | ASN | CB-CA-C | 5.38 | 121.13 | 110.42 |
| 17 | k | 217 | LEU | N-CA-CB | 5.38 | 119.58 | 110.49 |
| 19 | f | 344 | ARG | NE-CZ-NH1 | 5.38 | 126.88 | 121.50 |
| 14 | a | 266 | ASP | CA-CB-CG | 5.38 | 117.98 | 112.60 |
| 1 | 0 | 130 | GLY | CA-C-O | -5.38 | 117.39 | 122.39 |
| 1 | 0 | 1156 | LEU | N-CA-C | -5.38 | 106.49 | 112.57 |
| 7 | O | 455 | ASP | CA-C-N | 5.38 | 127.49 | 120.28 |
| 7 | O | 455 | ASP | C-N-CA | 5.38 | 127.49 | 120.28 |
| 9 | R | 685 | PRO | CA-C-O | -5.38 | 111.43 | 119.34 |
| 2 | Z | 879 | THR | CA-CB-OG1 | 5.38 | 117.67 | 109.60 |
| 2 | Z | 948 | ARG | CA-C-O | 5.38 | 125.56 | 119.27 |
| 4 | z | 715 | GLU | N-CA-C | 5.38 | 117.14 | 111.28 |
| 14 | h | 782 | TYR | CA-C-N | 5.38 | 126.09 | 120.12 |
| 14 | h | 782 | TYR | C-N-CA | 5.38 | 126.09 | 120.12 |
| 17 | d | 21 | GLY | N-CA-C | -5.38 | 106.79 | 115.08 |
| 17 | d | 194 | TYR | CA-C-N | 5.38 | 128.39 | 120.91 |
| 17 | d | 194 | TYR | C-N-CA | 5.38 | 128.39 | 120.91 |
| 14 | a | 914 | TYR | CB-CG-CD2 | -5.38 | 112.73 | 120.80 |
| 1 | 0 | 777 | ILE | N-CA-C | -5.38 | 104.37 | 111.09 |
| 5 | H | 391 | GLU | CA-C-O | 5.38 | 126.18 | 120.10 |
| 5 | K | 408 | ILE | N-CA-C | 5.38 | 115.58 | 110.42 |
| 7 | M | 310 | MET | CA-C-N | 5.38 | 127.93 | 120.29 |
| 7 | M | 310 | MET | C-N-CA | 5.38 | 127.93 | 120.29 |
| 8 | N | 903 | LEU | N-CA-C | 5.38 | 116.83 | 111.07 |
| 8 | N | 1239 | ASP | N-CA-C | -5.38 | 99.34 | 110.80 |
| 8 | P | 463 | PHE | CA-CB-CG | -5.38 | 108.42 | 113.80 |
| 8 | P | 1637 | VAL | CB-CA-C | -5.38 | 105.03 | 112.24 |
| 9 | Q | 74 | ALA | N-CA-CB | 5.38 | 118.03 | 110.12 |
| 9 | T | 781 | CYS | N-CA-C | 5.38 | 117.14 | 111.28 |
| 1 | Y | 293 | ILE | O-C-N | 5.38 | 129.29 | 122.57 |
| 1 | Y | 1158 | HIS | CE1-NE2-CD2 | -5.38 | 103.62 | 109.00 |
| 2 | Z | 754 | TYR | CA-C-N | 5.38 | 127.93 | 120.29 |
| 2 | Z | 754 | TYR | C-N-CA | 5.38 | 127.93 | 120.29 |
| 12 | u | 703 | GLN | CA-C-N | 5.38 | 127.34 | 120.56 |
| 12 | u | 703 | GLN | C-N-CA | 5.38 | 127.34 | 120.56 |
| 20 | n | 83 | ASP | CA-CB-CG | 5.38 | 117.98 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | n | 576 | ASN | CA-C-O | 5.38 | 125.53 | 119.18 |
| 20 | n | 691 | TYR | CA-C-N | 5.38 | 130.00 | 121.18 |
| 20 | n | 691 | TYR | C-N-CA | 5.38 | 130.00 | 121.18 |
| 20 | n | 975 | PHE | N-CA-C | -5.38 | 106.09 | 113.30 |
| 16 | c | 336 | ALA | N-CA-C | 5.38 | 118.06 | 111.82 |
| 19 | f | 186 | GLU | N-CA-C | -5.38 | 105.45 | 112.23 |
| 20 | g | 316 | ILE | CA-C-N | 5.38 | 127.49 | 120.28 |
| 20 | g | 316 | ILE | C-N-CA | 5.38 | 127.49 | 120.28 |
| 20 | g | 788 | TRP | CG-CD2-CE3 | 5.38 | 139.28 | 133.90 |
| 1 | 0 | 206 | ASP | N-CA-CB | 5.38 | 119.58 | 110.49 |
| 2 | 1 | 615 | ARG | NE-CZ-NH1 | 5.38 | 126.88 | 121.50 |
| 5 | E | 381 | GLU | CB-CG-CD | -5.38 | 103.46 | 112.60 |
| 8 | N | 614 | ILE | CA-C-N | 5.38 | 128.26 | 120.79 |
| 8 | N | 614 | ILE | C-N-CA | 5.38 | 128.26 | 120.79 |
| 8 | P | 560 | ASN | CB-CA-C | 5.38 | 122.87 | 116.63 |
| 9 | Q | 821 | GLN | N-CA-CB | 5.38 | 119.52 | 110.92 |
| 9 | R | 289 | LEU | CA-C-N | 5.38 | 127.75 | 120.44 |
| 9 | R | 289 | LEU | C-N-CA | 5.38 | 127.75 | 120.44 |
| 9 | R | 629 | ARG | NH1-CZ-NH2 | -5.38 | 112.31 | 119.30 |
| 13 | x | 1438 | GLU | CA-C-O | 5.38 | 126.25 | 120.55 |
| 15 | i | 169 | VAL | CA-C-O | 5.38 | 126.06 | 120.25 |
| 19 | m | 44 | SER | O-C-N | -5.38 | 116.28 | 122.09 |
| 21 | t | 72 | GLU | O-C-N | 5.38 | 129.54 | 122.93 |
| 16 | c | 500 | ASP | CA-CB-CG | -5.38 | 107.22 | 112.60 |
| 17 | d | 100 | ALA | CA-C-O | -5.38 | 114.92 | 120.89 |
| 14 | a | 331 | ILE | CB-CA-C | 5.38 | 118.15 | 110.84 |
| 2 | 1 | 905 | ARG | CB-CA-C | -5.38 | 100.69 | 110.63 |
| 7 | M | 126 | GLU | CA-CB-CG | 5.38 | 124.85 | 114.10 |
| 7 | O | 1448 | GLY | CA-C-O | -5.38 | 112.97 | 119.04 |
| 9 | Q | 638 | TYR | CA-C-O | -5.38 | 114.72 | 120.42 |
| 9 | S | 715 | MET | CA-C-N | 5.38 | 127.75 | 120.65 |
| 9 | S | 715 | MET | C-N-CA | 5.38 | 127.75 | 120.65 |
| 1 | Y | 118 | THR | CA-C-N | 5.38 | 125.67 | 119.92 |
| 1 | Y | 118 | THR | C-N-CA | 5.38 | 125.67 | 119.92 |
| 2 | Z | 1231 | GLU | CA-C-N | 5.38 | 127.48 | 120.28 |
| 2 | Z | 1231 | GLU | C-N-CA | 5.38 | 127.48 | 120.28 |
| 14 | h | 318 | ASN | O-C-N | 5.38 | 129.08 | 123.06 |
| 4 | D | 678 | GLN | CA-C-O | 5.37 | 126.46 | 120.82 |
| 6 | L | 335 | SER | CA-C-N | 5.37 | 129.81 | 120.68 |
| 6 | L | 335 | SER | C-N-CA | 5.37 | 129.81 | 120.68 |
| 7 | M | 223 | LEU | O-C-N | -5.37 | 116.93 | 123.27 |
| 7 | O | 110 | ARG | NE-CZ-NH1 | 5.37 | 126.87 | 121.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 149 | LYS | CA-C-N | 5.37 | 127.48 | 120.28 |
| 7 | O | 149 | LYS | C-N-CA | 5.37 | 127.48 | 120.28 |
| 7 | O | 875 | VAL | CA-C-O | -5.37 | 115.36 | 120.95 |
| 1 | Y | 1382 | GLU | N-CA-C | -5.37 | 106.66 | 113.43 |
| 4 | y | 700 | ILE | CA-C-N | 5.37 | 127.43 | 120.44 |
| 4 | y | 700 | ILE | C-N-CA | 5.37 | 127.43 | 120.44 |
| 16 | j | 301 | ASN | CA-C-O | 5.37 | 128.19 | 120.51 |
| 20 | n | 517 | PRO | N-CA-C | 5.37 | 117.25 | 110.70 |
| 21 | p | 21 | LYS | CA-C-O | -5.37 | 115.15 | 120.90 |
| 20 | g | 371 | SER | N-CA-CB | 5.37 | 119.11 | 111.05 |
| 2 | 1 | 922 | LYS | CA-C-N | 5.37 | 129.26 | 121.52 |
| 2 | 1 | 922 | LYS | C-N-CA | 5.37 | 129.26 | 121.52 |
| 7 | M | 335 | ASP | CA-CB-CG | 5.37 | 117.97 | 112.60 |
| 8 | P | 1033 | PHE | CA-C-N | 5.37 | 131.19 | 122.76 |
| 8 | P | 1033 | PHE | C-N-CA | 5.37 | 131.19 | 122.76 |
| 8 | P | 1594 | ASP | N-CA-C | -5.37 | 99.36 | 110.80 |
| 9 | R | 514 | LYS | N-CA-C | 5.37 | 122.24 | 110.80 |
| 9 | R | 601 | PRO | CA-C-O | -5.37 | 110.82 | 120.60 |
| 10 | U | 329 | GLN | CA-C-O | 5.37 | 125.93 | 119.59 |
| 1 | Y | 686 | THR | N-CA-C | 5.37 | 119.58 | 113.19 |
| 2 | Z | 413 | SER | O-C-N | 5.37 | 129.61 | 122.95 |
| 13 | x | 1444 | ASN | OD1-CG-ND2 | -5.37 | 117.23 | 122.60 |
| 21 | o | 19 | LYS | CA-C-N | 5.37 | 127.48 | 120.28 |
| 21 | o | 19 | LYS | C-N-CA | 5.37 | 127.48 | 120.28 |
| 14 | a | 940 | VAL | N-CA-C | -5.37 | 104.19 | 110.05 |
| 7 | M | 774 | ARG | O-C-N | 5.37 | 127.81 | 122.12 |
| 12 | u | 84 | ASN | CA-C-N | 5.37 | 131.80 | 121.54 |
| 12 | u | 84 | ASN | C-N-CA | 5.37 | 131.80 | 121.54 |
| 19 | m | 220 | ASN | CA-C-O | -5.37 | 115.56 | 120.50 |
| 20 | g | 201 | ASN | N-CA-CB | 5.37 | 119.57 | 110.49 |
| 14 | a | 484 | TYR | CA-CB-CG | -5.37 | 104.23 | 113.90 |
| 2 | 1 | 963 | THR | CB-CA-C | -5.37 | 101.88 | 110.79 |
| 5 | H | 330 | VAL | N-CA-C | -5.37 | 98.17 | 109.34 |
| 5 | H | 418 | GLN | N-CA-C | -5.37 | 105.99 | 112.54 |
| 6 | L | 396 | THR | CA-CB-OG1 | 5.37 | 117.65 | 109.60 |
| 8 | N | 1476 | VAL | CB-CA-C | -5.37 | 105.03 | 111.85 |
| 7 | O | 89 | CYS | N-CA-C | -5.37 | 105.87 | 112.90 |
| 7 | O | 1167 | LYS | N-CA-C | -5.37 | 106.86 | 113.41 |
| 9 | Q | 691 | ARG | NE-CZ-NH2 | -5.37 | 114.37 | 119.20 |
| 9 | S | 319 | SER | N-CA-C | -5.37 | 100.91 | 109.23 |
| 9 | T | 632 | ASP | CB-CA-C | -5.37 | 102.45 | 110.88 |
| 12 | u | 241 | THR | CB-CA-C | 5.37 | 118.61 | 109.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 382 | VAL | CA-CB-CG1 | -5.37 | 101.27 | 110.40 |
| 14 | h | 656 | ASP | CA-CB-CG | 5.37 | 117.97 | 112.60 |
| 16 | j | 202 | ARG | O-C-N | -5.37 | 116.05 | 122.65 |
| 20 | n | 805 | ALA | CA-C-N | 5.37 | 127.74 | 120.44 |
| 20 | n | 805 | ALA | C-N-CA | 5.37 | 127.74 | 120.44 |
| 20 | n | 1012 | GLU | N-CA-C | -5.37 | 105.95 | 112.88 |
| 16 | c | 650 | HIS | CE1-NE2-CD2 | -5.37 | 103.63 | 109.00 |
| 1 | 0 | 1442 | SER | N-CA-C | 5.37 | 117.88 | 111.71 |
| 7 | M | 513 | TRP | CE2-CD2-CE3 | -5.37 | 113.43 | 118.80 |
| 7 | O | 739 | ARG | NE-CZ-NH2 | 5.37 | 124.03 | 119.20 |
| 9 | Q | 336 | LEU | CA-C-N | 5.37 | 128.04 | 120.42 |
| 9 | Q | 336 | LEU | C-N-CA | 5.37 | 128.04 | 120.42 |
| 2 | Z | 1009 | PHE | CA-C-N | 5.37 | 131.81 | 121.18 |
| 2 | Z | 1009 | PHE | C-N-CA | 5.37 | 131.81 | 121.18 |
| 14 | h | 903 | ASN | N-CA-C | -5.37 | 106.41 | 113.17 |
| 15 | b | 315 | GLN | OE1-CD-NE2 | -5.37 | 117.23 | 122.60 |
| 15 | b | 510 | HIS | ND1-CE1-NE2 | 5.37 | 113.77 | 108.40 |
| 2 | 1 | 877 | SER | N-CA-C | -5.37 | 99.37 | 110.80 |
| 4 | G | 690 | GLN | OE1-CD-NE2 | -5.37 | 117.23 | 122.60 |
| 7 | M | 1550 | LEU | CA-C-N | 5.37 | 129.75 | 122.19 |
| 7 | M | 1550 | LEU | C-N-CA | 5.37 | 129.75 | 122.19 |
| 8 | P | 634 | ILE | N-CA-C | 5.37 | 116.74 | 110.62 |
| 8 | P | 956 | PHE | CA-CB-CG | 5.37 | 119.17 | 113.80 |
| 8 | P | 1253 | GLU | N-CA-C | 5.37 | 116.81 | 111.07 |
| 9 | R | 121 | ILE | N-CA-C | 5.37 | 115.57 | 110.42 |
| 12 | u | 176 | ASP | CA-CB-CG | 5.37 | 117.97 | 112.60 |
| 12 | v | 241 | THR | N-CA-CB | 5.37 | 119.38 | 110.63 |
| 13 | w | 1408 | ARG | CA-C-N | 5.37 | 128.46 | 120.31 |
| 13 | w | 1408 | ARG | C-N-CA | 5.37 | 128.46 | 120.31 |
| 19 | m | 535 | ARG | N-CA-C | 5.37 | 119.08 | 112.54 |
| 21 | q | 86 | PHE | CA-C-O | 5.37 | 126.88 | 120.28 |
| 16 | c | 408 | ASP | O-C-N | 5.37 | 127.60 | 122.07 |
| 16 | c | 552 | TYR | CD1-CG-CD2 | 5.37 | 126.15 | 118.10 |
| 18 | e | 335 | TYR | CA-C-O | -5.37 | 114.83 | 120.63 |
| 14 | a | 1020 | ASN | CA-C-N | 5.37 | 131.15 | 121.92 |
| 14 | a | 1020 | ASN | C-N-CA | 5.37 | 131.15 | 121.92 |
| 1 | 0 | 236 | THR | N-CA-C | -5.36 | 101.30 | 108.86 |
| 2 | 1 | 1161 | HIS | CE1-NE2-CD2 | -5.36 | 103.64 | 109.00 |
| 5 | H | 519 | GLY | N-CA-C | 5.36 | 119.63 | 112.77 |
| 7 | M | 685 | LEU | CB-CA-C | -5.36 | 102.75 | 111.06 |
| 8 | N | 1195 | GLN | N-CA-CB | 5.36 | 117.93 | 109.94 |
| 8 | P | 121 | ASP | N-CA-C | -5.36 | 106.69 | 113.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | Q | 467 | ILE | CA-CB-CG2 | -5.36 | 101.38 | 110.50 |
| 9 | S | 20 | LYS | N-CA-C | 5.36 | 117.21 | 111.36 |
| 9 | T | 86 | PHE | CA-C-N | 5.36 | 128.09 | 120.53 |
| 9 | T | 86 | PHE | C-N-CA | 5.36 | 128.09 | 120.53 |
| 9 | T | 136 | PHE | CA-C-N | 5.36 | 127.47 | 120.28 |
| 9 | T | 136 | PHE | C-N-CA | 5.36 | 127.47 | 120.28 |
| 13 | x | 1275 | ASN | CA-C-O | 5.36 | 126.14 | 119.97 |
| 14 | h | 186 | LEU | N-CA-C | -5.36 | 98.47 | 108.02 |
| 18 | l | 131 | ASP | CA-C-N | 5.36 | 131.92 | 121.41 |
| 18 | l | 131 | ASP | C-N-CA | 5.36 | 131.92 | 121.41 |
| 19 | m | 243 | TRP | CB-CA-C | 5.36 | 119.69 | 110.79 |
| 19 | m | 592 | LYS | CA-C-N | 5.36 | 130.18 | 120.79 |
| 19 | m | 592 | LYS | C-N-CA | 5.36 | 130.18 | 120.79 |
| 21 | p | 11 | VAL | CA-CB-CG1 | -5.36 | 101.28 | 110.40 |
| 15 | b | 158 | PHE | N-CA-C | 5.36 | 117.13 | 111.28 |
| 19 | f | 205 | ASN | N-CA-C | -5.36 | 99.37 | 110.80 |
| 14 | a | 680 | LEU | N-CA-CB | 5.36 | 118.00 | 110.12 |
| 2 | 1 | 815 | PHE | N-CA-C | 5.36 | 117.88 | 111.71 |
| 7 | O | 1331 | VAL | CA-C-N | 5.36 | 127.41 | 120.44 |
| 7 | O | 1331 | VAL | C-N-CA | 5.36 | 127.41 | 120.44 |
| 12 | v | 401 | ASP | O-C-N | -5.36 | 116.90 | 122.96 |
| 14 | h | 992 | ASP | CA-C-N | 5.36 | 131.62 | 121.97 |
| 14 | h | 992 | ASP | C-N-CA | 5.36 | 131.62 | 121.97 |
| 5 | K | 394 | THR | CA-CB-OG1 | 5.36 | 117.64 | 109.60 |
| 7 | M | 266 | ASP | N-CA-C | -5.36 | 107.11 | 113.38 |
| 8 | N | 1043 | LEU | CA-C-N | 5.36 | 128.21 | 120.38 |
| 8 | N | 1043 | LEU | C-N-CA | 5.36 | 128.21 | 120.38 |
| 7 | O | 972 | VAL | N-CA-C | -5.36 | 107.52 | 112.83 |
| 9 | R | 537 | ILE | N-CA-C | 5.36 | 116.13 | 110.72 |
| 9 | T | 121 | ILE | O-C-N | 5.36 | 127.07 | 121.87 |
| 9 | T | 736 | LEU | CA-C-O | -5.36 | 115.19 | 120.82 |
| 1 | Y | 577 | PHE | CA-C-N | -5.36 | 116.12 | 123.14 |
| 1 | Y | 577 | PHE | C-N-CA | -5.36 | 116.12 | 123.14 |
| 1 | Y | 1103 | LEU | N-CA-C | -5.36 | 105.00 | 112.45 |
| 1 | Y | 1261 | ARG | CA-C-N | 5.36 | 127.90 | 121.84 |
| 1 | Y | 1261 | ARG | C-N-CA | 5.36 | 127.90 | 121.84 |
| 2 | Z | 165 | ILE | O-C-N | 5.36 | 128.76 | 122.81 |
| 2 | Z | 212 | ASN | CA-CB-CG | 5.36 | 117.96 | 112.60 |
| 2 | Z | 947 | LEU | N-CA-C | 5.36 | 117.12 | 111.28 |
| 12 | u | 563 | GLN | CA-C-N | 5.36 | 127.41 | 120.44 |
| 12 | u | 563 | GLN | C-N-CA | 5.36 | 127.41 | 120.44 |
| 4 | z | 716 | THR | N-CA-CB | 5.36 | 118.09 | 110.16 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | i | 183 | ASN | CA-CB-CG | -5.36 | 107.24 | 112.60 |
| 19 | m | 724 | LEU | N-CA-C | -5.36 | 105.57 | 113.61 |
| 20 | g | 1064 | ARG | NH1-CZ-NH2 | -5.36 | 112.33 | 119.30 |
| 6 | L | 455 | GLU | CA-C-N | 5.36 | 127.46 | 120.28 |
| 6 | L | 455 | GLU | C-N-CA | 5.36 | 127.46 | 120.28 |
| 7 | M | 194 | SER | CA-C-N | 5.36 | 127.46 | 120.28 |
| 7 | M | 194 | SER | C-N-CA | 5.36 | 127.46 | 120.28 |
| 9 | T | 304 | LYS | CA-C-N | 5.36 | 130.02 | 121.34 |
| 9 | T | 304 | LYS | C-N-CA | 5.36 | 130.02 | 121.34 |
| 2 | Z | 576 | SER | CA-C-N | 5.36 | 131.78 | 121.54 |
| 2 | Z | 576 | SER | C-N-CA | 5.36 | 131.78 | 121.54 |
| 12 | v | 366 | LEU | CA-C-N | 5.36 | 126.54 | 119.84 |
| 12 | v | 366 | LEU | C-N-CA | 5.36 | 126.54 | 119.84 |
| 14 | h | 626 | HIS | ND1-CE1-NE2 | 5.36 | 113.76 | 108.40 |
| 19 | f | 178 | HIS | CB-CA-C | -5.36 | 102.02 | 110.86 |
| 20 | g | 141 | THR | CB-CA-C | 5.36 | 118.37 | 109.53 |
| 5 | H | 324 | TYR | CA-C-N | 5.36 | 127.90 | 120.29 |
| 5 | H | 324 | TYR | C-N-CA | 5.36 | 127.90 | 120.29 |
| 7 | M | 677 | SER | CA-C-N | 5.36 | 127.41 | 120.44 |
| 7 | M | 677 | SER | C-N-CA | 5.36 | 127.41 | 120.44 |
| 7 | O | 143 | ASN | N-CA-CB | 5.36 | 118.24 | 110.47 |
| 7 | O | 238 | PHE | N-CA-C | 5.36 | 117.87 | 111.71 |
| 8 | P | 1000 | LYS | CA-C-O | 5.36 | 125.87 | 119.60 |
| 9 | T | 103 | ILE | N-CA-CB | -5.36 | 102.39 | 111.23 |
| 1 | Y | 831 | LYS | CA-CB-CG | -5.36 | 103.39 | 114.10 |
| 12 | v | 551 | ASN | O-C-N | 5.36 | 127.59 | 122.07 |
| 15 | i | 608 | PRO | CB-CA-C | 5.36 | 119.13 | 111.04 |
| 18 | l | 156 | VAL | CA-CB-CG1 | 5.36 | 119.51 | 110.40 |
| 19 | m | 535 | ARG | NE-CZ-NH2 | -5.36 | 114.38 | 119.20 |
| 20 | n | 373 | ASN | CA-CB-CG | -5.36 | 107.24 | 112.60 |
| 14 | a | 89 | HIS | CA-C-O | -5.36 | 113.16 | 119.48 |
| 1 | 0 | 675 | ALA | CA-C-N | 5.36 | 130.59 | 122.56 |
| 1 | 0 | 675 | ALA | C-N-CA | 5.36 | 130.59 | 122.56 |
| 1 | 0 | 1281 | THR | N-CA-CB | 5.36 | 118.19 | 110.37 |
| 5 | H | 314 | ASN | CA-CB-CG | 5.36 | 117.95 | 112.60 |
| 6 | I | 393 | ASP | N-CA-CB | 5.36 | 117.78 | 110.01 |
| 8 | N | 218 | ASN | CA-CB-CG | 5.36 | 117.96 | 112.60 |
| 8 | N | 765 | PHE | N-CA-C | -5.36 | 106.12 | 113.30 |
| 8 | N | 1095 | GLU | CA-C-O | 5.36 | 128.17 | 120.51 |
| 7 | O | 429 | GLU | N-CA-C | 5.36 | 116.80 | 111.07 |
| 7 | O | 1090 | PRO | CA-C-N | 5.36 | 127.77 | 120.54 |
| 7 | O | 1090 | PRO | C-N-CA | 5.36 | 127.77 | 120.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1190 | ALA | CA-C-N | 5.36 | 127.45 | 120.28 |
| 8 | P | 1190 | ALA | C-N-CA | 5.36 | 127.45 | 120.28 |
| 8 | P | 1337 | LEU | N-CA-C | -5.36 | 105.39 | 112.94 |
| 2 | Z | 1100 | PHE | N-CA-C | 5.36 | 117.12 | 111.28 |
| 12 | u | 698 | ASN | CA-C-O | -5.36 | 115.20 | 120.82 |
| 16 | j | 197 | VAL | CA-C-N | -5.36 | 115.41 | 122.85 |
| 16 | j | 197 | VAL | C-N-CA | -5.36 | 115.41 | 122.85 |
| 20 | g | 694 | LEU | CA-C-O | -5.36 | 113.16 | 119.48 |
| 7 | M | 553 | ILE | N-CA-C | -5.35 | 100.76 | 108.42 |
| 7 | M | 1312 | ILE | N-CA-C | 5.35 | 115.80 | 110.23 |
| 8 | N | 1199 | TYR | N-CA-C | -5.35 | 105.89 | 112.90 |
| 7 | O | 616 | VAL | CA-C-O | 5.35 | 126.06 | 119.58 |
| 7 | O | 879 | GLN | N-CA-C | -5.35 | 107.40 | 114.31 |
| 1 | Y | 1005 | ARG | N-CA-C | 5.35 | 119.07 | 112.54 |
| 13 | w | 1361 | GLU | CA-C-N | 5.35 | 127.89 | 120.29 |
| 13 | w | 1361 | GLU | C-N-CA | 5.35 | 127.89 | 120.29 |
| 14 | h | 647 | PHE | CA-CB-CG | -5.35 | 108.45 | 113.80 |
| 17 | d | 201 | GLU | N-CA-C | -5.35 | 100.68 | 108.07 |
| 14 | a | 352 | ILE | CA-C-O | -5.35 | 117.97 | 122.63 |
| 1 | 0 | 459 | ALA | CA-C-N | 5.35 | 129.53 | 122.30 |
| 1 | 0 | 459 | ALA | C-N-CA | 5.35 | 129.53 | 122.30 |
| 2 | 1 | 1160 | ILE | CA-C-N | 5.35 | 127.89 | 120.29 |
| 2 | 1 | 1160 | ILE | C-N-CA | 5.35 | 127.89 | 120.29 |
| 5 | B | 387 | GLN | OE1-CD-NE2 | -5.35 | 117.25 | 122.60 |
| 5 | E | 410 | LYS | N-CA-C | 5.35 | 116.80 | 111.07 |
| 7 | M | 120 | ILE | CA-CB-CG1 | 5.35 | 119.50 | 110.40 |
| 8 | N | 204 | VAL | O-C-N | 5.35 | 126.23 | 121.41 |
| 8 | N | 720 | ARG | N-CA-C | 5.35 | 117.86 | 111.71 |
| 8 | N | 1452 | SER | CB-CA-C | 5.35 | 119.20 | 110.96 |
| 8 | N | 1593 | HIS | CE1-NE2-CD2 | -5.35 | 103.65 | 109.00 |
| 7 | O | 328 | ASP | CA-C-N | 5.35 | 129.16 | 120.60 |
| 7 | O | 328 | ASP | C-N-CA | 5.35 | 129.16 | 120.60 |
| 8 | P | 293 | GLU | O-C-N | -5.35 | 115.52 | 122.37 |
| 8 | P | 1384 | ASP | CA-CB-CG | -5.35 | 107.25 | 112.60 |
| 9 | Q | 268 | ILE | CA-C-N | 5.35 | 131.76 | 121.54 |
| 9 | Q | 268 | ILE | C-N-CA | 5.35 | 131.76 | 121.54 |
| 9 | T | 331 | VAL | CA-C-O | -5.35 | 112.78 | 119.95 |
| 2 | Z | 1271 | ARG | CA-C-O | 5.35 | 126.09 | 120.42 |
| 14 | h | 365 | ILE | CA-C-O | -5.35 | 115.06 | 120.31 |
| 14 | h | 381 | SER | CA-C-O | -5.35 | 114.85 | 121.06 |
| 14 | h | 487 | ASN | OD1-CG-ND2 | -5.35 | 117.25 | 122.60 |
| 15 | i | 285 | VAL | CA-C-O | -5.35 | 113.42 | 119.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | n | 312 | ILE | CA-CB-CG2 | -5.35 | 101.40 | 110.50 |
| 20 | n | 1025 | ASP | N-CA-C | -5.35 | 105.39 | 112.94 |
| 15 | b | 507 | LEU | CA-C-O | 5.35 | 126.18 | 120.24 |
| 19 | f | 186 | GLU | N-CA-CB | 5.35 | 118.54 | 110.30 |
| 1 | 0 | 1333 | HIS | CA-CB-CG | -5.35 | 108.45 | 113.80 |
| 7 | M | 256 | HIS | CA-CB-CG | 5.35 | 119.15 | 113.80 |
| 7 | M | 727 | GLU | CA-C-O | 5.35 | 128.16 | 120.51 |
| 7 | M | 918 | PHE | N-CA-C | -5.35 | 98.66 | 108.02 |
| 8 | N | 1465 | LEU | N-CA-CB | 5.35 | 118.16 | 110.40 |
| 9 | S | 494 | TYR | CA-C-N | 5.35 | 128.44 | 120.31 |
| 9 | S | 494 | TYR | C-N-CA | 5.35 | 128.44 | 120.31 |
| 2 | Z | 149 | GLU | N-CA-C | -5.35 | 106.34 | 112.92 |
| 14 | h | 352 | ILE | N-CA-C | 5.35 | 111.94 | 106.21 |
| 15 | i | 85 | LYS | O-C-N | 5.35 | 129.74 | 122.57 |
| 19 | f | 694 | VAL | CA-C-N | 5.35 | 129.72 | 121.53 |
| 19 | f | 694 | VAL | C-N-CA | 5.35 | 129.72 | 121.53 |
| 14 | a | 883 | GLU | N-CA-CB | 5.35 | 120.60 | 111.66 |
| 1 | 0 | 276 | HIS | CA-C-O | 5.35 | 126.38 | 120.71 |
| 1 | 0 | 1060 | TYR | CA-C-O | 5.35 | 124.51 | 119.59 |
| 1 | 0 | 1153 | ASN | CA-C-N | 5.35 | 131.76 | 121.54 |
| 1 | 0 | 1153 | ASN | C-N-CA | 5.35 | 131.76 | 121.54 |
| 8 | N | 964 | GLN | CA-C-N | 5.35 | 131.76 | 121.54 |
| 8 | N | 964 | GLN | C-N-CA | 5.35 | 131.76 | 121.54 |
| 7 | O | 642 | PHE | CA-C-O | -5.35 | 114.88 | 120.55 |
| 8 | P | 899 | GLN | CG-CD-NE2 | -5.35 | 108.38 | 116.40 |
| 9 | Q | 359 | ASN | OD1-CG-ND2 | 5.35 | 127.95 | 122.60 |
| 9 | S | 93 | ASN | CA-C-N | 5.35 | 127.39 | 120.44 |
| 9 | S | 93 | ASN | C-N-CA | 5.35 | 127.39 | 120.44 |
| 9 | S | 422 | ARG | NE-CZ-NH2 | -5.35 | 114.39 | 119.20 |
| 1 | Y | 1413 | VAL | CA-C-N | 5.35 | 127.45 | 120.28 |
| 1 | Y | 1413 | VAL | C-N-CA | 5.35 | 127.45 | 120.28 |
| 12 | u | 257 | SER | N-CA-CB | 5.35 | 117.98 | 110.12 |
| 14 | h | 362 | LYS | CA-C-O | 5.35 | 127.43 | 120.21 |
| 15 | i | 255 | ARG | O-C-N | 5.35 | 128.25 | 122.15 |
| 20 | g | 129 | ASN | O-C-N | -5.35 | 116.32 | 122.20 |
| 2 | 1 | 951 | VAL | N-CA-C | -5.35 | 105.32 | 110.72 |
| 6 | C | 279 | GLN | N-CA-CB | 5.35 | 117.77 | 110.01 |
| 8 | N | 179 | LEU | O-C-N | -5.35 | 116.56 | 122.07 |
| 7 | O | 1577 | LYS | CA-C-N | 5.35 | 128.01 | 120.42 |
| 7 | O | 1577 | LYS | C-N-CA | 5.35 | 128.01 | 120.42 |
| 8 | P | 680 | ASP | CA-C-N | 5.35 | 127.71 | 120.44 |
| 8 | P | 680 | ASP | C-N-CA | 5.35 | 127.71 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 1487 | TYR | CA-C-N | 5.35 | 127.78 | 120.46 |
| 1 | Y | 1487 | TYR | C-N-CA | 5.35 | 127.78 | 120.46 |
| 2 | Z | 1004 | VAL | CB-CA-C | -5.35 | 105.01 | 112.02 |
| 14 | h | 971 | ASN | CA-CB-CG | -5.35 | 107.25 | 112.60 |
| 17 | k | 154 | ALA | CA-C-O | -5.35 | 112.80 | 119.54 |
| 15 | b | 171 | ARG | N-CA-CB | -5.35 | 102.25 | 110.16 |
| 20 | g | 281 | ARG | NE-CZ-NH2 | 5.35 | 124.01 | 119.20 |
| 1 | 0 | 238 | MET | CG-SD-CE | -5.35 | 89.14 | 100.90 |
| 7 | M | 1212 | THR | N-CA-C | -5.35 | 106.77 | 113.72 |
| 8 | N | 519 | SER | CA-C-N | 5.35 | 130.00 | 120.70 |
| 8 | N | 519 | SER | C-N-CA | 5.35 | 130.00 | 120.70 |
| 8 | N | 1183 | PHE | CA-C-O | -5.35 | 113.48 | 119.79 |
| 7 | O | 1629 | LEU | N-CA-C | -5.35 | 107.06 | 113.21 |
| 9 | Q | 248 | THR | N-CA-CB | 5.35 | 118.57 | 110.28 |
| 1 | Y | 1075 | ASP | CA-CB-CG | -5.35 | 107.25 | 112.60 |
| 1 | Y | 1107 | LEU | CA-C-N | -5.35 | 112.35 | 121.97 |
| 1 | Y | 1107 | LEU | C-N-CA | -5.35 | 112.35 | 121.97 |
| 2 | Z | 828 | THR | CB-CA-C | 5.35 | 117.69 | 109.03 |
| 14 | h | 1034 | LEU | O-C-N | 5.35 | 129.65 | 122.49 |
| 15 | i | 544 | ASN | CA-C-N | 5.35 | 130.94 | 122.60 |
| 15 | i | 544 | ASN | C-N-CA | 5.35 | 130.94 | 122.60 |
| 2 | 1 | 1202 | LEU | CB-CA-C | -5.34 | 101.53 | 110.56 |
| 4 | A | 775 | THR | O-C-N | -5.34 | 114.90 | 122.06 |
| 6 | C | 276 | GLU | CA-C-N | 5.34 | 127.78 | 120.46 |
| 6 | C | 276 | GLU | C-N-CA | 5.34 | 127.78 | 120.46 |
| 6 | I | 456 | ARG | NE-CZ-NH1 | -5.34 | 116.16 | 121.50 |
| 7 | M | 639 | LEU | CA-C-N | 5.34 | 127.39 | 120.44 |
| 7 | M | 639 | LEU | C-N-CA | 5.34 | 127.39 | 120.44 |
| 7 | M | 720 | HIS | CE1-NE2-CD2 | -5.34 | 103.66 | 109.00 |
| 8 | N | 390 | ILE | CA-C-O | -5.34 | 115.09 | 119.47 |
| 9 | Q | 500 | GLU | N-CA-C | -5.34 | 106.81 | 113.38 |
| 9 | Q | 702 | ILE | CA-C-O | 5.34 | 127.46 | 120.78 |
| 9 | Q | 754 | ARG | CA-CB-CG | 5.34 | 124.79 | 114.10 |
| 1 | Y | 183 | TRP | CA-CB-CG | 5.34 | 123.75 | 113.60 |
| 12 | u | 629 | LYS | N-CA-C | -5.34 | 105.45 | 111.28 |
| 21 | q | 81 | ILE | N-CA-CB | 5.34 | 118.63 | 111.90 |
| 16 | c | 765 | GLU | N-CA-CB | 5.34 | 119.52 | 110.49 |
| 20 | g | 683 | GLU | N-CA-CB | -5.34 | 101.38 | 111.43 |
| 8 | P | 463 | PHE | CA-C-N | 5.34 | 131.74 | 121.54 |
| 8 | P | 463 | PHE | C-N-CA | 5.34 | 131.74 | 121.54 |
| 15 | b | 653 | ILE | N-CA-CB | 5.34 | 119.22 | 112.22 |
| 2 | 1 | 284 | TRP | N-CA-CB | 5.34 | 119.16 | 110.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | A | 745 | TYR | CA-C-N | 5.34 | 127.75 | 120.54 |
| 4 | A | 745 | TYR | C-N-CA | 5.34 | 127.75 | 120.54 |
| 5 | B | 358 | LEU | N-CA-CB | 5.34 | 117.97 | 110.12 |
| 5 | H | 299 | TRP | CD2-CE2-CZ2 | -5.34 | 117.06 | 122.40 |
| 7 | M | 527 | TYR | CA-C-N | 5.34 | 127.70 | 120.65 |
| 7 | M | 527 | TYR | C-N-CA | 5.34 | 127.70 | 120.65 |
| 8 | P | 1209 | ALA | N-CA-CB | 5.34 | 117.75 | 110.01 |
| 9 | S | 680 | ASN | N-CA-C | -5.34 | 102.97 | 110.50 |
| 11 | V | 280 | ILE | N-CA-CB | 5.34 | 118.58 | 111.64 |
| 19 | m | 474 | ASN | CB-CG-OD1 | 5.34 | 131.48 | 120.80 |
| 20 | g | 602 | SER | N-CA-C | -5.34 | 106.72 | 113.18 |
| 2 | 1 | 1208 | ASP | O-C-N | 5.34 | 128.70 | 122.24 |
| 6 | I | 329 | ASP | CA-CB-CG | 5.34 | 117.94 | 112.60 |
| 8 | N | 401 | ALA | CA-C-N | 5.34 | 128.43 | 120.31 |
| 8 | N | 401 | ALA | C-N-CA | 5.34 | 128.43 | 120.31 |
| 7 | O | 1451 | THR | CA-C-O | -5.34 | 113.83 | 119.97 |
| 9 | T | 19 | ASN | N-CA-C | 5.34 | 118.01 | 111.82 |
| 9 | T | 49 | LEU | CA-C-O | 5.34 | 128.15 | 120.51 |
| 1 | Y | 1282 | ASP | N-CA-CB | 5.34 | 119.51 | 110.49 |
| 2 | Z | 260 | VAL | N-CA-CB | 5.34 | 116.75 | 110.82 |
| 14 | h | 334 | LEU | N-CA-CB | 5.34 | 119.51 | 110.49 |
| 14 | h | 957 | ASP | N-CA-C | -5.34 | 101.17 | 108.38 |
| 19 | f | 217 | GLU | CA-C-O | -5.34 | 114.79 | 121.46 |
| 20 | g | 622 | ASN | OD1-CG-ND2 | 5.34 | 127.94 | 122.60 |
| 20 | g | 1025 | ASP | CB-CA-C | -5.34 | 102.37 | 111.02 |
| 14 | a | 844 | CYS | N-CA-C | -5.34 | 106.44 | 113.17 |
| 4 | A | 713 | ASN | OD1-CG-ND2 | 5.34 | 127.94 | 122.60 |
| 7 | O | 824 | ALA | CA-C-N | 5.34 | 124.60 | 120.33 |
| 7 | O | 824 | ALA | C-N-CA | 5.34 | 124.60 | 120.33 |
| 9 | Q | 138 | ASN | N-CA-C | 5.34 | 117.10 | 111.28 |
| 1 | Y | 693 | GLU | N-CA-CB | 5.34 | 119.51 | 110.49 |
| 14 | h | 389 | LEU | N-CA-C | -5.34 | 105.60 | 113.61 |
| 21 | p | 25 | LEU | CA-C-O | -5.34 | 114.89 | 120.55 |
| 21 | r | 50 | ASP | N-CA-CB | 5.34 | 117.97 | 110.12 |
| 17 | d | 15 | ALA | O-C-N | -5.34 | 118.18 | 123.62 |
| 4 | G | 648 | LEU | CA-C-O | 5.34 | 126.42 | 120.82 |
| 7 | M | 1594 | GLY | CA-C-N | 5.34 | 131.58 | 121.97 |
| 7 | M | 1594 | GLY | C-N-CA | 5.34 | 131.58 | 121.97 |
| 7 | O | 1467 | ALA | CA-C-N | 5.34 | 128.42 | 120.31 |
| 7 | O | 1467 | ALA | C-N-CA | 5.34 | 128.42 | 120.31 |
| 9 | S | 257 | TRP | N-CA-C | 5.34 | 118.01 | 111.82 |
| 2 | Z | 417 | ASN | CB-CA-C | -5.34 | 99.14 | 109.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | m | 643 | PHE | CA-C-O | 5.34 | 127.14 | 121.16 |
| 20 | n | 536 | GLU | O-C-N | 5.34 | 128.66 | 122.09 |
| 20 | n | 610 | LEU | CA-C-O | -5.34 | 113.18 | 119.48 |
| 15 | b | 482 | TRP | CA-C-N | 5.34 | 126.51 | 119.84 |
| 15 | b | 482 | TRP | C-N-CA | 5.34 | 126.51 | 119.84 |
| 16 | c | 294 | ILE | CA-C-N | 5.34 | 127.38 | 120.44 |
| 16 | c | 294 | ILE | C-N-CA | 5.34 | 127.38 | 120.44 |
| 1 | 0 | 260 | HIS | N-CA-CB | 5.33 | 119.50 | 110.49 |
| 2 | 1 | 1316 | VAL | CA-C-N | 5.33 | 131.73 | 121.54 |
| 2 | 1 | 1316 | VAL | C-N-CA | 5.33 | 131.73 | 121.54 |
| 2 | 1 | 1386 | ARG | N-CA-C | -5.33 | 100.63 | 108.79 |
| 7 | M | 423 | LEU | CA-C-N | 5.33 | 127.43 | 120.28 |
| 7 | M | 423 | LEU | C-N-CA | 5.33 | 127.43 | 120.28 |
| 8 | P | 610 | LYS | N-CA-C | -5.33 | 105.04 | 112.03 |
| 9 | Q | 256 | SER | N-CA-C | -5.33 | 105.91 | 112.90 |
| 9 | Q | 410 | ALA | CA-C-N | 5.33 | 127.77 | 120.46 |
| 9 | Q | 410 | ALA | C-N-CA | 5.33 | 127.77 | 120.46 |
| 1 | Y | 1327 | ILE | CB-CA-C | 5.33 | 118.66 | 111.94 |
| 4 | z | 657 | GLN | N-CA-C | 5.33 | 116.78 | 111.07 |
| 16 | c | 353 | ASN | CA-C-N | 5.33 | 129.47 | 120.29 |
| 16 | c | 353 | ASN | C-N-CA | 5.33 | 129.47 | 120.29 |
| 20 | g | 92 | MET | N-CA-C | -5.33 | 106.82 | 113.38 |
| 20 | g | 408 | ASN | N-CA-CB | 5.33 | 117.85 | 110.17 |
| 14 | a | 238 | THR | N-CA-C | -5.33 | 102.27 | 109.95 |
| 14 | a | 530 | LYS | CG-CD-CE | 5.33 | 123.57 | 111.30 |
| 2 | 1 | 1108 | PHE | N-CA-C | -5.33 | 106.15 | 113.30 |
| 7 | M | 101 | ASN | OD1-CG-ND2 | 5.33 | 127.93 | 122.60 |
| 7 | M | 274 | LYS | CA-C-N | 5.33 | 127.28 | 120.56 |
| 7 | M | 274 | LYS | C-N-CA | 5.33 | 127.28 | 120.56 |
| 8 | N | 326 | SER | N-CA-CB | -5.33 | 102.25 | 110.46 |
| 8 | N | 408 | PRO | N-CA-C | -5.33 | 106.77 | 114.18 |
| 8 | N | 747 | ILE | O-C-N | 5.33 | 127.04 | 121.87 |
| 8 | N | 1474 | LEU | O-C-N | -5.33 | 116.95 | 123.30 |
| 9 | S | 289 | LEU | CA-C-O | 5.33 | 124.77 | 118.90 |
| 9 | T | 354 | VAL | N-CA-C | -5.33 | 107.62 | 113.43 |
| 2 | Z | 795 | MET | N-CA-C | -5.33 | 104.36 | 111.24 |
| 12 | u | 85 | ASP | CB-CA-C | -5.33 | 99.81 | 110.42 |
| 4 | z | 709 | ASN | N-CA-C | 5.33 | 117.09 | 111.28 |
| 14 | h | 802 | TYR | CA-C-O | -5.33 | 114.57 | 120.33 |
| 20 | n | 1150 | TYR | CB-CA-C | 5.33 | 118.39 | 109.80 |
| 21 | t | 56 | THR | CA-C-O | -5.33 | 112.88 | 120.51 |
| 17 | d | 282 | LYS | CA-CB-CG | 5.33 | 124.77 | 114.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | a | 1030 | LEU | N-CA-CB | 5.33 | 119.78 | 110.98 |
| 1 | 0 | 1147 | GLU | N-CA-CB | 5.33 | 118.43 | 110.22 |
| 5 | B | 356 | GLU | N-CA-C | -5.33 | 107.43 | 114.04 |
| 4 | J | 756 | ASN | N-CA-CB | 5.33 | 117.74 | 110.01 |
| 8 | N | 1058 | GLU | CA-C-N | 5.33 | 131.19 | 121.97 |
| 8 | N | 1058 | GLU | C-N-CA | 5.33 | 131.19 | 121.97 |
| 7 | O | 692 | TYR | N-CA-CB | 5.33 | 117.67 | 110.10 |
| 7 | O | 993 | ALA | N-CA-CB | 5.33 | 119.50 | 110.49 |
| 9 | S | 74 | ALA | CA-C-O | -5.33 | 114.90 | 120.55 |
| 9 | T | 310 | ASP | CA-CB-CG | -5.33 | 107.27 | 112.60 |
| 11 | X | 292 | GLY | N-CA-C | -5.33 | 100.54 | 113.18 |
| 1 | Y | 392 | SER | CA-C-O | -5.33 | 115.65 | 121.89 |
| 15 | i | 602 | GLU | CA-C-O | 5.33 | 124.82 | 118.69 |
| 18 | l | 176 | SER | CA-C-O | 5.33 | 127.02 | 121.15 |
| 19 | m | 243 | TRP | CA-CB-CG | 5.33 | 123.73 | 113.60 |
| 19 | m | 343 | ILE | N-CA-C | -5.33 | 104.83 | 112.35 |
| 16 | c | 393 | GLN | N-CA-CB | 5.33 | 119.10 | 110.41 |
| 20 | g | 856 | LYS | N-CA-CB | 5.33 | 119.50 | 110.49 |
| 14 | a | 114 | GLU | O-C-N | 5.33 | 129.68 | 122.59 |
| 2 | 1 | 541 | SER | N-CA-C | -5.33 | 99.45 | 110.80 |
| 14 | a | 407 | GLY | N-CA-C | -5.33 | 105.86 | 113.86 |
| 2 | 1 | 171 | TYR | O-C-N | -5.33 | 115.63 | 122.72 |
| 2 | 1 | 909 | HIS | N-CA-C | 5.33 | 119.50 | 112.89 |
| 7 | M | 930 | VAL | N-CA-C | -5.33 | 105.09 | 112.50 |
| 8 | N | 1008 | THR | O-C-N | -5.33 | 115.19 | 121.32 |
| 8 | P | 1290 | SER | CA-C-N | 5.33 | 125.03 | 119.92 |
| 8 | P | 1290 | SER | C-N-CA | 5.33 | 125.03 | 119.92 |
| 9 | S | 700 | ALA | CA-C-O | 5.33 | 126.10 | 119.97 |
| 12 | u | 275 | GLU | N-CA-CB | 5.33 | 119.50 | 110.49 |
| 14 | h | 364 | GLN | CA-C-N | -5.33 | 115.76 | 123.11 |
| 14 | h | 364 | GLN | C-N-CA | -5.33 | 115.76 | 123.11 |
| 15 | i | 274 | LEU | N-CA-CB | 5.33 | 118.74 | 110.80 |
| 15 | i | 571 | TYR | CB-CA-C | -5.33 | 100.82 | 109.13 |
| 2 | 1 | 121 | LEU | N-CA-CB | 5.33 | 117.98 | 110.36 |
| 8 | N | 686 | GLY | N-CA-C | -5.33 | 100.55 | 113.18 |
| 8 | P | 1501 | SER | CB-CA-C | -5.33 | 101.95 | 110.79 |
| 1 | Y | 1420 | GLY | N-CA-C | -5.33 | 107.68 | 115.72 |
| 2 | Z | 599 | LEU | N-CA-C | 5.33 | 122.15 | 110.80 |
| 2 | Z | 1318 | HIS | CA-C-O | 5.33 | 126.41 | 120.82 |
| 15 | i | 661 | HIS | CE1-NE2-CD2 | -5.33 | 103.67 | 109.00 |
| 21 | t | 27 | ILE | N-CA-C | 5.33 | 116.05 | 110.62 |
| 14 | a | 980 | VAL | N-CA-C | -5.33 | 107.62 | 113.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 442 | GLY | CA-C-O | -5.33 | 115.26 | 120.75 |
| 6 | C | 327 | LYS | CA-C-O | -5.33 | 114.91 | 120.55 |
| 5 | H | 423 | LYS | CA-C-O | -5.33 | 111.75 | 120.80 |
| 7 | M | 1168 | ILE | CA-C-N | 5.33 | 127.95 | 120.28 |
| 7 | M | 1168 | ILE | C-N-CA | 5.33 | 127.95 | 120.28 |
| 8 | N | 1190 | ALA | N-CA-CB | 5.33 | 118.05 | 110.06 |
| 7 | O | 1002 | LEU | CB-CA-C | 5.33 | 119.14 | 110.24 |
| 9 | Q | 789 | LEU | CA-C-N | 5.33 | 131.96 | 122.06 |
| 9 | Q | 789 | LEU | C-N-CA | 5.33 | 131.96 | 122.06 |
| 9 | R | 457 | TYR | CA-C-N | 5.33 | 131.44 | 122.87 |
| 9 | R | 457 | TYR | C-N-CA | 5.33 | 131.44 | 122.87 |
| 14 | h | 949 | LEU | CA-C-N | 5.33 | 127.68 | 120.44 |
| 14 | h | 949 | LEU | C-N-CA | 5.33 | 127.68 | 120.44 |
| 15 | i | 339 | ILE | CA-C-N | 5.33 | 126.98 | 120.22 |
| 15 | i | 339 | ILE | C-N-CA | 5.33 | 126.98 | 120.22 |
| 16 | j | 412 | LEU | O-C-N | -5.33 | 115.67 | 121.53 |
| 20 | n | 910 | ASP | N-CA-C | -5.33 | 104.36 | 111.87 |
| 15 | b | 531 | LEU | CA-C-N | -5.33 | 114.45 | 120.89 |
| 15 | b | 531 | LEU | C-N-CA | -5.33 | 114.45 | 120.89 |
| 17 | d | 12 | ILE | CA-C-O | -5.33 | 114.78 | 120.85 |
| 20 | g | 103 | LYS | O-C-N | 5.33 | 128.64 | 122.25 |
| 20 | g | 588 | ILE | CA-C-O | 5.33 | 126.45 | 119.85 |
| 1 | 0 | 1333 | HIS | N-CA-C | -5.32 | 105.44 | 112.94 |
| 2 | 1 | 633 | HIS | ND1-CE1-NE2 | 5.32 | 113.72 | 108.40 |
| 5 | K | 525 | GLU | N-CA-CB | 5.32 | 118.53 | 110.28 |
| 9 | S | 505 | HIS | CA-C-N | 5.32 | 127.36 | 120.44 |
| 9 | S | 505 | HIS | C-N-CA | 5.32 | 127.36 | 120.44 |
| 9 | T | 596 | ASP | O-C-N | 5.32 | 129.67 | 122.59 |
| 1 | Y | 169 | THR | N-CA-CB | 5.32 | 119.15 | 110.37 |
| 4 | y | 676 | ILE | N-CA-C | 5.32 | 115.53 | 110.42 |
| 14 | h | 209 | THR | CA-C-O | 5.32 | 128.05 | 121.87 |
| 18 | l | 9 | ASP | CA-CB-CG | -5.32 | 107.28 | 112.60 |
| 18 | l | 54 | HIS | CA-C-O | -5.32 | 115.58 | 121.33 |
| 21 | t | 43 | GLY | O-C-N | -5.32 | 117.08 | 122.19 |
| 16 | c | 558 | ASN | CB-CA-C | 5.32 | 120.02 | 110.81 |
| 17 | d | 284 | ASN | CA-CB-CG | 5.32 | 117.92 | 112.60 |
| 9 | T | 101 | PRO | CB-CA-C | 5.32 | 115.96 | 110.00 |
| 12 | u | 380 | ILE | CB-CA-C | -5.32 | 104.34 | 110.41 |
| 12 | v | 327 | LEU | CA-C-N | 5.32 | 131.52 | 122.37 |
| 12 | v | 327 | LEU | C-N-CA | 5.32 | 131.52 | 122.37 |
| 12 | v | 408 | LEU | N-CA-C | -5.32 | 100.73 | 109.40 |
| 17 | d | 83 | LYS | CA-C-O | -5.32 | 114.15 | 120.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 1387 | ILE | CA-CB-CG1 | 5.32 | 119.45 | 110.40 |
| 7 | M | 288 | TRP | N-CA-C | 5.32 | 119.03 | 112.54 |
| 7 | O | 697 | THR | O-C-N | 5.32 | 127.76 | 122.12 |
| 8 | P | 1034 | ILE | N-CA-C | -5.32 | 107.11 | 112.17 |
| 9 | R | 226 | ARG | CA-C-N | 5.32 | 127.36 | 120.44 |
| 9 | R | 226 | ARG | C-N-CA | 5.32 | 127.36 | 120.44 |
| 9 | T | 809 | VAL | CA-CB-CG1 | 5.32 | 119.45 | 110.40 |
| 18 | l | 310 | VAL | N-CA-CB | 5.32 | 118.06 | 111.41 |
| 19 | m | 461 | GLN | N-CA-CB | 5.32 | 117.94 | 110.12 |
| 15 | b | 383 | VAL | N-CA-CB | 5.32 | 120.01 | 111.23 |
| 19 | f | 593 | GLY | CA-C-N | 5.32 | 127.97 | 120.42 |
| 19 | f | 593 | GLY | C-N-CA | 5.32 | 127.97 | 120.42 |
| 19 | f | 637 | ASP | N-CA-CB | 5.32 | 117.86 | 109.83 |
| 1 | 0 | 1357 | LYS | CA-C-O | -5.32 | 115.63 | 120.95 |
| 7 | M | 146 | SER | CA-C-N | 5.32 | 127.41 | 120.28 |
| 7 | M | 146 | SER | C-N-CA | 5.32 | 127.41 | 120.28 |
| 7 | M | 315 | GLU | N-CA-C | -5.32 | 106.81 | 113.72 |
| 8 | N | 745 | HIS | CE1-NE2-CD2 | -5.32 | 103.68 | 109.00 |
| 7 | O | 1312 | ILE | CA-C-O | -5.32 | 115.88 | 121.41 |
| 9 | Q | 411 | VAL | N-CA-C | -5.32 | 105.19 | 110.62 |
| 10 | U | 255 | ILE | O-C-N | -5.32 | 117.72 | 123.14 |
| 1 | Y | 465 | ILE | N-CA-CB | 5.32 | 119.86 | 111.99 |
| 2 | 1 | 102 | SER | CA-C-N | 5.32 | 127.84 | 120.29 |
| 2 | 1 | 102 | SER | C-N-CA | 5.32 | 127.84 | 120.29 |
| 5 | H | 434 | GLU | N-CA-CB | 5.32 | 119.48 | 110.49 |
| 7 | M | 529 | MET | CA-C-O | -5.32 | 113.86 | 119.97 |
| 7 | M | 1313 | ILE | CA-C-N | 5.32 | 129.47 | 120.64 |
| 7 | M | 1313 | ILE | C-N-CA | 5.32 | 129.47 | 120.64 |
| 8 | N | 1316 | LEU | CA-C-O | -5.32 | 112.91 | 120.51 |
| 7 | O | 820 | GLN | CA-C-N | 5.32 | 131.69 | 121.54 |
| 7 | O | 820 | GLN | C-N-CA | 5.32 | 131.69 | 121.54 |
| 7 | O | 1187 | ASN | CA-C-N | 5.32 | 131.70 | 121.54 |
| 7 | O | 1187 | ASN | C-N-CA | 5.32 | 131.70 | 121.54 |
| 9 | R | 234 | ILE | CA-C-N | 5.32 | 127.35 | 120.44 |
| 9 | R | 234 | ILE | C-N-CA | 5.32 | 127.35 | 120.44 |
| 9 | R | 405 | ASP | CA-C-N | 5.32 | 124.83 | 119.19 |
| 9 | R | 405 | ASP | C-N-CA | 5.32 | 124.83 | 119.19 |
| 1 | Y | 164 | PHE | CA-C-O | 5.32 | 125.71 | 119.28 |
| 2 | Z | 752 | VAL | O-C-N | 5.32 | 127.12 | 121.91 |
| 12 | u | 145 | LEU | CA-C-O | 5.32 | 126.10 | 120.36 |
| 14 | h | 234 | LEU | N-CA-C | -5.32 | 99.43 | 108.26 |
| 16 | j | 187 | ASP | CA-C-N | 5.32 | 127.97 | 120.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 16 | j | 187 | ASP | C-N-CA | 5.32 | 127.97 | 120.42 |
| 19 | m | 416 | TYR | O-C-N | 5.32 | 127.55 | 122.07 |
| 20 | n | 856 | LYS | N-CA-CB | 5.32 | 119.47 | 110.49 |
| 20 | n | 994 | THR | N-CA-C | 5.32 | 117.94 | 110.23 |
| 19 | f | 524 | VAL | CA-C-O | -5.32 | 114.13 | 120.78 |
| 20 | g | 950 | ASN | N-CA-CB | 5.32 | 118.45 | 110.53 |
| 14 | a | 129 | LEU | CA-C-O | 5.32 | 127.33 | 121.11 |
| 14 | a | 153 | GLN | OE1-CD-NE2 | 5.32 | 127.92 | 122.60 |
| 1 | 0 | 696 | ARG | CD-NE-CZ | -5.32 | 116.96 | 124.40 |
| 5 | B | 296 | LYS | N-CA-C | -5.32 | 99.48 | 110.80 |
| 7 | M | 524 | SER | CA-C-N | 5.32 | 127.40 | 120.28 |
| 7 | M | 524 | SER | C-N-CA | 5.32 | 127.40 | 120.28 |
| 7 | M | 632 | SER | O-C-N | -5.32 | 116.48 | 122.12 |
| 7 | M | 1053 | ILE | N-CA-CB | 5.32 | 118.55 | 110.58 |
| 8 | N | 893 | TYR | N-CA-C | -5.32 | 100.99 | 109.23 |
| 7 | O | 253 | LYS | N-CA-C | 5.32 | 118.93 | 112.23 |
| 7 | O | 1579 | ASN | N-CA-CB | 5.32 | 117.72 | 110.01 |
| 9 | R | 621 | HIS | CG-CD2-NE2 | 5.32 | 112.52 | 107.20 |
| 11 | X | 274 | PHE | N-CA-C | -5.32 | 102.30 | 109.95 |
| 12 | u | 67 | ASP | N-CA-C | -5.32 | 106.84 | 113.38 |
| 15 | i | 253 | VAL | N-CA-C | 5.32 | 116.04 | 110.62 |
| 15 | i | 596 | SER | N-CA-CB | 5.32 | 118.94 | 110.65 |
| 16 | j | 364 | SER | N-CA-CB | 5.32 | 119.83 | 110.37 |
| 15 | b | 415 | CYS | N-CA-C | 5.32 | 117.07 | 111.28 |
| 17 | d | 108 | ALA | N-CA-C | 5.32 | 117.23 | 109.84 |
| 19 | f | 657 | ALA | CA-C-N | 5.32 | 127.40 | 120.28 |
| 19 | f | 657 | ALA | C-N-CA | 5.32 | 127.40 | 120.28 |
| 20 | g | 405 | GLU | CB-CG-CD | -5.32 | 103.56 | 112.60 |
| 7 | M | 622 | GLN | CB-CA-C | -5.31 | 102.41 | 111.02 |
| 8 | N | 979 | ASN | OD1-CG-ND2 | 5.31 | 127.91 | 122.60 |
| 7 | O | 632 | SER | CA-C-O | -5.31 | 114.92 | 120.55 |
| 8 | P | 660 | PHE | CA-CB-CG | 5.31 | 119.11 | 113.80 |
| 1 | Y | 954 | ALA | CB-CA-C | -5.31 | 101.05 | 109.82 |
| 1 | Y | 1428 | TYR | CA-C-N | 5.31 | 128.02 | 120.53 |
| 1 | Y | 1428 | TYR | C-N-CA | 5.31 | 128.02 | 120.53 |
| 19 | f | 430 | PRO | O-C-N | 5.31 | 128.87 | 122.23 |
| 2 | 1 | 1212 | PRO | CB-CA-C | 5.31 | 120.33 | 111.56 |
| 4 | A | 699 | TYR | N-CA-C | -5.31 | 105.40 | 111.14 |
| 5 | K | 310 | ALA | CA-C-O | -5.31 | 115.73 | 121.36 |
| 7 | O | 1489 | ILE | N-CA-CB | 5.31 | 117.76 | 110.54 |
| 8 | P | 889 | THR | CA-C-N | 5.31 | 131.69 | 121.54 |
| 8 | P | 889 | THR | C-N-CA | 5.31 | 131.69 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1049 | ASP | O-C-N | 5.31 | 129.13 | 122.86 |
| 8 | P | 1491 | LEU | N-CA-C | 5.31 | 117.07 | 111.28 |
| 9 | S | 549 | ASP | N-CA-C | -5.31 | 97.66 | 108.12 |
| 1 | Y | 436 | LEU | CB-CA-C | -5.31 | 98.63 | 109.94 |
| 15 | i | 598 | ASN | CA-CB-CG | -5.31 | 107.29 | 112.60 |
| 16 | j | 452 | TYR | CA-C-O | -5.31 | 115.24 | 120.82 |
| 16 | j | 526 | ILE | CA-CB-CG2 | 5.31 | 119.53 | 110.50 |
| 19 | m | 392 | LEU | CA-C-N | 5.31 | 127.40 | 120.28 |
| 19 | m | 392 | LEU | C-N-CA | 5.31 | 127.40 | 120.28 |
| 20 | n | 986 | ILE | N-CA-C | -5.31 | 105.35 | 110.72 |
| 15 | b | 302 | THR | O-C-N | -5.31 | 115.57 | 122.37 |
| 19 | f | 43 | ARG | CB-CA-C | -5.31 | 102.51 | 110.90 |
| 19 | f | 662 | PHE | N-CA-C | 5.31 | 117.98 | 111.82 |
| 7 | M | 1354 | VAL | CA-C-N | 5.31 | 129.63 | 121.19 |
| 7 | M | 1354 | VAL | C-N-CA | 5.31 | 129.63 | 121.19 |
| 7 | O | 55 | GLU | CA-C-N | 5.31 | 127.62 | 120.50 |
| 7 | O | 55 | GLU | C-N-CA | 5.31 | 127.62 | 120.50 |
| 20 | g | 1104 | ILE | CA-C-N | 5.31 | 130.56 | 122.65 |
| 20 | g | 1104 | ILE | C-N-CA | 5.31 | 130.56 | 122.65 |
| 2 | 1 | 1167 | ALA | O-C-N | 5.31 | 127.75 | 122.12 |
| 5 | B | 461 | ALA | CA-C-N | 5.31 | 127.39 | 120.28 |
| 5 | B | 461 | ALA | C-N-CA | 5.31 | 127.39 | 120.28 |
| 6 | C | 359 | THR | CA-CB-OG1 | 5.31 | 117.57 | 109.60 |
| 7 | M | 214 | LEU | N-CA-C | 5.31 | 116.75 | 111.07 |
| 7 | O | 701 | THR | CA-CB-OG1 | 5.31 | 117.56 | 109.60 |
| 7 | O | 1385 | PHE | CA-C-O | -5.31 | 115.23 | 120.70 |
| 7 | O | 1605 | PHE | CA-C-N | 5.31 | 127.34 | 120.44 |
| 7 | O | 1605 | PHE | C-N-CA | 5.31 | 127.34 | 120.44 |
| 8 | P | 88 | PHE | O-C-N | 5.31 | 129.24 | 123.13 |
| 9 | S | 777 | ILE | CB-CA-C | 5.31 | 117.78 | 111.20 |
| 9 | T | 64 | LYS | N-CA-C | 5.31 | 115.40 | 108.07 |
| 10 | U | 262 | ILE | CA-C-N | 5.31 | 127.39 | 120.28 |
| 10 | U | 262 | ILE | C-N-CA | 5.31 | 127.39 | 120.28 |
| 11 | X | 399 | LYS | O-C-N | -5.31 | 117.74 | 123.42 |
| 4 | z | 658 | TYR | N-CA-CB | 5.31 | 117.71 | 110.01 |
| 14 | h | 528 | ILE | CA-C-O | -5.31 | 115.03 | 120.71 |
| 16 | j | 557 | GLN | OE1-CD-NE2 | -5.31 | 117.29 | 122.60 |
| 16 | c | 290 | GLU | N-CA-CB | 5.31 | 118.51 | 110.28 |
| 16 | c | 544 | LEU | CA-C-N | 5.31 | 127.66 | 120.65 |
| 16 | c | 544 | LEU | C-N-CA | 5.31 | 127.66 | 120.65 |
| 19 | f | 244 | ARG | NE-CZ-NH2 | 5.31 | 123.98 | 119.20 |
| 14 | a | 342 | LEU | N-CA-C | -5.31 | 99.49 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | a | 738 | ARG | N-CA-CB | 5.31 | 119.00 | 111.19 |
| 1 | 0 | 618 | THR | N-CA-C | -5.31 | 99.67 | 108.75 |
| 2 | 1 | 367 | LEU | CA-C-N | 5.31 | 128.20 | 120.98 |
| 2 | 1 | 367 | LEU | C-N-CA | 5.31 | 128.20 | 120.98 |
| 7 | M | 848 | VAL | CA-CB-CG1 | 5.31 | 119.42 | 110.40 |
| 7 | M | 1150 | PHE | N-CA-C | 5.31 | 117.06 | 111.28 |
| 7 | M | 1527 | ARG | CA-C-N | 5.31 | 127.45 | 120.60 |
| 7 | M | 1527 | ARG | C-N-CA | 5.31 | 127.45 | 120.60 |
| 8 | N | 345 | ASP | CB-CG-OD2 | -5.31 | 106.19 | 118.40 |
| 8 | N | 1319 | LEU | N-CA-CB | 5.31 | 117.76 | 109.85 |
| 9 | Q | 244 | SER | CA-C-O | -5.31 | 115.64 | 121.58 |
| 9 | Q | 321 | LYS | CB-CG-CD | 5.31 | 123.51 | 111.30 |
| 13 | x | 1310 | VAL | CA-C-N | 5.31 | 127.39 | 120.28 |
| 13 | x | 1310 | VAL | C-N-CA | 5.31 | 127.39 | 120.28 |
| 4 | z | 686 | ALA | CA-C-N | 5.31 | 127.66 | 120.65 |
| 4 | z | 686 | ALA | C-N-CA | 5.31 | 127.66 | 120.65 |
| 20 | n | 220 | VAL | CA-C-N | 5.31 | 130.23 | 122.85 |
| 20 | n | 220 | VAL | C-N-CA | 5.31 | 130.23 | 122.85 |
| 16 | c | 548 | TYR | O-C-N | 5.31 | 130.05 | 123.15 |
| 5 | H | 396 | SER | CB-CA-C | -5.31 | 102.52 | 110.90 |
| 8 | N | 187 | PHE | CA-C-N | 5.31 | 127.73 | 120.46 |
| 8 | N | 187 | PHE | C-N-CA | 5.31 | 127.73 | 120.46 |
| 8 | N | 770 | HIS | ND1-CE1-NE2 | 5.31 | 113.71 | 108.40 |
| 7 | O | 621 | TYR | CA-C-N | 5.31 | 131.29 | 122.54 |
| 7 | O | 621 | TYR | C-N-CA | 5.31 | 131.29 | 122.54 |
| 8 | P | 1207 | TRP | CB-CG-CD2 | -5.31 | 119.37 | 126.80 |
| 16 | c | 328 | ASN | N-CA-CB | 5.31 | 119.46 | 110.49 |
| 19 | f | 330 | ARG | NH1-CZ-NH2 | -5.31 | 112.40 | 119.30 |
| 20 | g | 804 | ILE | CA-C-N | 5.31 | 127.70 | 120.54 |
| 20 | g | 804 | ILE | C-N-CA | 5.31 | 127.70 | 120.54 |
| 14 | a | 974 | GLU | CA-C-O | 5.31 | 127.54 | 121.28 |
| 5 | B | 404 | ARG | CA-C-N | 5.30 | 127.39 | 120.28 |
| 5 | B | 404 | ARG | C-N-CA | 5.30 | 127.39 | 120.28 |
| 6 | I | 405 | LEU | N-CA-CB | 5.30 | 119.45 | 110.49 |
| 7 | M | 719 | ILE | CA-C-O | -5.30 | 114.80 | 121.11 |
| 8 | N | 1463 | SER | O-C-N | -5.30 | 115.83 | 122.35 |
| 7 | O | 1238 | ASP | CA-CB-CG | 5.30 | 117.90 | 112.60 |
| 9 | Q | 79 | SER | CA-C-N | 5.30 | 131.67 | 121.54 |
| 9 | Q | 79 | SER | C-N-CA | 5.30 | 131.67 | 121.54 |
| 9 | S | 163 | ILE | CB-CA-C | -5.30 | 104.90 | 112.22 |
| 9 | T | 271 | VAL | CB-CA-C | -5.30 | 104.98 | 112.14 |
| 2 | Z | 1314 | ALA | N-CA-C | -5.30 | 106.49 | 113.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | u | 228 | ASN | OD1-CG-ND2 | 5.30 | 127.90 | 122.60 |
| 4 | y | 661 | LYS | CA-C-N | 5.30 | 127.73 | 120.46 |
| 4 | y | 661 | LYS | C-N-CA | 5.30 | 127.73 | 120.46 |
| 18 | l | 325 | ASP | CA-CB-CG | 5.30 | 117.91 | 112.60 |
| 15 | b | 711 | GLU | O-C-N | -5.30 | 115.52 | 122.20 |
| 18 | e | 241 | ARG | CD-NE-CZ | 5.30 | 131.83 | 124.40 |
| 9 | S | 303 | ASN | CA-C-O | -5.30 | 114.35 | 120.24 |
| 1 | Y | 1205 | SER | CA-C-N | 5.30 | 127.39 | 120.28 |
| 1 | Y | 1205 | SER | C-N-CA | 5.30 | 127.39 | 120.28 |
| 2 | 1 | 184 | ASN | CA-C-N | 5.30 | 127.24 | 120.56 |
| 2 | 1 | 184 | ASN | C-N-CA | 5.30 | 127.24 | 120.56 |
| 2 | 1 | 1330 | GLU | CA-C-N | 5.30 | 131.43 | 122.26 |
| 2 | 1 | 1330 | GLU | C-N-CA | 5.30 | 131.43 | 122.26 |
| 6 | F | 292 | HIS | CA-C-O | -5.30 | 115.43 | 121.00 |
| 5 | H | 466 | LEU | N-CA-C | 5.30 | 117.06 | 111.28 |
| 8 | N | 840 | LEU | CA-C-N | 5.30 | 127.02 | 120.34 |
| 8 | N | 840 | LEU | C-N-CA | 5.30 | 127.02 | 120.34 |
| 7 | O | 1196 | SER | CA-C-O | -5.30 | 113.07 | 118.90 |
| 7 | O | 1392 | ILE | CA-C-N | 5.30 | 130.99 | 122.83 |
| 7 | O | 1392 | ILE | C-N-CA | 5.30 | 130.99 | 122.83 |
| 9 | Q | 470 | GLY | CA-C-N | 5.30 | 126.47 | 119.84 |
| 9 | Q | 470 | GLY | C-N-CA | 5.30 | 126.47 | 119.84 |
| 9 | Q | 810 | ALA | N-CA-C | 5.30 | 117.81 | 111.71 |
| 1 | Y | 214 | VAL | CA-CB-CG1 | -5.30 | 101.39 | 110.40 |
| 1 | Y | 1026 | TYR | N-CA-C | -5.30 | 106.83 | 113.72 |
| 1 | Y | 1183 | LEU | O-C-N | -5.30 | 115.22 | 121.32 |
| 20 | n | 97 | GLY | N-CA-C | -5.30 | 102.74 | 111.38 |
| 21 | t | 58 | HIS | O-C-N | -5.30 | 116.89 | 123.36 |
| 16 | c | 610 | TRP | CB-CG-CD2 | -5.30 | 119.38 | 126.80 |
| 20 | g | 1047 | LEU | O-C-N | -5.30 | 115.75 | 122.27 |
| 4 | D | 774 | ASN | N-CA-C | 5.30 | 117.80 | 111.71 |
| 4 | G | 753 | GLU | CA-C-N | 5.30 | 132.45 | 121.32 |
| 4 | G | 753 | GLU | C-N-CA | 5.30 | 132.45 | 121.32 |
| 5 | K | 294 | LYS | N-CA-C | -5.30 | 100.47 | 108.52 |
| 5 | K | 345 | PRO | CA-C-N | 5.30 | 130.15 | 122.36 |
| 5 | K | 345 | PRO | C-N-CA | 5.30 | 130.15 | 122.36 |
| 7 | M | 910 | ARG | NE-CZ-NH1 | -5.30 | 116.20 | 121.50 |
| 8 | N | 1076 | SER | O-C-N | 5.30 | 127.53 | 122.07 |
| 8 | N | 1638 | LYS | CA-C-N | 5.30 | 125.82 | 119.94 |
| 8 | N | 1638 | LYS | C-N-CA | 5.30 | 125.82 | 119.94 |
| 7 | O | 636 | SER | N-CA-CB | 5.30 | 118.38 | 110.22 |
| 10 | W | 273 | PHE | N-CA-C | -5.30 | 106.68 | 112.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 11 | X | 376 | ILE | N-CA-C | -5.30 | 99.93 | 107.77 |
| 1 | Y | 1095 | LYS | N-CA-C | 5.30 | 117.74 | 111.33 |
| 12 | u | 662 | LEU | CA-C-N | 5.30 | 127.38 | 120.28 |
| 12 | u | 662 | LEU | C-N-CA | 5.30 | 127.38 | 120.28 |
| 15 | i | 608 | PRO | N-CA-CB | -5.30 | 98.17 | 103.20 |
| 16 | j | 584 | ASN | CA-C-N | 5.30 | 127.77 | 120.67 |
| 16 | j | 584 | ASN | C-N-CA | 5.30 | 127.77 | 120.67 |
| 19 | f | 273 | ASN | CA-CB-CG | -5.30 | 107.30 | 112.60 |
| 20 | g | 440 | ARG | N-CA-CB | 5.30 | 119.71 | 110.81 |
| 2 | 1 | 393 | VAL | CA-C-N | 5.30 | 128.61 | 120.82 |
| 2 | 1 | 393 | VAL | C-N-CA | 5.30 | 128.61 | 120.82 |
| 1 | Y | 442 | GLY | O-C-N | 5.30 | 127.28 | 122.19 |
| 12 | u | 280 | LYS | CA-C-O | -5.30 | 114.72 | 120.81 |
| 15 | i | 637 | ARG | CA-C-N | 5.30 | 131.66 | 121.54 |
| 15 | i | 637 | ARG | C-N-CA | 5.30 | 131.66 | 121.54 |
| 19 | f | 589 | HIS | ND1-CE1-NE2 | 5.30 | 113.70 | 108.40 |
| 2 | 1 | 1374 | PRO | O-C-N | 5.30 | 129.42 | 122.27 |
| 5 | B | 410 | LYS | N-CA-CB | 5.30 | 117.91 | 110.12 |
| 6 | I | 352 | VAL | CA-C-N | 5.30 | 127.33 | 120.44 |
| 6 | I | 352 | VAL | C-N-CA | 5.30 | 127.33 | 120.44 |
| 8 | P | 1446 | PHE | CB-CA-C | 5.30 | 119.11 | 110.96 |
| 9 | R | 211 | LYS | CB-CG-CD | 5.30 | 123.48 | 111.30 |
| 9 | S | 467 | ILE | CA-CB-CG2 | -5.30 | 101.50 | 110.50 |
| 9 | S | 562 | LEU | N-CA-C | -5.30 | 106.50 | 113.17 |
| 9 | T | 557 | LEU | CB-CA-C | 5.30 | 116.32 | 109.28 |
| 1 | Y | 1026 | TYR | CB-CG-CD1 | 5.30 | 128.74 | 120.80 |
| 12 | u | 92 | GLU | N-CA-CB | 5.30 | 119.06 | 110.43 |
| 12 | u | 190 | ASP | N-CA-C | -5.30 | 107.19 | 113.97 |
| 15 | i | 238 | LYS | CA-C-O | 5.30 | 125.73 | 119.48 |
| 15 | i | 617 | THR | N-CA-C | -5.30 | 106.50 | 113.12 |
| 17 | k | 285 | LEU | N-CA-CB | 5.30 | 119.44 | 110.49 |
| 20 | n | 620 | ASN | N-CA-C | -5.30 | 101.71 | 109.81 |
| 20 | n | 1076 | PHE | O-C-N | -5.30 | 117.71 | 121.84 |
| 21 | t | 53 | TYR | N-CA-C | -5.30 | 105.67 | 113.61 |
| 14 | a | 62 | LEU | N-CA-C | -5.30 | 99.52 | 110.80 |
| 6 | C | 302 | ASP | O-C-N | -5.29 | 115.75 | 122.26 |
| 6 | C | 348 | GLN | O-C-N | 5.29 | 127.73 | 122.12 |
| 1 | Y | 1438 | ASP | CA-CB-CG | -5.29 | 107.31 | 112.60 |
| 4 | z | 659 | THR | N-CA-C | 5.29 | 117.05 | 111.28 |
| 19 | m | 97 | HIS | N-CA-C | 5.29 | 116.56 | 109.83 |
| 2 | 1 | 1177 | VAL | N-CA-C | -5.29 | 104.63 | 112.04 |
| 7 | O | 109 | ARG | CB-CA-C | -5.29 | 102.00 | 110.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 752 | TYR | CA-C-N | 5.29 | 127.81 | 120.29 |
| 7 | O | 752 | TYR | C-N-CA | 5.29 | 127.81 | 120.29 |
| 9 | S | 503 | ALA | CA-C-O | 5.29 | 126.16 | 120.55 |
| 11 | X | 361 | ASN | CA-CB-CG | -5.29 | 107.31 | 112.60 |
| 12 | u | 300 | THR | O-C-N | -5.29 | 115.84 | 122.35 |
| 12 | u | 666 | GLU | CA-C-O | -5.29 | 115.26 | 120.82 |
| 14 | h | 166 | LEU | CA-C-N | 5.29 | 130.57 | 122.95 |
| 14 | h | 166 | LEU | C-N-CA | 5.29 | 130.57 | 122.95 |
| 14 | h | 473 | VAL | CA-C-O | 5.29 | 127.27 | 120.76 |
| 15 | i | 344 | ARG | N-CA-C | -5.29 | 106.13 | 112.59 |
| 16 | j | 330 | PRO | CA-C-N | 5.29 | 127.32 | 120.44 |
| 16 | j | 330 | PRO | C-N-CA | 5.29 | 127.32 | 120.44 |
| 19 | m | 698 | ASN | N-CA-C | -5.29 | 106.50 | 113.17 |
| 15 | b | 552 | ILE | O-C-N | -5.29 | 116.38 | 121.83 |
| 5 | H | 439 | GLN | N-CA-C | 5.29 | 117.96 | 111.82 |
| 7 | M | 622 | GLN | OE1-CD-NE2 | -5.29 | 117.31 | 122.60 |
| 8 | N | 325 | TRP | CZ3-CH2-CZ2 | -5.29 | 114.62 | 121.50 |
| 9 | Q | 419 | ASP | CB-CA-C | -5.29 | 103.01 | 112.27 |
| 9 | T | 344 | GLY | CA-C-O | 5.29 | 125.70 | 119.46 |
| 2 | Z | 1297 | ILE | CA-C-N | 5.29 | 127.90 | 120.28 |
| 2 | Z | 1297 | ILE | C-N-CA | 5.29 | 127.90 | 120.28 |
| 14 | h | 67 | TYR | CA-C-N | 5.29 | 129.12 | 121.18 |
| 14 | h | 67 | TYR | C-N-CA | 5.29 | 129.12 | 121.18 |
| 14 | h | 230 | HIS | CA-C-N | 5.29 | 130.25 | 122.63 |
| 14 | h | 230 | HIS | C-N-CA | 5.29 | 130.25 | 122.63 |
| 15 | i | 736 | ASN | OD1-CG-ND2 | 5.29 | 127.89 | 122.60 |
| 17 | d | 122 | ASP | CA-CB-CG | 5.29 | 117.89 | 112.60 |
| 18 | e | 72 | ILE | CB-CA-C | 5.29 | 119.16 | 110.69 |
| 14 | a | 490 | VAL | N-CA-CB | 5.29 | 119.96 | 111.23 |
| 14 | a | 836 | ASN | CA-CB-CG | 5.29 | 117.89 | 112.60 |
| 7 | M | 430 | PHE | CA-CB-CG | -5.29 | 108.51 | 113.80 |
| 7 | O | 793 | TYR | CB-CA-C | -5.29 | 102.45 | 111.02 |
| 12 | v | 234 | TYR | CA-C-N | 5.29 | 128.35 | 120.31 |
| 12 | v | 234 | TYR | C-N-CA | 5.29 | 128.35 | 120.31 |
| 12 | v | 359 | GLU | CA-C-N | 5.29 | 129.51 | 122.95 |
| 12 | v | 359 | GLU | C-N-CA | 5.29 | 129.51 | 122.95 |
| 13 | w | 1303 | ILE | CA-C-O | 5.29 | 126.46 | 120.85 |
| 20 | n | 463 | LYS | CB-CA-C | 5.29 | 119.98 | 111.36 |
| 20 | n | 673 | ILE | CA-CB-CG1 | 5.29 | 119.39 | 110.40 |
| 15 | b | 550 | HIS | O-C-N | 5.29 | 129.59 | 122.82 |
| 1 | 0 | 1415 | ILE | CA-CB-CG1 | 5.29 | 119.39 | 110.40 |
| 7 | M | 785 | TYR | CA-C-N | 5.29 | 127.63 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 785 | TYR | C-N-CA | 5.29 | 127.63 | 120.44 |
| 8 | P | 586 | LEU | O-C-N | 5.29 | 129.08 | 122.63 |
| 8 | P | 731 | SER | CA-C-O | -5.29 | 115.37 | 121.19 |
| 9 | R | 805 | SER | O-C-N | -5.29 | 116.51 | 122.12 |
| 9 | T | 422 | ARG | N-CA-CB | 5.29 | 117.95 | 109.28 |
| 1 | Y | 684 | PHE | CA-C-N | 5.29 | 127.22 | 120.56 |
| 1 | Y | 684 | PHE | C-N-CA | 5.29 | 127.22 | 120.56 |
| 1 | Y | 840 | GLU | O-C-N | 5.29 | 128.77 | 122.27 |
| 2 | Z | 757 | SER | N-CA-CB | 5.29 | 119.17 | 110.39 |
| 12 | u | 276 | TYR | CB-CA-C | -5.29 | 103.08 | 111.17 |
| 12 | v | 353 | ARG | NE-CZ-NH2 | 5.29 | 123.96 | 119.20 |
| 16 | j | 480 | GLN | OE1-CD-NE2 | 5.29 | 127.89 | 122.60 |
| 17 | k | 77 | GLY | N-CA-C | -5.29 | 108.19 | 114.48 |
| 19 | m | 600 | TRP | CA-C-N | 5.29 | 127.37 | 120.28 |
| 19 | m | 600 | TRP | C-N-CA | 5.29 | 127.37 | 120.28 |
| 20 | n | 1017 | ILE | CA-C-O | -5.29 | 112.86 | 119.95 |
| 16 | c | 629 | GLU | CB-CA-C | 5.29 | 119.39 | 109.71 |
| 14 | a | 119 | VAL | N-CA-C | -5.29 | 98.84 | 106.88 |
| 5 | E | 357 | GLY | CA-C-N | 5.29 | 127.31 | 120.44 |
| 5 | E | 357 | GLY | C-N-CA | 5.29 | 127.31 | 120.44 |
| 8 | N | 651 | TYR | CA-C-N | 5.29 | 127.68 | 120.54 |
| 8 | N | 651 | TYR | C-N-CA | 5.29 | 127.68 | 120.54 |
| 8 | N | 660 | PHE | CA-C-N | 5.29 | 132.05 | 122.27 |
| 8 | N | 660 | PHE | C-N-CA | 5.29 | 132.05 | 122.27 |
| 8 | P | 320 | MET | CA-C-N | 5.29 | 131.49 | 121.97 |
| 8 | P | 320 | MET | C-N-CA | 5.29 | 131.49 | 121.97 |
| 9 | T | 785 | MET | CA-C-N | 5.29 | 127.33 | 120.56 |
| 9 | T | 785 | MET | C-N-CA | 5.29 | 127.33 | 120.56 |
| 16 | j | 653 | GLU | N-CA-CB | 5.29 | 118.53 | 110.44 |
| 17 | d | 39 | GLU | N-CA-C | -5.29 | 104.09 | 110.44 |
| 4 | D | 714 | PHE | CA-CB-CG | -5.29 | 108.52 | 113.80 |
| 7 | M | 261 | LYS | CB-CA-C | -5.29 | 100.85 | 110.63 |
| 8 | N | 390 | ILE | CA-C-N | 5.29 | 126.45 | 119.84 |
| 8 | N | 390 | ILE | C-N-CA | 5.29 | 126.45 | 119.84 |
| 7 | O | 159 | LYS | N-CA-CB | 5.29 | 117.67 | 110.01 |
| 7 | O | 690 | GLU | CA-CB-CG | 5.29 | 124.67 | 114.10 |
| 7 | O | 1160 | TYR | N-CA-CB | 5.29 | 121.52 | 111.00 |
| 8 | P | 1288 | PHE | CB-CG-CD2 | -5.29 | 111.72 | 120.70 |
| 1 | Y | 426 | VAL | O-C-N | -5.29 | 115.99 | 122.97 |
| 1 | Y | 1083 | TYR | CG-CD2-CE2 | 5.29 | 129.13 | 121.20 |
| 1 | Y | 1356 | LYS | CA-C-O | 5.29 | 127.43 | 121.51 |
| 12 | u | 312 | ASN | N-CA-C | -5.29 | 99.54 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 173 | PHE | N-CA-CB | 5.29 | 119.42 | 110.49 |
| 14 | h | 411 | LEU | CA-C-N | 5.29 | 127.89 | 120.28 |
| 14 | h | 411 | LEU | C-N-CA | 5.29 | 127.89 | 120.28 |
| 14 | h | 816 | THR | N-CA-CB | 5.29 | 119.42 | 110.49 |
| 15 | i | 677 | LEU | CA-C-O | 5.29 | 128.07 | 120.51 |
| 20 | n | 649 | PHE | CB-CG-CD1 | -5.29 | 111.72 | 120.70 |
| 16 | c | 445 | LEU | CA-C-N | 5.29 | 128.73 | 120.75 |
| 16 | c | 445 | LEU | C-N-CA | 5.29 | 128.73 | 120.75 |
| 20 | g | 834 | THR | N-CA-C | -5.29 | 104.84 | 111.92 |
| 2 | 1 | 383 | HIS | CG-CD2-NE2 | 5.28 | 112.48 | 107.20 |
| 2 | 1 | 577 | PHE | N-CA-C | -5.28 | 105.63 | 113.40 |
| 7 | M | 564 | ASP | CA-CB-CG | 5.28 | 117.88 | 112.60 |
| 8 | N | 104 | SER | N-CA-CB | 5.28 | 118.39 | 109.78 |
| 8 | N | 1543 | VAL | O-C-N | -5.28 | 116.98 | 123.00 |
| 7 | O | 1477 | ASP | N-CA-C | 5.28 | 117.04 | 111.28 |
| 9 | Q | 554 | VAL | CB-CA-C | -5.28 | 106.41 | 111.06 |
| 2 | Z | 196 | GLU | N-CA-C | -5.28 | 106.06 | 112.88 |
| 2 | Z | 1196 | ASN | O-C-N | -5.28 | 116.50 | 122.68 |
| 12 | v | 539 | ILE | CA-C-N | 5.28 | 127.70 | 120.46 |
| 12 | v | 539 | ILE | C-N-CA | 5.28 | 127.70 | 120.46 |
| 14 | h | 954 | ARG | CD-NE-CZ | -5.28 | 117.00 | 124.40 |
| 15 | i | 223 | TYR | N-CA-C | -5.28 | 106.22 | 113.30 |
| 20 | n | 284 | TYR | N-CA-CB | 5.28 | 118.57 | 110.70 |
| 20 | n | 480 | LYS | N-CA-CB | 5.28 | 119.48 | 110.50 |
| 20 | g | 494 | VAL | O-C-N | 5.28 | 129.32 | 122.77 |
| 20 | g | 782 | ASP | CA-CB-CG | 5.28 | 117.88 | 112.60 |
| 14 | a | 169 | VAL | CB-CA-C | -5.28 | 105.57 | 111.80 |
| 2 | 1 | 924 | SER | N-CA-C | -5.28 | 99.55 | 110.80 |
| 6 | I | 439 | ILE | CA-C-N | 5.28 | 130.06 | 122.72 |
| 6 | I | 439 | ILE | C-N-CA | 5.28 | 130.06 | 122.72 |
| 8 | N | 212 | TRP | CA-CB-CG | 5.28 | 123.64 | 113.60 |
| 9 | R | 593 | ILE | N-CA-C | 5.28 | 115.46 | 107.75 |
| 9 | T | 696 | TYR | CA-CB-CG | -5.28 | 104.39 | 113.90 |
| 11 | V | 395 | LEU | CA-C-N | 5.28 | 127.36 | 120.28 |
| 11 | V | 395 | LEU | C-N-CA | 5.28 | 127.36 | 120.28 |
| 14 | a | 164 | HIS | CG-CD2-NE2 | 5.28 | 112.48 | 107.20 |
| 1 | 0 | 1259 | ALA | CA-C-N | 5.28 | 131.62 | 121.54 |
| 1 | 0 | 1259 | ALA | C-N-CA | 5.28 | 131.62 | 121.54 |
| 4 | D | 719 | GLU | N-CA-CB | 5.28 | 119.28 | 110.41 |
| 4 | J | 679 | LEU | CA-C-N | 5.28 | 128.13 | 120.79 |
| 4 | J | 679 | LEU | C-N-CA | 5.28 | 128.13 | 120.79 |
| 7 | M | 194 | SER | CB-CA-C | -5.28 | 102.02 | 110.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1239 | ASP | N-CA-C | -5.28 | 106.22 | 113.30 |
| 9 | Q | 123 | MET | CA-C-N | 5.28 | 127.30 | 120.44 |
| 9 | Q | 123 | MET | C-N-CA | 5.28 | 127.30 | 120.44 |
| 2 | Z | 975 | ASP | N-CA-CB | 5.28 | 118.48 | 110.45 |
| 12 | u | 252 | GLN | N-CA-CB | 5.28 | 117.67 | 110.01 |
| 12 | v | 389 | TRP | CA-C-N | 5.28 | 127.36 | 120.28 |
| 12 | v | 389 | TRP | C-N-CA | 5.28 | 127.36 | 120.28 |
| 13 | w | 1404 | GLU | CA-C-N | 5.28 | 127.36 | 120.28 |
| 13 | w | 1404 | GLU | C-N-CA | 5.28 | 127.36 | 120.28 |
| 14 | h | 120 | ASN | OD1-CG-ND2 | 5.28 | 127.88 | 122.60 |
| 21 | t | 47 | LYS | N-CA-CB | 5.28 | 117.67 | 110.01 |
| 16 | c | 394 | ILE | N-CA-CB | 5.28 | 119.94 | 111.23 |
| 16 | c | 480 | GLN | CA-C-O | -5.28 | 114.82 | 120.42 |
| 14 | a | 990 | ASP | CA-CB-CG | 5.28 | 117.88 | 112.60 |
| 6 | C | 446 | GLU | CB-CA-C | -5.28 | 102.03 | 110.79 |
| 6 | L | 381 | GLU | CB-CG-CD | -5.28 | 103.62 | 112.60 |
| 7 | M | 1572 | ASN | N-CA-CB | 5.28 | 117.73 | 109.97 |
| 7 | O | 784 | ILE | CA-C-O | -5.28 | 115.92 | 121.41 |
| 1 | 0 | 1161 | MET | CA-C-N | 5.28 | 127.61 | 120.38 |
| 1 | 0 | 1161 | MET | C-N-CA | 5.28 | 127.61 | 120.38 |
| 7 | O | 152 | HIS | CE1-NE2-CD2 | -5.28 | 103.72 | 109.00 |
| 9 | R | 800 | GLY | N-CA-C | 5.28 | 120.44 | 113.37 |
| 9 | S | 233 | ASP | CA-CB-CG | 5.28 | 117.88 | 112.60 |
| 9 | S | 286 | THR | CA-C-O | -5.28 | 115.28 | 120.82 |
| 9 | T | 45 | SER | N-CA-CB | 5.28 | 119.41 | 110.49 |
| 2 | Z | 666 | SER | CA-C-O | 5.28 | 126.34 | 120.90 |
| 12 | u | 650 | SER | O-C-N | 5.28 | 127.72 | 122.12 |
| 21 | q | 33 | ASP | N-CA-C | 5.28 | 118.98 | 112.54 |
| 21 | t | 54 | GLY | CA-C-N | 5.28 | 129.79 | 121.56 |
| 21 | t | 54 | GLY | C-N-CA | 5.28 | 129.79 | 121.56 |
| 19 | f | 262 | ALA | O-C-N | 5.28 | 127.72 | 122.12 |
| 1 | 0 | 1146 | TYR | CB-CG-CD1 | -5.28 | 112.89 | 120.80 |
| 1 | 0 | 1333 | HIS | O-C-N | -5.28 | 115.81 | 122.19 |
| 6 | C | 301 | HIS | ND1-CE1-NE2 | 5.28 | 113.67 | 108.40 |
| 7 | M | 639 | LEU | CA-C-O | -5.28 | 114.83 | 120.42 |
| 8 | N | 344 | SER | O-C-N | 5.28 | 127.58 | 122.09 |
| 8 | N | 1159 | ASP | CA-CB-CG | 5.28 | 117.88 | 112.60 |
| 7 | O | 167 | ILE | CB-CA-C | 5.28 | 116.45 | 111.44 |
| 8 | P | 1416 | GLY | CA-C-N | 5.28 | 128.34 | 120.90 |
| 8 | P | 1416 | GLY | C-N-CA | 5.28 | 128.34 | 120.90 |
| 9 | R | 369 | THR | CA-C-N | 5.28 | 129.04 | 120.60 |
| 9 | R | 369 | THR | C-N-CA | 5.28 | 129.04 | 120.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | S | 24 | GLU | CB-CA-C | -5.28 | 100.87 | 110.63 |
| 2 | Z | 1166 | ILE | CA-C-N | 5.28 | 127.30 | 120.44 |
| 2 | Z | 1166 | ILE | C-N-CA | 5.28 | 127.30 | 120.44 |
| 15 | i | 646 | LEU | N-CA-C | -5.28 | 99.56 | 110.80 |
| 19 | m | 584 | ILE | CA-C-N | 5.28 | 127.78 | 120.29 |
| 19 | m | 584 | ILE | C-N-CA | 5.28 | 127.78 | 120.29 |
| 20 | g | 868 | HIS | CA-C-N | 5.28 | 128.33 | 120.31 |
| 20 | g | 868 | HIS | C-N-CA | 5.28 | 128.33 | 120.31 |
| 14 | a | 436 | HIS | CG-CD2-NE2 | 5.28 | 112.47 | 107.20 |
| 8 | N | 1022 | TYR | N-CA-CB | 5.27 | 117.80 | 109.94 |
| 12 | v | 598 | LEU | CA-C-N | 5.27 | 127.30 | 120.44 |
| 12 | v | 598 | LEU | C-N-CA | 5.27 | 127.30 | 120.44 |
| 19 | f | 361 | SER | CA-C-N | 5.27 | 127.87 | 120.28 |
| 19 | f | 361 | SER | C-N-CA | 5.27 | 127.87 | 120.28 |
| 5 | B | 524 | ASN | CA-C-O | -5.27 | 115.28 | 120.82 |
| 6 | C | 299 | ILE | CA-C-O | 5.27 | 123.97 | 119.38 |
| 4 | D | 641 | VAL | N-CA-CB | 5.27 | 119.36 | 110.56 |
| 5 | H | 473 | ILE | CB-CA-C | 5.27 | 115.82 | 110.65 |
| 7 | M | 1290 | ILE | CA-C-O | -5.27 | 115.20 | 121.05 |
| 8 | N | 753 | TYR | CA-C-N | 5.27 | 131.61 | 121.54 |
| 8 | N | 753 | TYR | C-N-CA | 5.27 | 131.61 | 121.54 |
| 8 | N | 1002 | SER | N-CA-C | 5.27 | 117.03 | 111.28 |
| 8 | N | 1090 | THR | CA-CB-OG1 | 5.27 | 117.51 | 109.60 |
| 8 | N | 1414 | GLU | CA-C-N | 5.27 | 130.06 | 121.62 |
| 8 | N | 1414 | GLU | C-N-CA | 5.27 | 130.06 | 121.62 |
| 7 | O | 1669 | LEU | O-C-N | 5.27 | 127.57 | 122.09 |
| 9 | T | 259 | ILE | CA-C-N | 5.27 | 127.34 | 120.28 |
| 9 | T | 259 | ILE | C-N-CA | 5.27 | 127.34 | 120.28 |
| 9 | T | 320 | TRP | CA-C-O | -5.27 | 115.25 | 121.16 |
| 9 | T | 673 | PRO | N-CA-C | 5.27 | 119.51 | 111.34 |
| 16 | j | 277 | GLY | N-CA-C | 5.27 | 123.09 | 112.34 |
| 17 | k | 202 | GLY | N-CA-C | -5.27 | 107.73 | 114.37 |
| 20 | n | 628 | HIS | CE1-NE2-CD2 | -5.27 | 103.73 | 109.00 |
| 20 | n | 645 | ILE | CA-CB-CG1 | 5.27 | 119.36 | 110.40 |
| 20 | g | 1047 | LEU | CA-C-O | 5.27 | 126.03 | 119.97 |
| 14 | a | 418 | GLN | N-CA-C | 5.27 | 117.71 | 111.33 |
| 1 | 0 | 361 | ILE | N-CA-CB | 5.27 | 120.96 | 111.21 |
| 6 | F | 358 | LEU | CA-C-O | 5.27 | 124.48 | 118.47 |
| 8 | N | 901 | ILE | CA-C-N | 5.27 | 127.66 | 120.54 |
| 8 | N | 901 | ILE | C-N-CA | 5.27 | 127.66 | 120.54 |
| 19 | m | 561 | ASN | N-CA-C | -5.27 | 106.79 | 114.12 |
| 20 | n | 641 | VAL | CA-CB-CG2 | 5.27 | 119.36 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 804 | SER | N-CA-CB | 5.27 | 118.45 | 110.28 |
| 2 | 1 | 1162 | GLU | N-CA-CB | -5.27 | 102.37 | 110.12 |
| 6 | F | 377 | ILE | O-C-N | 5.27 | 126.98 | 121.87 |
| 6 | L | 333 | ILE | N-CA-C | 5.27 | 115.48 | 110.42 |
| 8 | P | 836 | GLY | O-C-N | 5.27 | 128.02 | 122.28 |
| 8 | P | 1597 | ARG | CB-CG-CD | 5.27 | 123.42 | 111.30 |
| 9 | T | 737 | SER | CA-C-N | 5.27 | 127.77 | 120.29 |
| 9 | T | 737 | SER | C-N-CA | 5.27 | 127.77 | 120.29 |
| 1 | Y | 1303 | SER | N-CA-CB | 5.27 | 119.40 | 110.49 |
| 2 | Z | 1119 | ALA | N-CA-C | -5.27 | 105.56 | 112.41 |
| 2 | Z | 1184 | ASP | CB-CA-C | -5.27 | 101.46 | 109.89 |
| 12 | v | 525 | LEU | N-CA-C | -5.27 | 105.45 | 111.14 |
| 13 | x | 1342 | GLN | CA-C-N | 5.27 | 127.34 | 120.28 |
| 13 | x | 1342 | GLN | C-N-CA | 5.27 | 127.34 | 120.28 |
| 14 | h | 952 | ASN | CA-CB-CG | 5.27 | 117.87 | 112.60 |
| 20 | n | 504 | PHE | CA-CB-CG | 5.27 | 119.07 | 113.80 |
| 21 | s | 22 | GLU | N-CA-CB | 5.27 | 117.86 | 110.12 |
| 5 | H | 311 | PHE | CA-CB-CG | 5.27 | 119.07 | 113.80 |
| 7 | M | 685 | LEU | N-CA-C | -5.27 | 106.62 | 112.57 |
| 7 | M | 1553 | LEU | N-CA-C | -5.27 | 105.71 | 113.61 |
| 8 | N | 1098 | ASN | OD1-CG-ND2 | 5.27 | 127.87 | 122.60 |
| 8 | N | 1129 | LYS | O-C-N | 5.27 | 128.91 | 122.96 |
| 7 | O | 793 | TYR | CA-C-N | 5.27 | 129.84 | 122.05 |
| 7 | O | 793 | TYR | C-N-CA | 5.27 | 129.84 | 122.05 |
| 7 | O | 1563 | LEU | N-CA-CB | 5.27 | 118.07 | 109.69 |
| 7 | O | 1578 | VAL | CA-C-N | 5.27 | 127.29 | 120.44 |
| 7 | O | 1578 | VAL | C-N-CA | 5.27 | 127.29 | 120.44 |
| 8 | P | 507 | PRO | N-CA-CB | 5.27 | 108.19 | 103.08 |
| 8 | P | 595 | ILE | N-CA-CB | 5.27 | 117.70 | 110.54 |
| 1 | Y | 226 | PRO | N-CD-CG | 5.27 | 111.10 | 103.20 |
| 12 | u | 407 | GLY | O-C-N | -5.27 | 116.72 | 122.41 |
| 13 | x | 1338 | GLN | CA-C-O | -5.27 | 115.29 | 120.82 |
| 4 | y | 646 | ASN | N-CA-C | 5.27 | 116.71 | 111.07 |
| 14 | h | 75 | ARG | CA-C-O | 5.27 | 125.16 | 119.15 |
| 14 | h | 151 | HIS | N-CA-C | -5.27 | 99.70 | 108.34 |
| 14 | h | 950 | SER | CA-C-O | -5.27 | 115.27 | 120.70 |
| 15 | i | 594 | ILE | CA-CB-CG2 | 5.27 | 119.45 | 110.50 |
| 19 | m | 144 | TRP | CE2-CD2-CE3 | 5.27 | 124.07 | 118.80 |
| 20 | n | 493 | PHE | N-CA-C | -5.27 | 104.44 | 111.87 |
| 20 | n | 918 | SER | N-CA-C | -5.27 | 106.36 | 112.89 |
| 17 | d | 234 | TRP | N-CA-CB | 5.27 | 117.71 | 109.97 |
| 20 | g | 901 | ASN | N-CA-C | -5.27 | 105.21 | 111.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | a | 344 | VAL | CB-CA-C | 5.27 | 118.55 | 111.28 |
| 6 | I | 334 | SER | CA-C-N | 5.27 | 127.34 | 120.28 |
| 6 | I | 334 | SER | C-N-CA | 5.27 | 127.34 | 120.28 |
| 7 | O | 1327 | PHE | CA-CB-CG | -5.27 | 108.53 | 113.80 |
| 8 | P | 1289 | LYS | N-CA-C | -5.27 | 100.82 | 109.40 |
| 15 | i | 676 | LEU | CA-C-N | 5.27 | 131.60 | 121.54 |
| 15 | i | 676 | LEU | C-N-CA | 5.27 | 131.60 | 121.54 |
| 18 | l | 300 | HIS | CE1-NE2-CD2 | -5.27 | 103.73 | 109.00 |
| 1 | 0 | 680 | SER | CA-C-N | 5.26 | 127.33 | 120.28 |
| 1 | 0 | 680 | SER | C-N-CA | 5.26 | 127.33 | 120.28 |
| 1 | 0 | 1428 | TYR | N-CA-CB | 5.26 | 117.92 | 110.13 |
| 2 | 1 | 1056 | HIS | CG-CD2-NE2 | 5.26 | 112.47 | 107.20 |
| 2 | 1 | 1333 | GLU | N-CA-C | -5.26 | 100.44 | 108.76 |
| 5 | H | 355 | PHE | CA-CB-CG | -5.26 | 108.54 | 113.80 |
| 7 | M | 1286 | PHE | N-CA-CB | 5.26 | 117.78 | 109.94 |
| 8 | N | 832 | THR | CB-CA-C | 5.26 | 118.91 | 111.86 |
| 8 | N | 982 | ILE | CB-CA-C | 5.26 | 117.35 | 111.45 |
| 7 | O | 521 | LEU | CA-C-N | 5.26 | 127.33 | 120.28 |
| 7 | O | 521 | LEU | C-N-CA | 5.26 | 127.33 | 120.28 |
| 8 | P | 450 | THR | CA-C-N | 5.26 | 127.59 | 120.38 |
| 8 | P | 450 | THR | C-N-CA | 5.26 | 127.59 | 120.38 |
| 8 | P | 852 | PHE | CA-CB-CG | 5.26 | 119.06 | 113.80 |
| 8 | P | 865 | ASN | N-CA-C | -5.26 | 99.71 | 108.34 |
| 9 | R | 215 | TYR | CA-C-N | 5.26 | 127.33 | 120.28 |
| 9 | R | 215 | TYR | C-N-CA | 5.26 | 127.33 | 120.28 |
| 9 | S | 164 | GLN | CA-C-O | 5.26 | 126.00 | 120.42 |
| 12 | u | 324 | LEU | N-CA-C | -5.26 | 100.82 | 109.40 |
| 19 | m | 397 | ASP | N-CA-CB | 5.26 | 117.86 | 110.12 |
| 20 | n | 855 | LYS | N-CA-C | -5.26 | 106.72 | 112.72 |
| 17 | d | 149 | ASN | N-CA-C | -5.26 | 107.40 | 113.88 |
| 14 | a | 393 | HIS | CB-CA-C | 5.26 | 119.69 | 110.64 |
| 7 | O | 1406 | TYR | N-CA-C | -5.26 | 104.46 | 112.04 |
| 21 | o | 86 | PHE | CA-C-N | 5.26 | 130.58 | 123.11 |
| 21 | o | 86 | PHE | C-N-CA | 5.26 | 130.58 | 123.11 |
| 21 | p | 70 | THR | CA-C-O | 5.26 | 128.02 | 121.81 |
| 8 | N | 1202 | SER | N-CA-CB | 5.26 | 118.45 | 110.14 |
| 7 | O | 675 | LEU | CA-C-N | 5.26 | 127.33 | 120.28 |
| 7 | O | 675 | LEU | C-N-CA | 5.26 | 127.33 | 120.28 |
| 7 | O | 1054 | SER | N-CA-C | 5.26 | 117.01 | 111.28 |
| 9 | T | 248 | THR | CA-C-N | 5.26 | 127.33 | 120.28 |
| 9 | T | 248 | THR | C-N-CA | 5.26 | 127.33 | 120.28 |
| 9 | T | 319 | SER | N-CA-C | -5.26 | 99.59 | 110.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 12 | v | 146 | LYS | N-CA-C | -5.26 | 102.27 | 110.42 |
| 15 | i | 200 | ASN | CA-C-N | 5.26 | 127.76 | 120.29 |
| 15 | i | 200 | ASN | C-N-CA | 5.26 | 127.76 | 120.29 |
| 17 | k | 16 | VAL | O-C-N | 5.26 | 128.73 | 123.10 |
| 20 | n | 1114 | TYR | CA-C-N | 5.26 | 130.35 | 121.14 |
| 20 | n | 1114 | TYR | C-N-CA | 5.26 | 130.35 | 121.14 |
| 15 | b | 657 | TYR | N-CA-C | -5.26 | 102.73 | 110.52 |
| 1 | 0 | 231 | LEU | CA-C-O | 5.26 | 125.93 | 120.30 |
| 2 | 1 | 928 | LEU | CA-C-O | 5.26 | 124.31 | 118.52 |
| 7 | M | 754 | ASP | CA-C-N | 5.26 | 127.59 | 120.65 |
| 7 | M | 754 | ASP | C-N-CA | 5.26 | 127.59 | 120.65 |
| 8 | P | 1334 | ASP | CA-C-O | -5.26 | 115.31 | 121.10 |
| 9 | R | 413 | LYS | O-C-N | -5.26 | 115.20 | 122.46 |
| 9 | R | 700 | ALA | N-CA-C | 5.26 | 117.42 | 111.11 |
| 2 | Z | 810 | SER | N-CA-CB | 5.26 | 118.32 | 110.22 |
| 12 | u | 70 | HIS | CE1-NE2-CD2 | -5.26 | 103.74 | 109.00 |
| 12 | u | 702 | LEU | N-CA-CB | 5.26 | 117.85 | 110.12 |
| 13 | w | 1116 | ASN | CB-CA-C | 5.26 | 120.09 | 110.10 |
| 4 | z | 657 | GLN | CA-C-N | 5.26 | 127.28 | 120.44 |
| 4 | z | 657 | GLN | C-N-CA | 5.26 | 127.28 | 120.44 |
| 15 | i | 582 | GLU | N-CA-C | -5.26 | 102.41 | 110.14 |
| 19 | m | 333 | SER | O-C-N | 5.26 | 127.69 | 122.12 |
| 17 | d | 239 | GLU | N-CA-C | 5.26 | 116.70 | 111.07 |
| 20 | g | 893 | ASP | N-CA-C | -5.26 | 99.60 | 110.80 |
| 4 | A | 717 | LYS | O-C-N | -5.26 | 115.80 | 122.27 |
| 4 | G | 646 | ASN | O-C-N | 5.26 | 128.14 | 122.15 |
| 7 | M | 109 | ARG | CA-C-O | -5.26 | 114.98 | 120.55 |
| 7 | O | 1104 | ASN | CA-CB-CG | 5.26 | 117.86 | 112.60 |
| 8 | P | 1064 | GLU | CA-C-N | 5.26 | 131.50 | 122.09 |
| 8 | P | 1064 | GLU | C-N-CA | 5.26 | 131.50 | 122.09 |
| 9 | T | 426 | PRO | O-C-N | -5.26 | 114.65 | 122.12 |
| 16 | j | 636 | SER | N-CA-CB | 5.26 | 119.38 | 110.49 |
| 19 | m | 608 | SER | CA-C-N | 5.26 | 129.41 | 122.42 |
| 19 | m | 608 | SER | C-N-CA | 5.26 | 129.41 | 122.42 |
| 20 | n | 100 | ASN | CA-CB-CG | 5.26 | 117.86 | 112.60 |
| 14 | a | 507 | PHE | N-CA-C | 5.26 | 117.01 | 111.28 |
| 2 | 1 | 269 | THR | CA-C-N | 5.26 | 131.71 | 121.41 |
| 2 | 1 | 269 | THR | C-N-CA | 5.26 | 131.71 | 121.41 |
| 4 | G | 801 | PHE | CA-CB-CG | -5.26 | 108.54 | 113.80 |
| 7 | M | 118 | SER | N-CA-CB | 5.26 | 117.77 | 109.94 |
| 7 | M | 324 | ILE | CA-CB-CG1 | 5.26 | 119.34 | 110.40 |
| 7 | M | 1531 | THR | N-CA-CB | 5.26 | 117.63 | 110.01 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 973 | THR | CB-CA-C | 5.26 | 120.88 | 110.42 |
| 8 | P | 840 | LEU | N-CA-CB | 5.26 | 119.12 | 110.39 |
| 8 | P | 1043 | LEU | N-CA-CB | 5.26 | 119.65 | 110.98 |
| 12 | v | 590 | ALA | CA-C-N | 5.26 | 127.32 | 120.28 |
| 12 | v | 590 | ALA | C-N-CA | 5.26 | 127.32 | 120.28 |
| 13 | w | 1230 | GLU | CA-C-N | 5.26 | 127.27 | 120.44 |
| 13 | w | 1230 | GLU | C-N-CA | 5.26 | 127.27 | 120.44 |
| 13 | x | 1396 | LEU | O-C-N | 5.26 | 127.69 | 122.12 |
| 4 | y | 722 | LEU | O-C-N | 5.26 | 127.69 | 122.12 |
| 14 | h | 430 | ASN | CA-CB-CG | 5.26 | 117.86 | 112.60 |
| 17 | k | 91 | GLN | O-C-N | -5.26 | 115.16 | 122.41 |
| 17 | d | 29 | SER | N-CA-CB | 5.26 | 118.57 | 110.21 |
| 20 | g | 322 | ASP | CA-CB-CG | 5.26 | 117.86 | 112.60 |
| 2 | 1 | 929 | ASP | N-CA-CB | 5.25 | 118.19 | 110.57 |
| 7 | M | 1276 | ASP | CA-C-O | 5.25 | 126.12 | 120.55 |
| 7 | O | 1028 | VAL | CA-C-N | 5.25 | 127.75 | 120.29 |
| 7 | O | 1028 | VAL | C-N-CA | 5.25 | 127.75 | 120.29 |
| 7 | O | 1536 | SER | N-CA-CB | 5.25 | 117.63 | 110.01 |
| 8 | P | 727 | ASN | N-CA-CB | 5.25 | 118.76 | 110.56 |
| 11 | X | 396 | ALA | CA-C-N | 5.25 | 131.71 | 121.41 |
| 11 | X | 396 | ALA | C-N-CA | 5.25 | 131.71 | 121.41 |
| 1 | Y | 290 | GLY | CA-C-N | 5.25 | 131.58 | 121.54 |
| 1 | Y | 290 | GLY | C-N-CA | 5.25 | 131.58 | 121.54 |
| 20 | n | 875 | PHE | CA-C-O | -5.25 | 114.85 | 120.42 |
| 20 | g | 435 | SER | N-CA-CB | 5.25 | 119.37 | 110.49 |
| 2 | 1 | 255 | VAL | O-C-N | -5.25 | 117.37 | 122.99 |
| 5 | E | 475 | SER | N-CA-C | -5.25 | 105.63 | 111.36 |
| 4 | J | 816 | LYS | N-CA-C | 5.25 | 119.40 | 112.89 |
| 9 | T | 469 | TYR | CA-CB-CG | -5.25 | 104.44 | 113.90 |
| 1 | Y | 1406 | HIS | CG-CD2-NE2 | 5.25 | 112.45 | 107.20 |
| 12 | u | 681 | ASP | N-CA-C | 5.25 | 116.69 | 111.07 |
| 14 | h | 708 | ASN | CA-CB-CG | -5.25 | 107.35 | 112.60 |
| 14 | h | 884 | GLU | N-CA-CB | 5.25 | 119.37 | 110.49 |
| 19 | m | 398 | ILE | CB-CA-C | -5.25 | 104.97 | 112.22 |
| 1 | 0 | 1381 | SER | N-CA-CB | 5.25 | 119.36 | 110.49 |
| 2 | 1 | 796 | ASN | CA-C-N | 5.25 | 127.32 | 120.28 |
| 2 | 1 | 796 | ASN | C-N-CA | 5.25 | 127.32 | 120.28 |
| 6 | C | 403 | THR | N-CA-C | 5.25 | 119.31 | 113.01 |
| 5 | H | 394 | THR | N-CA-C | -5.25 | 106.20 | 113.18 |
| 6 | I | 401 | ILE | CB-CA-C | -5.25 | 104.97 | 112.22 |
| 8 | N | 268 | THR | CA-CB-CG2 | -5.25 | 101.57 | 110.50 |
| 8 | N | 1174 | ASN | CB-CA-C | -5.25 | 99.01 | 109.99 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 1318 | LEU | CB-CA-C | -5.25 | 100.59 | 110.67 |
| 7 | O | 710 | LEU | CA-C-N | 5.25 | 127.27 | 120.44 |
| 7 | O | 710 | LEU | C-N-CA | 5.25 | 127.27 | 120.44 |
| 2 | Z | 97 | PHE | CA-CB-CG | -5.25 | 108.55 | 113.80 |
| 12 | v | 340 | ASP | N-CA-C | -5.25 | 101.22 | 109.25 |
| 14 | h | 639 | LEU | N-CA-C | -5.25 | 107.00 | 113.41 |
| 19 | m | 235 | GLN | N-CA-C | 5.25 | 118.41 | 110.64 |
| 19 | m | 716 | ASP | N-CA-C | -5.25 | 105.61 | 112.23 |
| 20 | n | 921 | GLU | N-CA-C | 5.25 | 117.91 | 111.82 |
| 15 | b | 644 | GLN | CA-C-O | 5.25 | 125.79 | 119.59 |
| 19 | f | 289 | HIS | CG-CD2-NE2 | 5.25 | 112.45 | 107.20 |
| 14 | a | 168 | TYR | CA-C-N | -5.25 | 116.38 | 122.63 |
| 14 | a | 168 | TYR | C-N-CA | -5.25 | 116.38 | 122.63 |
| 1 | 0 | 911 | ASN | CA-C-N | 5.25 | 128.28 | 122.77 |
| 1 | 0 | 911 | ASN | C-N-CA | 5.25 | 128.28 | 122.77 |
| 7 | O | 1547 | ILE | CA-C-O | -5.25 | 115.61 | 121.17 |
| 9 | R | 728 | PHE | CA-C-O | -5.25 | 114.98 | 120.55 |
| 2 | Z | 1070 | ASP | CA-C-N | 5.25 | 128.29 | 120.31 |
| 2 | Z | 1070 | ASP | C-N-CA | 5.25 | 128.29 | 120.31 |
| 12 | u | 637 | GLN | N-CA-C | 5.25 | 117.00 | 111.28 |
| 12 | v | 411 | GLU | O-C-N | 5.25 | 129.68 | 123.33 |
| 20 | n | 435 | SER | N-CA-CB | 5.25 | 119.36 | 110.49 |
| 20 | g | 524 | GLN | CB-CG-CD | -5.25 | 103.67 | 112.60 |
| 4 | G | 756 | ASN | CA-C-N | 5.25 | 128.29 | 120.31 |
| 4 | G | 756 | ASN | C-N-CA | 5.25 | 128.29 | 120.31 |
| 5 | H | 508 | LYS | CA-C-O | 5.25 | 126.11 | 120.55 |
| 8 | N | 755 | ASN | N-CA-C | -5.25 | 105.59 | 112.41 |
| 8 | N | 934 | GLU | CB-CG-CD | -5.25 | 103.68 | 112.60 |
| 9 | T | 644 | TYR | CA-C-N | 5.25 | 127.84 | 120.28 |
| 9 | T | 644 | TYR | C-N-CA | 5.25 | 127.84 | 120.28 |
| 15 | i | 457 | TYR | CA-C-O | 5.25 | 126.05 | 119.59 |
| 16 | j | 317 | HIS | CA-CB-CG | 5.25 | 119.05 | 113.80 |
| 15 | b | 553 | ILE | CB-CA-C | -5.25 | 106.15 | 112.19 |
| 1 | 0 | 393 | ILE | CA-C-N | 5.25 | 134.60 | 121.80 |
| 1 | 0 | 393 | ILE | C-N-CA | 5.25 | 134.60 | 121.80 |
| 4 | D | 646 | ASN | CA-C-N | 5.25 | 129.48 | 120.72 |
| 4 | D | 646 | ASN | C-N-CA | 5.25 | 129.48 | 120.72 |
| 7 | M | 117 | VAL | CA-C-N | 5.25 | 127.62 | 120.54 |
| 7 | M | 117 | VAL | C-N-CA | 5.25 | 127.62 | 120.54 |
| 7 | O | 950 | GLU | CB-CG-CD | -5.25 | 103.68 | 112.60 |
| 8 | P | 948 | LEU | N-CA-C | -5.25 | 106.90 | 113.72 |
| 8 | P | 1171 | ARG | NH1-CZ-NH2 | 5.25 | 126.12 | 119.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | R | 24 | GLU | N-CA-CB | 5.25 | 117.92 | 110.16 |
| 9 | S | 794 | TYR | N-CA-C | -5.25 | 98.68 | 108.02 |
| 10 | W | 251 | HIS | CE1-NE2-CD2 | -5.25 | 103.75 | 109.00 |
| 1 | Y | 156 | ILE | CA-C-O | -5.25 | 115.14 | 119.76 |
| 18 | e | 303 | HIS | CE1-NE2-CD2 | -5.25 | 103.75 | 109.00 |
| 6 | C | 452 | ASP | CA-CB-CG | 5.25 | 117.84 | 112.60 |
| 5 | E | 299 | TRP | N-CA-CB | 5.25 | 119.36 | 110.49 |
| 4 | G | 800 | HIS | CE1-NE2-CD2 | -5.25 | 103.75 | 109.00 |
| 7 | O | 610 | SER | O-C-N | -5.25 | 116.56 | 122.12 |
| 8 | P | 390 | ILE | CB-CA-C | -5.25 | 105.74 | 110.88 |
| 13 | x | 1287 | ASN | N-CA-C | -5.25 | 105.00 | 111.40 |
| 17 | k | 12 | ILE | CA-C-O | -5.25 | 114.87 | 120.85 |
| 21 | s | 55 | ASN | OD1-CG-ND2 | -5.25 | 117.36 | 122.60 |
| 17 | d | 105 | VAL | N-CA-CB | 5.25 | 120.08 | 111.58 |
| 5 | B | 302 | ASN | CA-CB-CG | 5.24 | 117.84 | 112.60 |
| 5 | B | 515 | ASN | CB-CG-OD1 | -5.24 | 110.31 | 120.80 |
| 7 | M | 1108 | ARG | N-CA-C | 5.24 | 117.74 | 111.71 |
| 7 | M | 1313 | ILE | N-CA-CB | 5.24 | 116.12 | 110.62 |
| 7 | M | 1663 | LEU | N-CA-C | -5.24 | 99.63 | 110.80 |
| 8 | N | 418 | ASN | N-CA-C | 5.24 | 117.45 | 110.53 |
| 7 | O | 70 | PHE | N-CA-CB | -5.24 | 102.23 | 110.30 |
| 7 | O | 711 | GLN | CA-C-N | 5.24 | 127.26 | 120.44 |
| 7 | O | 711 | GLN | C-N-CA | 5.24 | 127.26 | 120.44 |
| 8 | P | 601 | VAL | CA-C-N | 5.24 | 131.41 | 121.97 |
| 8 | P | 601 | VAL | C-N-CA | 5.24 | 131.41 | 121.97 |
| 9 | Q | 352 | VAL | N-CA-CB | -5.24 | 105.54 | 112.36 |
| 9 | S | 623 | ILE | N-CA-CB | 5.24 | 117.28 | 110.57 |
| 19 | m | 120 | TRP | O-C-N | 5.24 | 127.68 | 122.12 |
| 19 | m | 579 | GLN | N-CA-CB | 5.24 | 117.61 | 110.01 |
| 16 | c | 277 | GLY | CA-C-N | 5.24 | 124.56 | 118.85 |
| 16 | c | 277 | GLY | C-N-CA | 5.24 | 124.56 | 118.85 |
| 16 | c | 374 | GLU | N-CA-C | -5.24 | 105.62 | 112.23 |
| 17 | d | 63 | HIS | CA-C-O | -5.24 | 115.24 | 120.96 |
| 19 | f | 55 | ASN | N-CA-CB | 5.24 | 118.41 | 110.28 |
| 6 | F | 301 | HIS | N-CA-C | -5.24 | 106.39 | 112.89 |
| 6 | L | 347 | THR | CA-C-N | 5.24 | 127.25 | 120.44 |
| 6 | L | 347 | THR | C-N-CA | 5.24 | 127.25 | 120.44 |
| 7 | M | 673 | SER | N-CA-CB | 5.24 | 117.83 | 110.12 |
| 2 | 1 | 1171 | ASP | N-CA-CB | 5.24 | 119.09 | 110.39 |
| 2 | 1 | 1290 | ASN | CB-CA-C | -5.24 | 99.82 | 109.15 |
| 5 | H | 406 | VAL | N-CA-CB | 5.24 | 120.26 | 110.77 |
| 7 | M | 819 | VAL | N-CA-C | -5.24 | 106.77 | 113.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 448 | ILE | N-CA-C | -5.24 | 101.97 | 108.89 |
| 8 | N | 664 | LEU | N-CA-CB | 5.24 | 118.23 | 110.53 |
| 9 | S | 786 | ILE | CA-C-N | 5.24 | 127.73 | 120.29 |
| 9 | S | 786 | ILE | C-N-CA | 5.24 | 127.73 | 120.29 |
| 2 | Z | 486 | GLN | N-CA-C | -5.24 | 106.20 | 112.59 |
| 2 | Z | 1279 | THR | N-CA-C | -5.24 | 100.86 | 109.40 |
| 14 | h | 343 | ASN | O-C-N | 5.24 | 126.72 | 121.85 |
| 14 | h | 940 | VAL | CB-CA-C | 5.24 | 119.91 | 110.48 |
| 20 | n | 950 | ASN | CA-C-N | 5.24 | 128.28 | 120.31 |
| 20 | n | 950 | ASN | C-N-CA | 5.24 | 128.28 | 120.31 |
| 18 | e | 203 | HIS | CE1-NE2-CD2 | -5.24 | 103.76 | 109.00 |
| 19 | f | 349 | SER | CB-CA-C | -5.24 | 102.09 | 110.79 |
| 20 | g | 511 | PRO | CA-C-N | -5.24 | 116.33 | 122.93 |
| 20 | g | 511 | PRO | C-N-CA | -5.24 | 116.33 | 122.93 |
| 14 | a | 574 | LEU | CA-C-O | 5.24 | 126.83 | 121.07 |
| 14 | a | 734 | HIS | CA-CB-CG | -5.24 | 108.56 | 113.80 |
| 1 | 0 | 1276 | LEU | N-CA-C | 5.24 | 117.82 | 109.96 |
| 7 | M | 1240 | HIS | CA-CB-CG | 5.24 | 119.04 | 113.80 |
| 7 | M | 1249 | ILE | CA-C-O | -5.24 | 115.50 | 120.95 |
| 8 | P | 661 | MET | CA-C-N | 5.24 | 131.86 | 122.38 |
| 8 | P | 661 | MET | C-N-CA | 5.24 | 131.86 | 122.38 |
| 8 | P | 1066 | VAL | N-CA-CB | 5.24 | 117.67 | 110.54 |
| 9 | Q | 231 | ASN | N-CA-CB | 5.24 | 119.84 | 111.56 |
| 9 | Q | 474 | PHE | N-CA-C | -5.24 | 106.91 | 113.72 |
| 2 | Z | 709 | PHE | CA-C-N | 5.24 | 127.25 | 120.44 |
| 2 | Z | 709 | PHE | C-N-CA | 5.24 | 127.25 | 120.44 |
| 12 | u | 629 | LYS | N-CA-CB | 5.24 | 117.82 | 110.12 |
| 4 | y | 639 | ASP | CA-C-N | 5.24 | 127.30 | 120.28 |
| 4 | y | 639 | ASP | C-N-CA | 5.24 | 127.30 | 120.28 |
| 19 | m | 554 | ASN | CA-C-N | 5.24 | 129.34 | 120.64 |
| 19 | m | 554 | ASN | C-N-CA | 5.24 | 129.34 | 120.64 |
| 2 | 1 | 487 | LYS | CA-C-O | 5.24 | 126.09 | 120.70 |
| 2 | 1 | 619 | GLU | N-CA-C | -5.24 | 107.06 | 113.50 |
| 2 | 1 | 1124 | ASP | N-CA-C | -5.24 | 106.28 | 113.30 |
| 7 | M | 352 | ILE | N-CA-C | -5.24 | 101.38 | 107.61 |
| 9 | R | 124 | SER | CA-C-O | -5.24 | 115.31 | 121.07 |
| 12 | u | 212 | LEU | N-CA-C | -5.24 | 102.17 | 108.25 |
| 4 | y | 660 | LYS | O-C-N | 5.24 | 127.67 | 122.12 |
| 20 | n | 517 | PRO | N-CA-CB | 5.24 | 108.16 | 103.08 |
| 18 | e | 41 | ASP | CA-CB-CG | 5.24 | 117.84 | 112.60 |
| 20 | g | 250 | LYS | O-C-N | -5.24 | 116.24 | 120.38 |
| 1 | 0 | 652 | TYR | CA-C-O | -5.24 | 115.43 | 121.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 896 | MET | CA-C-N | 5.24 | 127.63 | 120.46 |
| 1 | 0 | 896 | MET | C-N-CA | 5.24 | 127.63 | 120.46 |
| 6 | L | 358 | LEU | N-CA-C | -5.24 | 105.88 | 113.21 |
| 7 | M | 478 | LEU | CA-C-O | -5.24 | 115.00 | 120.55 |
| 7 | M | 1089 | ASN | CA-C-N | 5.24 | 126.39 | 119.84 |
| 7 | M | 1089 | ASN | C-N-CA | 5.24 | 126.39 | 119.84 |
| 7 | O | 1037 | ASN | CA-C-O | -5.24 | 113.02 | 120.51 |
| 7 | O | 1623 | VAL | CB-CA-C | -5.24 | 104.27 | 111.65 |
| 8 | P | 1031 | LYS | N-CA-C | -5.24 | 106.68 | 114.64 |
| 8 | P | 1170 | ASP | CA-CB-CG | 5.24 | 117.83 | 112.60 |
| 9 | Q | 672 | GLN | N-CA-CB | 5.24 | 116.19 | 111.27 |
| 9 | T | 225 | SER | CA-CB-OG | 5.24 | 121.57 | 111.10 |
| 1 | Y | 911 | ASN | CB-CA-C | -5.24 | 100.92 | 109.56 |
| 1 | Y | 1227 | ILE | CA-C-O | 5.24 | 127.01 | 121.67 |
| 2 | Z | 604 | LEU | N-CA-C | -5.24 | 101.17 | 109.96 |
| 14 | h | 352 | ILE | CA-C-N | 5.24 | 129.12 | 122.37 |
| 14 | h | 352 | ILE | C-N-CA | 5.24 | 129.12 | 122.37 |
| 21 | q | 60 | ILE | CB-CG1-CD1 | 5.24 | 124.80 | 113.80 |
| 16 | c | 376 | GLU | CA-C-N | 5.24 | 130.77 | 122.60 |
| 16 | c | 376 | GLU | C-N-CA | 5.24 | 130.77 | 122.60 |
| 20 | g | 832 | TYR | CA-C-N | 5.24 | 129.84 | 122.09 |
| 20 | g | 832 | TYR | C-N-CA | 5.24 | 129.84 | 122.09 |
| 20 | g | 1151 | GLU | CA-C-O | 5.24 | 124.28 | 118.52 |
| 1 | 0 | 956 | ASN | OD1-CG-ND2 | 5.23 | 127.83 | 122.60 |
| 7 | M | 154 | GLN | N-CA-CB | 5.23 | 117.74 | 109.94 |
| 8 | P | 109 | ARG | NH1-CZ-NH2 | 5.23 | 126.10 | 119.30 |
| 8 | P | 721 | GLU | CB-CA-C | -5.23 | 103.86 | 111.14 |
| 9 | Q | 704 | ARG | NE-CZ-NH2 | -5.23 | 114.49 | 119.20 |
| 9 | R | 371 | PHE | CA-C-N | 5.23 | 127.29 | 120.28 |
| 9 | R | 371 | PHE | C-N-CA | 5.23 | 127.29 | 120.28 |
| 9 | T | 262 | SER | O-C-N | -5.23 | 116.10 | 122.22 |
| 1 | Y | 1344 | PHE | CB-CA-C | -5.23 | 101.95 | 110.85 |
| 15 | i | 493 | ALA | N-CA-C | -5.23 | 106.40 | 112.89 |
| 18 | e | 155 | LYS | N-CA-CB | 5.23 | 118.18 | 109.60 |
| 1 | 0 | 140 | ASN | CA-CB-CG | -5.23 | 107.37 | 112.60 |
| 6 | I | 301 | HIS | CE1-NE2-CD2 | -5.23 | 103.77 | 109.00 |
| 7 | M | 82 | ASN | CA-CB-CG | 5.23 | 117.83 | 112.60 |
| 7 | M | 140 | LEU | N-CA-C | 5.23 | 116.98 | 111.28 |
| 7 | M | 1382 | TYR | N-CA-CB | 5.23 | 117.55 | 109.91 |
| 8 | N | 356 | HIS | CG-CD2-NE2 | 5.23 | 112.43 | 107.20 |
| 8 | N | 1429 | HIS | CG-CD2-NE2 | 5.23 | 112.43 | 107.20 |
| 8 | P | 362 | LEU | O-C-N | -5.23 | 116.68 | 122.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1335 | GLN | N-CA-CB | 5.23 | 119.33 | 110.49 |
| 9 | R | 132 | ALA | N-CA-C | 5.23 | 116.98 | 111.28 |
| 10 | W | 310 | GLY | CA-C-N | 5.23 | 127.56 | 120.44 |
| 10 | W | 310 | GLY | C-N-CA | 5.23 | 127.56 | 120.44 |
| 10 | W | 354 | ALA | CA-C-O | 5.23 | 124.94 | 119.03 |
| 12 | u | 650 | SER | CA-C-N | 5.23 | 127.81 | 120.28 |
| 12 | u | 650 | SER | C-N-CA | 5.23 | 127.81 | 120.28 |
| 14 | h | 558 | LEU | CA-C-N | 5.23 | 131.53 | 121.54 |
| 14 | h | 558 | LEU | C-N-CA | 5.23 | 131.53 | 121.54 |
| 21 | s | 28 | SER | CA-C-N | 5.23 | 127.29 | 120.28 |
| 21 | s | 28 | SER | C-N-CA | 5.23 | 127.29 | 120.28 |
| 20 | g | 356 | CYS | N-CA-C | -5.23 | 101.31 | 108.38 |
| 20 | g | 991 | LEU | CA-C-O | 5.23 | 127.08 | 120.65 |
| 14 | a | 493 | TRP | N-CA-C | -5.23 | 105.56 | 112.94 |
| 1 | 0 | 1412 | ILE | N-CA-C | -5.23 | 105.50 | 110.42 |
| 2 | 1 | 1191 | LEU | CA-C-N | 5.23 | 127.29 | 120.28 |
| 2 | 1 | 1191 | LEU | C-N-CA | 5.23 | 127.29 | 120.28 |
| 5 | B | 337 | GLN | CA-C-N | 5.23 | 127.81 | 120.28 |
| 5 | B | 337 | GLN | C-N-CA | 5.23 | 127.81 | 120.28 |
| 5 | B | 512 | ILE | CA-C-N | 5.23 | 127.72 | 120.29 |
| 5 | B | 512 | ILE | C-N-CA | 5.23 | 127.72 | 120.29 |
| 7 | M | 1360 | LEU | CA-C-O | 5.23 | 125.76 | 119.59 |
| 8 | N | 935 | VAL | CB-CA-C | -5.23 | 106.40 | 111.05 |
| 8 | P | 1163 | LEU | N-CA-C | -5.23 | 106.29 | 113.30 |
| 1 | Y | 834 | ILE | CA-CB-CG1 | 5.23 | 119.29 | 110.40 |
| 1 | Y | 1176 | ASP | CA-C-N | 5.23 | 128.39 | 120.75 |
| 1 | Y | 1176 | ASP | C-N-CA | 5.23 | 128.39 | 120.75 |
| 15 | b | 452 | GLU | CB-CG-CD | -5.23 | 103.71 | 112.60 |
| 19 | f | 578 | ASP | CB-CG-OD1 | 5.23 | 130.43 | 118.40 |
| 14 | a | 782 | TYR | O-C-N | -5.23 | 116.27 | 121.19 |
| 2 | 1 | 452 | LYS | CA-C-O | -5.23 | 115.33 | 120.98 |
| 7 | M | 1299 | ASN | CB-CA-C | -5.23 | 102.44 | 110.81 |
| 7 | O | 296 | ARG | NE-CZ-NH2 | -5.23 | 114.49 | 119.20 |
| 9 | S | 565 | GLY | CA-C-N | 5.23 | 126.38 | 119.84 |
| 9 | S | 565 | GLY | C-N-CA | 5.23 | 126.38 | 119.84 |
| 12 | v | 55 | HIS | ND1-CE1-NE2 | 5.23 | 113.63 | 108.40 |
| 13 | x | 1229 | MET | N-CA-C | -5.23 | 106.85 | 113.18 |
| 14 | h | 676 | ALA | N-CA-C | 5.23 | 116.67 | 111.07 |
| 14 | h | 844 | CYS | N-CA-C | -5.23 | 106.58 | 113.17 |
| 19 | f | 186 | GLU | CA-C-N | 5.23 | 127.72 | 120.29 |
| 19 | f | 186 | GLU | C-N-CA | 5.23 | 127.72 | 120.29 |
| 2 | 1 | 810 | SER | CA-C-N | 5.23 | 127.81 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 810 | SER | C-N-CA | 5.23 | 127.81 | 120.28 |
| 2 | 1 | 1108 | PHE | CA-CB-CG | -5.23 | 108.57 | 113.80 |
| 4 | A | 774 | ASN | CA-C-N | 5.23 | 131.18 | 122.66 |
| 4 | A | 774 | ASN | C-N-CA | 5.23 | 131.18 | 122.66 |
| 6 | C | 405 | LEU | N-CA-C | -5.23 | 105.63 | 113.89 |
| 5 | E | 462 | ARG | NE-CZ-NH1 | 5.23 | 126.73 | 121.50 |
| 6 | I | 343 | ASP | N-CA-C | -5.23 | 106.49 | 112.92 |
| 4 | J | 753 | GLU | N-CA-C | -5.23 | 106.58 | 113.17 |
| 7 | M | 909 | LEU | CA-C-N | 5.23 | 128.25 | 120.31 |
| 7 | M | 909 | LEU | C-N-CA | 5.23 | 128.25 | 120.31 |
| 8 | P | 1318 | LEU | N-CA-C | 5.23 | 117.72 | 111.71 |
| 11 | V | 290 | HIS | CA-C-O | 5.23 | 125.47 | 119.35 |
| 1 | Y | 388 | GLU | N-CA-C | -5.23 | 102.26 | 110.36 |
| 1 | Y | 1182 | ILE | CB-CA-C | -5.23 | 105.84 | 111.59 |
| 1 | Y | 1265 | ALA | CA-C-N | 5.23 | 127.60 | 120.54 |
| 1 | Y | 1265 | ALA | C-N-CA | 5.23 | 127.60 | 120.54 |
| 2 | Z | 950 | VAL | CA-CB-CG2 | 5.23 | 119.29 | 110.40 |
| 13 | x | 1118 | ALA | O-C-N | -5.23 | 117.77 | 123.26 |
| 14 | h | 740 | PHE | CA-CB-CG | -5.23 | 108.57 | 113.80 |
| 14 | h | 987 | MET | CA-C-N | 5.23 | 127.28 | 120.28 |
| 14 | h | 987 | MET | C-N-CA | 5.23 | 127.28 | 120.28 |
| 15 | i | 88 | TYR | CA-CB-CG | -5.23 | 104.49 | 113.90 |
| 19 | m | 393 | ALA | O-C-N | 5.23 | 127.66 | 122.12 |
| 20 | n | 82 | ASN | N-CA-CB | 5.23 | 119.31 | 110.79 |
| 20 | n | 599 | LYS | CA-C-N | 5.23 | 127.24 | 120.44 |
| 20 | n | 599 | LYS | C-N-CA | 5.23 | 127.24 | 120.44 |
| 20 | n | 933 | LEU | N-CA-C | -5.23 | 101.75 | 110.17 |
| 15 | b | 521 | TRP | CD2-CE2-CZ2 | 5.23 | 127.63 | 122.40 |
| 1 | 0 | 1054 | MET | N-CA-C | -5.23 | 105.26 | 111.69 |
| 4 | D | 789 | GLU | N-CA-C | -5.23 | 107.57 | 114.31 |
| 7 | M | 1608 | ILE | O-C-N | 5.23 | 127.03 | 121.91 |
| 8 | N | 672 | VAL | CA-C-N | 5.23 | 127.28 | 120.28 |
| 8 | N | 672 | VAL | C-N-CA | 5.23 | 127.28 | 120.28 |
| 9 | T | 825 | PRO | CA-C-N | 5.23 | 127.59 | 120.54 |
| 9 | T | 825 | PRO | C-N-CA | 5.23 | 127.59 | 120.54 |
| 1 | Y | 1222 | THR | N-CA-CB | 5.23 | 119.92 | 110.83 |
| 12 | u | 358 | ARG | N-CA-CB | 5.23 | 121.24 | 111.52 |
| 14 | h | 517 | ALA | N-CA-CB | 5.23 | 117.65 | 110.07 |
| 20 | n | 1134 | HIS | ND1-CE1-NE2 | 5.23 | 113.63 | 108.40 |
| 20 | g | 591 | PHE | CA-C-O | -5.23 | 113.96 | 119.97 |
| 5 | H | 463 | LEU | CA-C-N | 5.22 | 127.28 | 120.28 |
| 5 | H | 463 | LEU | C-N-CA | 5.22 | 127.28 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 125 | HIS | CB-CG-CD2 | -5.22 | 124.41 | 131.20 |
| 8 | P | 1090 | THR | N-CA-CB | 5.22 | 117.80 | 110.12 |
| 9 | T | 740 | GLU | N-CA-CB | 5.22 | 117.64 | 110.07 |
| 15 | i | 302 | THR | CA-CB-OG1 | 5.22 | 117.44 | 109.60 |
| 19 | f | 306 | ASN | N-CA-C | 5.22 | 118.92 | 111.92 |
| 20 | g | 91 | ASP | N-CA-C | -5.22 | 101.36 | 109.72 |
| 20 | g | 365 | THR | CB-CA-C | -5.22 | 102.19 | 110.81 |
| 14 | a | 220 | TYR | CA-C-O | -5.22 | 115.87 | 121.56 |
| 2 | 1 | 350 | SER | N-CA-C | -5.22 | 104.58 | 112.99 |
| 2 | 1 | 1279 | THR | N-CA-C | -5.22 | 100.98 | 108.60 |
| 5 | E | 405 | ASN | CA-CB-CG | 5.22 | 117.82 | 112.60 |
| 5 | E | 460 | TRP | CA-C-N | 5.22 | 127.71 | 120.29 |
| 5 | E | 460 | TRP | C-N-CA | 5.22 | 127.71 | 120.29 |
| 6 | L | 372 | PHE | CA-C-O | -5.22 | 114.89 | 120.42 |
| 8 | N | 839 | ILE | CA-CB-CG1 | 5.22 | 119.28 | 110.40 |
| 7 | O | 1258 | HIS | CG-CD2-NE2 | 5.22 | 112.42 | 107.20 |
| 8 | P | 1533 | ILE | N-CA-C | 5.22 | 115.43 | 110.42 |
| 9 | Q | 586 | PHE | N-CA-CB | -5.22 | 102.94 | 110.56 |
| 9 | R | 130 | ASN | CA-C-N | 5.22 | 125.89 | 119.99 |
| 9 | R | 130 | ASN | C-N-CA | 5.22 | 125.89 | 119.99 |
| 1 | Y | 124 | ARG | O-C-N | -5.22 | 116.20 | 122.15 |
| 2 | Z | 1112 | ALA | CA-C-O | 5.22 | 125.95 | 120.42 |
| 12 | v | 531 | ILE | N-CA-C | -5.22 | 105.45 | 110.72 |
| 15 | b | 473 | LEU | N-CA-C | -5.22 | 107.08 | 113.50 |
| 16 | c | 578 | PRO | N-CA-CB | 5.22 | 108.73 | 103.25 |
| 2 | 1 | 379 | ILE | N-CA-CB | 5.22 | 119.84 | 111.23 |
| 5 | B | 326 | LYS | O-C-N | -5.22 | 116.46 | 121.94 |
| 7 | M | 483 | LEU | CA-C-N | 5.22 | 127.28 | 120.28 |
| 7 | M | 483 | LEU | C-N-CA | 5.22 | 127.28 | 120.28 |
| 16 | c | 268 | LEU | CA-C-N | 5.22 | 129.44 | 120.72 |
| 16 | c | 268 | LEU | C-N-CA | 5.22 | 129.44 | 120.72 |
| 17 | d | 132 | GLU | CA-C-N | 5.22 | 130.75 | 122.60 |
| 17 | d | 132 | GLU | C-N-CA | 5.22 | 130.75 | 122.60 |
| 1 | 0 | 225 | VAL | CA-C-N | 5.22 | 126.36 | 119.84 |
| 1 | 0 | 225 | VAL | C-N-CA | 5.22 | 126.36 | 119.84 |
| 2 | 1 | 719 | LEU | CA-C-O | 5.22 | 125.97 | 119.97 |
| 2 | 1 | 1116 | TYR | CA-C-N | 5.22 | 131.51 | 121.18 |
| 2 | 1 | 1116 | TYR | C-N-CA | 5.22 | 131.51 | 121.18 |
| 4 | J | 809 | ASP | CA-CB-CG | 5.22 | 117.82 | 112.60 |
| 5 | K | 362 | ASN | N-CA-C | 5.22 | 116.65 | 111.07 |
| 5 | K | 537 | TYR | N-CA-CB | 5.22 | 118.82 | 110.73 |
| 7 | M | 438 | VAL | N-CA-CB | 5.22 | 117.64 | 110.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 1336 | ILE | O-C-N | -5.22 | 117.08 | 120.42 |
| 7 | O | 659 | ASN | CA-CB-CG | -5.22 | 107.38 | 112.60 |
| 8 | P | 571 | ASN | OD1-CG-ND2 | 5.22 | 127.82 | 122.60 |
| 8 | P | 1397 | ASN | CB-CG-ND2 | -5.22 | 108.57 | 116.40 |
| 13 | x | 1354 | ALA | CB-CA-C | -5.22 | 102.69 | 110.88 |
| 14 | h | 541 | PRO | N-CA-CB | 5.22 | 107.89 | 103.19 |
| 20 | n | 151 | LEU | N-CA-CB | 5.22 | 119.31 | 110.49 |
| 21 | t | 58 | HIS | CE1-NE2-CD2 | -5.22 | 103.78 | 109.00 |
| 19 | f | 142 | SER | N-CA-CB | 5.22 | 119.31 | 110.49 |
| 20 | g | 1107 | ASN | CA-CB-CG | 5.22 | 117.82 | 112.60 |
| 2 | 1 | 603 | VAL | CA-C-O | -5.22 | 115.23 | 121.28 |
| 4 | D | 750 | THR | N-CA-CB | 5.22 | 118.31 | 110.53 |
| 8 | N | 415 | PHE | CA-C-N | 5.22 | 130.35 | 122.68 |
| 8 | N | 415 | PHE | C-N-CA | 5.22 | 130.35 | 122.68 |
| 9 | Q | 284 | GLN | N-CA-C | 5.22 | 118.81 | 112.23 |
| 1 | Y | 631 | GLN | CB-CA-C | -5.22 | 99.08 | 109.99 |
| 20 | n | 1049 | ASN | CA-C-O | 5.22 | 125.39 | 119.18 |
| 15 | b | 217 | GLY | CA-C-N | 5.22 | 128.61 | 120.68 |
| 15 | b | 217 | GLY | C-N-CA | 5.22 | 128.61 | 120.68 |
| 1 | 0 | 1235 | PHE | CB-CA-C | -5.22 | 100.98 | 110.63 |
| 2 | 1 | 1184 | ASP | CA-CB-CG | 5.22 | 117.82 | 112.60 |
| 6 | F | 276 | GLU | O-C-N | -5.22 | 116.20 | 122.15 |
| 8 | N | 504 | LEU | N-CA-C | -5.22 | 98.89 | 108.02 |
| 8 | P | 688 | THR | CA-CB-OG1 | 5.22 | 117.43 | 109.60 |
| 8 | P | 1643 | ASP | N-CA-C | -5.22 | 105.28 | 110.97 |
| 1 | Y | 980 | SER | N-CA-C | -5.22 | 106.86 | 113.43 |
| 2 | Z | 1107 | HIS | CA-C-N | 5.22 | 127.27 | 120.28 |
| 2 | Z | 1107 | HIS | C-N-CA | 5.22 | 127.27 | 120.28 |
| 12 | v | 254 | GLN | N-CA-CB | 5.22 | 117.79 | 110.12 |
| 13 | w | 1445 | THR | N-CA-CB | 5.22 | 117.88 | 110.16 |
| 18 | l | 328 | VAL | CB-CA-C | -5.22 | 103.55 | 111.69 |
| 20 | n | 869 | ASP | CA-C-N | 5.22 | 127.33 | 120.60 |
| 20 | n | 869 | ASP | C-N-CA | 5.22 | 127.33 | 120.60 |
| 15 | b | 519 | ILE | N-CA-CB | 5.22 | 119.84 | 111.23 |
| 20 | g | 870 | VAL | N-CA-C | 5.22 | 116.57 | 110.62 |
| 1 | 0 | 443 | GLY | N-CA-C | -5.21 | 107.84 | 115.72 |
| 6 | C | 401 | ILE | O-C-N | 5.21 | 127.69 | 121.80 |
| 5 | E | 337 | GLN | CA-C-N | 5.21 | 127.27 | 120.28 |
| 5 | E | 337 | GLN | C-N-CA | 5.21 | 127.27 | 120.28 |
| 6 | F | 298 | THR | N-CA-C | -5.21 | 105.63 | 112.41 |
| 7 | M | 1579 | ASN | O-C-N | 5.21 | 127.44 | 122.07 |
| 8 | N | 190 | GLN | O-C-N | 5.21 | 127.65 | 122.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1311 | LEU | CB-CA-C | -5.21 | 102.69 | 110.88 |
| 9 | Q | 773 | ASN | CA-C-N | 5.21 | 127.69 | 120.29 |
| 9 | Q | 773 | ASN | C-N-CA | 5.21 | 127.69 | 120.29 |
| 9 | R | 816 | TYR | CA-C-O | 5.21 | 125.99 | 120.10 |
| 9 | S | 608 | GLN | CA-C-O | -5.21 | 113.02 | 120.16 |
| 1 | Y | 929 | PHE | N-CA-C | -5.21 | 103.78 | 111.81 |
| 1 | Y | 1051 | VAL | O-C-N | 5.21 | 127.02 | 121.91 |
| 1 | Y | 1282 | ASP | CA-C-N | 5.21 | 129.69 | 121.56 |
| 1 | Y | 1282 | ASP | C-N-CA | 5.21 | 129.69 | 121.56 |
| 1 | Y | 1334 | GLU | N-CA-C | -5.21 | 107.94 | 114.56 |
| 12 | v | 264 | ASN | N-CA-C | -5.21 | 102.06 | 110.14 |
| 13 | x | 1366 | LEU | N-CA-C | 5.21 | 118.90 | 112.54 |
| 15 | i | 278 | CYS | CA-C-N | 5.21 | 127.27 | 120.28 |
| 15 | i | 278 | CYS | C-N-CA | 5.21 | 127.27 | 120.28 |
| 19 | m | 310 | THR | CA-C-O | 5.21 | 125.45 | 119.35 |
| 20 | n | 211 | MET | N-CA-CB | 5.21 | 118.91 | 110.41 |
| 21 | p | 63 | LYS | CA-C-N | -5.21 | 114.67 | 122.39 |
| 21 | p | 63 | LYS | C-N-CA | -5.21 | 114.67 | 122.39 |
| 16 | c | 194 | ILE | N-CA-C | -5.21 | 105.30 | 110.62 |
| 20 | g | 875 | PHE | N-CA-C | 5.21 | 117.04 | 111.36 |
| 14 | a | 134 | PRO | CB-CA-C | 5.21 | 117.78 | 110.95 |
| 14 | a | 158 | PHE | N-CA-CB | 5.21 | 119.23 | 111.51 |
| 2 | 1 | 867 | LEU | N-CA-C | 5.21 | 119.12 | 112.34 |
| 7 | O | 1501 | SER | CA-C-N | 5.21 | 131.26 | 122.87 |
| 7 | O | 1501 | SER | C-N-CA | 5.21 | 131.26 | 122.87 |
| 8 | P | 1412 | LEU | O-C-N | 5.21 | 127.65 | 122.12 |
| 9 | Q | 212 | PHE | N-CA-C | 5.21 | 116.65 | 111.07 |
| 2 | Z | 677 | PRO | N-CA-CB | 5.21 | 108.72 | 103.25 |
| 12 | v | 335 | MET | CG-SD-CE | -5.21 | 89.43 | 100.90 |
| 20 | n | 648 | GLN | OE1-CD-NE2 | 5.21 | 127.81 | 122.60 |
| 8 | N | 1603 | SER | CA-CB-OG | 5.21 | 121.53 | 111.10 |
| 7 | O | 565 | TYR | O-C-N | -5.21 | 115.86 | 122.27 |
| 9 | Q | 551 | ARG | CA-C-N | 5.21 | 129.29 | 120.64 |
| 9 | Q | 551 | ARG | C-N-CA | 5.21 | 129.29 | 120.64 |
| 9 | T | 787 | HIS | CE1-NE2-CD2 | -5.21 | 103.79 | 109.00 |
| 10 | W | 254 | ILE | N-CA-CB | 5.21 | 117.40 | 110.26 |
| 2 | Z | 1270 | ILE | N-CA-C | 5.21 | 115.88 | 110.82 |
| 2 | Z | 1365 | GLN | N-CA-C | -5.21 | 104.09 | 110.61 |
| 12 | v | 284 | PRO | CA-C-O | -5.21 | 115.47 | 121.36 |
| 15 | i | 297 | LYS | O-C-N | -5.21 | 115.85 | 122.26 |
| 19 | m | 512 | TYR | N-CA-C | -5.21 | 106.60 | 113.17 |
| 21 | p | 69 | VAL | CA-C-O | 5.21 | 126.51 | 120.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | b | 684 | ASP | N-CA-C | -5.21 | 100.91 | 109.40 |
| 15 | b | 691 | VAL | CB-CA-C | 5.21 | 119.84 | 111.29 |
| 19 | f | 232 | ASN | CB-CA-C | -5.21 | 102.34 | 110.37 |
| 19 | f | 559 | CYS | N-CA-CB | 5.21 | 119.30 | 110.49 |
| 14 | a | 803 | HIS | CB-CG-CD2 | -5.21 | 124.43 | 131.20 |
| 9 | R | 745 | LEU | CA-C-N | 5.21 | 126.35 | 119.84 |
| 9 | R | 745 | LEU | C-N-CA | 5.21 | 126.35 | 119.84 |
| 10 | U | 258 | TYR | N-CA-C | -5.21 | 102.27 | 110.14 |
| 1 | Y | 463 | GLU | CB-CG-CD | -5.21 | 103.74 | 112.60 |
| 20 | g | 883 | GLY | CA-C-N | -5.21 | 111.59 | 121.54 |
| 20 | g | 883 | GLY | C-N-CA | -5.21 | 111.59 | 121.54 |
| 14 | a | 771 | ASP | N-CA-CB | 5.21 | 118.32 | 110.30 |
| 2 | 1 | 1122 | ASP | N-CA-CB | 5.21 | 118.90 | 110.41 |
| 8 | N | 447 | LEU | CA-C-N | 5.21 | 128.85 | 121.66 |
| 8 | N | 447 | LEU | C-N-CA | 5.21 | 128.85 | 121.66 |
| 7 | O | 1617 | SER | N-CA-CB | 5.21 | 117.56 | 110.01 |
| 9 | S | 630 | ARG | NE-CZ-NH2 | 5.21 | 123.89 | 119.20 |
| 9 | T | 81 | GLU | CA-C-N | 5.21 | 131.49 | 121.54 |
| 9 | T | 81 | GLU | C-N-CA | 5.21 | 131.49 | 121.54 |
| 1 | Y | 230 | HIS | CG-CD2-NE2 | 5.21 | 112.41 | 107.20 |
| 2 | Z | 661 | ALA | CA-C-O | -5.21 | 113.98 | 119.97 |
| 2 | Z | 1256 | VAL | CA-C-N | 5.21 | 126.90 | 120.34 |
| 2 | Z | 1256 | VAL | C-N-CA | 5.21 | 126.90 | 120.34 |
| 12 | u | 74 | SER | CA-C-O | -5.21 | 113.98 | 119.97 |
| 12 | v | 560 | LEU | CB-CA-C | -5.21 | 102.70 | 110.88 |
| 16 | j | 415 | ASP | CB-CA-C | -5.21 | 101.42 | 109.80 |
| 19 | m | 111 | GLN | OE1-CD-NE2 | 5.21 | 127.81 | 122.60 |
| 19 | m | 432 | TYR | N-CA-C | -5.21 | 96.81 | 107.70 |
| 20 | n | 1046 | VAL | O-C-N | -5.21 | 116.82 | 121.87 |
| 20 | g | 278 | LYS | N-CA-C | -5.21 | 106.16 | 112.88 |
| 14 | a | 930 | SER | N-CA-C | -5.21 | 106.72 | 114.64 |
| 2 | 1 | 981 | GLN | CG-CD-NE2 | 5.21 | 124.21 | 116.40 |
| 5 | K | 351 | GLN | OE1-CD-NE2 | 5.21 | 127.81 | 122.60 |
| 7 | M | 838 | LYS | CA-C-N | 5.21 | 127.78 | 120.28 |
| 7 | M | 838 | LYS | C-N-CA | 5.21 | 127.78 | 120.28 |
| 7 | M | 1154 | ARG | NH1-CZ-NH2 | -5.21 | 112.53 | 119.30 |
| 8 | N | 1611 | TYR | CB-CG-CD1 | 5.21 | 128.61 | 120.80 |
| 7 | O | 418 | TYR | CA-C-N | 5.21 | 131.49 | 121.54 |
| 7 | O | 418 | TYR | C-N-CA | 5.21 | 131.49 | 121.54 |
| 9 | Q | 89 | ASP | CA-C-N | 5.21 | 127.21 | 120.44 |
| 9 | Q | 89 | ASP | C-N-CA | 5.21 | 127.21 | 120.44 |
| 9 | R | 429 | THR | CA-CB-CG2 | -5.21 | 101.65 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | T | 301 | ASN | CB-CA-C | -5.21 | 99.43 | 110.31 |
| 2 | Z | 377 | VAL | CB-CA-C | 5.21 | 119.02 | 110.69 |
| 12 | v | 141 | CYS | N-CA-C | -5.21 | 100.69 | 109.07 |
| 14 | h | 729 | ILE | CB-CA-C | -5.21 | 105.11 | 112.14 |
| 19 | m | 549 | PHE | CA-C-O | 5.21 | 125.44 | 119.35 |
| 20 | n | 539 | PHE | CA-CB-CG | 5.21 | 119.01 | 113.80 |
| 15 | b | 537 | GLU | CA-CB-CG | -5.21 | 103.69 | 114.10 |
| 20 | g | 201 | ASN | N-CA-C | -5.21 | 99.71 | 110.80 |
| 20 | g | 284 | TYR | CB-CG-CD1 | -5.21 | 112.99 | 120.80 |
| 14 | a | 177 | PHE | CA-CB-CG | -5.21 | 108.59 | 113.80 |
| 14 | a | 884 | GLU | N-CA-C | -5.21 | 99.71 | 110.80 |
| 1 | 0 | 1001 | ILE | CB-CG1-CD1 | 5.21 | 124.73 | 113.80 |
| 2 | 1 | 340 | GLU | CA-C-O | 5.21 | 126.62 | 120.58 |
| 6 | F | 439 | ILE | N-CA-C | 5.21 | 115.93 | 110.62 |
| 8 | N | 639 | PHE | CA-CB-CG | 5.21 | 119.00 | 113.80 |
| 2 | Z | 365 | SER | N-CA-CB | 5.21 | 118.72 | 110.55 |
| 12 | v | 395 | LYS | N-CA-CB | 5.21 | 117.56 | 110.01 |
| 14 | h | 105 | ARG | N-CA-C | -5.21 | 106.90 | 113.20 |
| 16 | c | 652 | ARG | CD-NE-CZ | 5.21 | 131.69 | 124.40 |
| 17 | d | 142 | ASP | N-CA-C | -5.21 | 100.92 | 109.40 |
| 20 | g | 571 | VAL | N-CA-CB | 5.21 | 116.08 | 110.62 |
| 2 | 1 | 1004 | VAL | N-CA-C | -5.20 | 105.42 | 110.42 |
| 4 | A | 754 | ASN | OD1-CG-ND2 | 5.20 | 127.80 | 122.60 |
| 6 | L | 292 | HIS | ND1-CG-CD2 | -5.20 | 100.90 | 106.10 |
| 7 | M | 1460 | LEU | CA-C-N | 5.20 | 127.68 | 120.29 |
| 7 | M | 1460 | LEU | C-N-CA | 5.20 | 127.68 | 120.29 |
| 8 | N | 794 | ILE | CA-CB-CG2 | -5.20 | 101.65 | 110.50 |
| 9 | R | 64 | LYS | CA-C-N | 5.20 | 131.48 | 121.54 |
| 9 | R | 64 | LYS | C-N-CA | 5.20 | 131.48 | 121.54 |
| 2 | Z | 972 | ASP | CA-C-N | 5.20 | 127.25 | 120.28 |
| 2 | Z | 972 | ASP | C-N-CA | 5.20 | 127.25 | 120.28 |
| 12 | u | 579 | ARG | N-CA-CB | 5.20 | 117.77 | 110.12 |
| 13 | w | 1289 | GLN | CA-C-N | 5.20 | 127.25 | 120.28 |
| 13 | w | 1289 | GLN | C-N-CA | 5.20 | 127.25 | 120.28 |
| 13 | w | 1355 | LYS | O-C-N | 5.20 | 127.64 | 122.12 |
| 13 | x | 1217 | THR | CA-C-N | 5.20 | 127.25 | 120.28 |
| 13 | x | 1217 | THR | C-N-CA | 5.20 | 127.25 | 120.28 |
| 14 | h | 671 | ASP | CA-CB-CG | -5.20 | 107.40 | 112.60 |
| 18 | l | 135 | ARG | CA-C-N | 5.20 | 130.47 | 122.77 |
| 18 | l | 135 | ARG | C-N-CA | 5.20 | 130.47 | 122.77 |
| 18 | l | 206 | ALA | O-C-N | 5.20 | 128.56 | 122.99 |
| 16 | c | 265 | HIS | CG-CD2-NE2 | 5.20 | 112.40 | 107.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | a | 603 | SER | N-CA-C | 5.20 | 118.04 | 109.72 |
| 1 | 0 | 376 | THR | N-CA-C | -5.20 | 100.42 | 108.90 |
| 2 | 1 | 197 | ILE | O-C-N | 5.20 | 128.43 | 122.97 |
| 2 | 1 | 867 | LEU | N-CA-CB | 5.20 | 119.54 | 110.18 |
| 6 | C | 293 | HIS | CG-CD2-NE2 | 5.20 | 112.40 | 107.20 |
| 8 | P | 115 | SER | CA-C-N | 5.20 | 127.20 | 120.44 |
| 8 | P | 115 | SER | C-N-CA | 5.20 | 127.20 | 120.44 |
| 8 | P | 851 | SER | N-CA-C | 5.20 | 117.69 | 111.71 |
| 9 | Q | 295 | ASN | CA-CB-CG | 5.20 | 117.80 | 112.60 |
| 14 | h | 335 | VAL | N-CA-C | -5.20 | 102.47 | 108.82 |
| 20 | n | 671 | ASN | CA-C-N | 5.20 | 128.94 | 121.71 |
| 20 | n | 671 | ASN | C-N-CA | 5.20 | 128.94 | 121.71 |
| 1 | 0 | 1296 | THR | N-CA-CB | 5.20 | 119.28 | 110.49 |
| 4 | J | 704 | GLN | CA-C-N | 5.20 | 129.41 | 120.72 |
| 4 | J | 704 | GLN | C-N-CA | 5.20 | 129.41 | 120.72 |
| 4 | J | 704 | GLN | OE1-CD-NE2 | 5.20 | 127.80 | 122.60 |
| 7 | M | 1022 | LEU | N-CA-C | 5.20 | 116.76 | 111.14 |
| 8 | N | 1494 | ILE | N-CA-C | 5.20 | 115.41 | 110.42 |
| 7 | O | 428 | GLN | N-CA-CB | 5.20 | 117.55 | 110.01 |
| 8 | P | 707 | PHE | CB-CG-CD1 | 5.20 | 129.54 | 120.70 |
| 8 | P | 1284 | ILE | CA-C-O | 5.20 | 125.56 | 119.89 |
| 9 | T | 301 | ASN | O-C-N | 5.20 | 129.40 | 122.43 |
| 11 | V | 396 | ALA | CA-C-N | 5.20 | 127.82 | 121.06 |
| 11 | V | 396 | ALA | C-N-CA | 5.20 | 127.82 | 121.06 |
| 1 | Y | 1482 | ASP | CA-C-O | -5.20 | 114.99 | 119.72 |
| 2 | Z | 1133 | CYS | CA-C-N | 5.20 | 127.20 | 120.44 |
| 2 | Z | 1133 | CYS | C-N-CA | 5.20 | 127.20 | 120.44 |
| 14 | h | 545 | THR | CB-CA-C | 5.20 | 118.93 | 109.62 |
| 17 | k | 52 | HIS | ND1-CE1-NE2 | 5.20 | 113.60 | 108.40 |
| 18 | l | 87 | ASP | N-CA-C | -5.20 | 103.59 | 110.40 |
| 20 | n | 922 | LEU | CA-C-O | -5.20 | 115.34 | 120.70 |
| 15 | b | 312 | LYS | CA-C-N | 5.20 | 130.81 | 121.66 |
| 15 | b | 312 | LYS | C-N-CA | 5.20 | 130.81 | 121.66 |
| 20 | g | 1082 | ASP | CA-C-N | 5.20 | 131.47 | 121.54 |
| 20 | g | 1082 | ASP | C-N-CA | 5.20 | 131.47 | 121.54 |
| 20 | g | 1096 | SER | N-CA-C | 5.20 | 118.88 | 112.54 |
| 1 | 0 | 276 | HIS | N-CA-C | -5.20 | 101.22 | 109.59 |
| 4 | A | 651 | SER | N-CA-C | 5.20 | 117.03 | 111.36 |
| 5 | B | 383 | SER | N-CA-CB | 5.20 | 117.85 | 110.16 |
| 6 | I | 345 | LEU | N-CA-CB | 5.20 | 118.34 | 110.28 |
| 7 | M | 435 | PHE | N-CA-C | -5.20 | 106.20 | 112.54 |
| 8 | N | 574 | HIS | CG-CD2-NE2 | 5.20 | 112.40 | 107.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 475 | TYR | O-C-N | -5.20 | 117.66 | 123.48 |
| 8 | P | 997 | VAL | CB-CA-C | -5.20 | 105.56 | 110.65 |
| 1 | Y | 433 | ASN | N-CA-CB | 5.20 | 118.39 | 110.44 |
| 12 | v | 39 | GLN | N-CA-CB | 5.20 | 117.42 | 109.94 |
| 4 | y | 766 | ILE | CB-CA-C | -5.20 | 105.12 | 112.14 |
| 14 | h | 734 | HIS | CA-C-O | 5.20 | 125.77 | 119.38 |
| 15 | i | 213 | ASN | OD1-CG-ND2 | -5.20 | 117.40 | 122.60 |
| 18 | l | 345 | ILE | CA-C-N | 5.20 | 131.06 | 121.70 |
| 18 | l | 345 | ILE | C-N-CA | 5.20 | 131.06 | 121.70 |
| 19 | m | 651 | ILE | N-CA-C | -5.20 | 107.28 | 111.91 |
| 21 | o | 91 | THR | CB-CA-C | 5.20 | 120.77 | 110.42 |
| 21 | p | 26 | THR | N-CA-CB | 5.20 | 117.61 | 110.07 |
| 18 | e | 77 | TYR | O-C-N | 5.20 | 130.08 | 122.39 |
| 20 | g | 357 | ASN | CB-CA-C | 5.20 | 117.45 | 109.03 |
| 1 | 0 | 916 | GLU | CA-C-N | 5.20 | 127.58 | 120.77 |
| 1 | 0 | 916 | GLU | C-N-CA | 5.20 | 127.58 | 120.77 |
| 8 | N | 1179 | SER | N-CA-CB | 5.20 | 118.56 | 109.72 |
| 8 | N | 1256 | GLU | CA-C-N | 5.20 | 127.24 | 120.28 |
| 8 | N | 1256 | GLU | C-N-CA | 5.20 | 127.24 | 120.28 |
| 7 | O | 249 | ASP | O-C-N | 5.20 | 127.63 | 122.12 |
| 9 | T | 672 | GLN | N-CA-C | -5.20 | 102.16 | 108.14 |
| 10 | W | 268 | LEU | N-CA-C | 5.20 | 116.94 | 111.28 |
| 20 | n | 439 | MET | CA-C-N | 5.20 | 128.09 | 120.71 |
| 20 | n | 439 | MET | C-N-CA | 5.20 | 128.09 | 120.71 |
| 15 | b | 726 | THR | N-CA-C | -5.20 | 101.41 | 109.72 |
| 14 | a | 886 | LEU | CA-C-O | 5.20 | 127.94 | 120.51 |
| 2 | 1 | 972 | ASP | CA-C-O | 5.20 | 125.36 | 119.18 |
| 4 | G | 805 | ARG | NH1-CZ-NH2 | 5.20 | 126.06 | 119.30 |
| 7 | M | 547 | PHE | CB-CA-C | -5.20 | 101.12 | 110.37 |
| 7 | M | 1643 | ARG | CA-C-N | 5.20 | 127.24 | 120.28 |
| 7 | M | 1643 | ARG | C-N-CA | 5.20 | 127.24 | 120.28 |
| 8 | P | 1635 | GLU | CA-C-N | 5.20 | 128.61 | 120.82 |
| 8 | P | 1635 | GLU | C-N-CA | 5.20 | 128.61 | 120.82 |
| 9 | R | 630 | ARG | N-CA-C | -5.20 | 104.56 | 112.04 |
| 9 | R | 791 | GLU | CB-CG-CD | -5.20 | 103.77 | 112.60 |
| 2 | Z | 727 | ARG | NE-CZ-NH1 | -5.20 | 116.31 | 121.50 |
| 14 | h | 684 | SER | CA-C-N | 5.20 | 127.67 | 120.29 |
| 14 | h | 684 | SER | C-N-CA | 5.20 | 127.67 | 120.29 |
| 16 | j | 604 | ASP | CA-CB-CG | 5.20 | 117.80 | 112.60 |
| 20 | g | 776 | ASN | N-CA-C | -5.20 | 105.68 | 112.23 |
| 20 | g | 1058 | LEU | CA-C-N | 5.20 | 127.24 | 120.28 |
| 20 | g | 1058 | LEU | C-N-CA | 5.20 | 127.24 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 420 | THR | N-CA-C | -5.19 | 106.90 | 114.12 |
| 8 | N | 1211 | ILE | N-CA-C | -5.19 | 105.43 | 110.42 |
| 8 | P | 265 | PHE | CA-C-N | 5.19 | 127.55 | 120.54 |
| 8 | P | 265 | PHE | C-N-CA | 5.19 | 127.55 | 120.54 |
| 9 | Q | 660 | LEU | CB-CA-C | -5.19 | 102.17 | 110.79 |
| 14 | h | 429 | GLU | N-CA-C | -5.19 | 106.18 | 112.88 |
| 20 | g | 422 | ASN | N-CA-CB | 5.19 | 119.27 | 110.49 |
| 1 | 0 | 1225 | PHE | CA-C-O | 5.19 | 127.81 | 121.68 |
| 5 | H | 294 | LYS | CA-CB-CG | 5.19 | 124.48 | 114.10 |
| 7 | M | 265 | ASP | CA-CB-CG | 5.19 | 117.79 | 112.60 |
| 7 | M | 672 | TRP | CA-C-N | 5.19 | 127.24 | 120.28 |
| 7 | M | 672 | TRP | C-N-CA | 5.19 | 127.24 | 120.28 |
| 7 | M | 1604 | ILE | CA-C-O | -5.19 | 115.55 | 120.95 |
| 8 | N | 202 | THR | CA-C-N | 5.19 | 131.46 | 121.54 |
| 8 | N | 202 | THR | C-N-CA | 5.19 | 131.46 | 121.54 |
| 8 | N | 348 | LYS | CA-C-O | 5.19 | 126.05 | 120.55 |
| 8 | N | 845 | SER | CA-C-N | 5.19 | 127.24 | 120.28 |
| 8 | N | 845 | SER | C-N-CA | 5.19 | 127.24 | 120.28 |
| 7 | O | 248 | PRO | CA-C-O | -5.19 | 115.44 | 122.08 |
| 7 | O | 772 | ASN | CA-C-N | 5.19 | 127.76 | 120.28 |
| 7 | O | 772 | ASN | C-N-CA | 5.19 | 127.76 | 120.28 |
| 8 | P | 458 | LYS | CG-CD-CE | 5.19 | 123.24 | 111.30 |
| 9 | R | 135 | ASP | O-C-N | 5.19 | 127.42 | 122.07 |
| 9 | T | 607 | ARG | CA-C-O | 5.19 | 125.86 | 120.30 |
| 12 | u | 86 | ASN | OD1-CG-ND2 | -5.19 | 117.41 | 122.60 |
| 12 | v | 65 | LEU | O-C-N | 5.19 | 128.77 | 122.85 |
| 14 | h | 480 | ASN | OD1-CG-ND2 | -5.19 | 117.41 | 122.60 |
| 14 | h | 672 | LYS | N-CA-C | -5.19 | 106.97 | 113.72 |
| 15 | b | 421 | ALA | N-CA-C | -5.19 | 106.72 | 113.16 |
| 2 | 1 | 195 | ASP | N-CA-C | -5.19 | 99.75 | 110.80 |
| 2 | 1 | 1062 | TRP | CG-CD2-CE3 | -5.19 | 128.71 | 133.90 |
| 4 | D | 677 | SER | O-C-N | 5.19 | 127.62 | 122.12 |
| 6 | F | 462 | GLN | O-C-N | -5.19 | 116.23 | 122.15 |
| 8 | N | 775 | PHE | N-CA-C | -5.19 | 99.74 | 110.80 |
| 9 | Q | 704 | ARG | N-CA-CB | 5.19 | 117.75 | 110.12 |
| 1 | Y | 1265 | ALA | N-CA-CB | 5.19 | 118.27 | 110.53 |
| 12 | v | 65 | LEU | N-CA-C | -5.19 | 103.54 | 110.55 |
| 14 | h | 910 | GLN | CG-CD-OE1 | 5.19 | 131.18 | 120.80 |
| 16 | j | 261 | LYS | N-CA-C | 5.19 | 116.94 | 111.28 |
| 19 | m | 74 | PHE | CB-CA-C | 5.19 | 119.10 | 110.90 |
| 19 | m | 459 | LYS | N-CA-CB | -5.19 | 102.47 | 110.20 |
| 14 | a | 128 | PHE | CA-CB-CG | 5.19 | 118.99 | 113.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 126 | TYR | N-CA-CB | 5.19 | 120.33 | 111.66 |
| 1 | 0 | 1438 | ASP | CA-CB-CG | -5.19 | 107.41 | 112.60 |
| 6 | I | 312 | VAL | CA-CB-CG2 | -5.19 | 101.58 | 110.40 |
| 16 | j | 559 | LEU | N-CA-CB | 5.19 | 117.99 | 110.26 |
| 19 | m | 318 | PRO | CA-C-N | 5.19 | 131.45 | 121.54 |
| 19 | m | 318 | PRO | C-N-CA | 5.19 | 131.45 | 121.54 |
| 21 | o | 32 | LEU | CA-C-O | -5.19 | 114.24 | 120.10 |
| 21 | p | 86 | PHE | N-CA-CB | 5.19 | 119.40 | 110.68 |
| 15 | b | 518 | ASP | CA-CB-CG | 5.19 | 117.79 | 112.60 |
| 5 | B | 326 | LYS | CA-C-N | 5.19 | 125.17 | 120.03 |
| 5 | B | 326 | LYS | C-N-CA | 5.19 | 125.17 | 120.03 |
| 6 | I | 309 | PRO | N-CA-CB | 5.19 | 109.02 | 103.52 |
| 8 | N | 119 | ASN | CA-C-O | -5.19 | 113.05 | 120.16 |
| 8 | P | 1188 | THR | O-C-N | 5.19 | 127.41 | 122.07 |
| 9 | S | 163 | ILE | N-CA-CB | 5.19 | 118.36 | 110.58 |
| 9 | S | 791 | GLU | CB-CA-C | -5.19 | 100.10 | 110.42 |
| 9 | T | 86 | PHE | CA-C-O | -5.19 | 115.05 | 120.55 |
| 2 | Z | 227 | LEU | CA-C-O | 5.19 | 125.34 | 119.27 |
| 2 | Z | 1090 | LYS | CA-C-N | 5.19 | 130.64 | 122.34 |
| 2 | Z | 1090 | LYS | C-N-CA | 5.19 | 130.64 | 122.34 |
| 12 | v | 254 | GLN | CA-C-N | 5.19 | 127.18 | 120.44 |
| 12 | v | 254 | GLN | C-N-CA | 5.19 | 127.18 | 120.44 |
| 16 | j | 563 | SER | N-CA-C | 5.19 | 118.88 | 112.24 |
| 15 | b | 66 | PRO | CA-C-N | 5.19 | 128.70 | 121.02 |
| 15 | b | 66 | PRO | C-N-CA | 5.19 | 128.70 | 121.02 |
| 18 | e | 212 | LYS | CA-CB-CG | 5.19 | 124.48 | 114.10 |
| 20 | g | 181 | ILE | CB-CA-C | -5.19 | 106.43 | 111.05 |
| 20 | g | 1126 | ASP | CA-CB-CG | 5.19 | 117.79 | 112.60 |
| 14 | a | 406 | ARG | CB-CG-CD | 5.19 | 123.23 | 111.30 |
| 14 | a | 992 | ASP | N-CA-CB | 5.19 | 119.25 | 110.49 |
| 2 | 1 | 1389 | GLY | O-C-N | -5.19 | 115.96 | 122.70 |
| 6 | F | 382 | LYS | N-CA-CB | 5.19 | 117.69 | 110.07 |
| 6 | L | 357 | LEU | CA-C-N | 5.19 | 128.06 | 119.35 |
| 6 | L | 357 | LEU | C-N-CA | 5.19 | 128.06 | 119.35 |
| 7 | M | 1531 | THR | CA-C-N | 5.19 | 128.00 | 120.79 |
| 7 | M | 1531 | THR | C-N-CA | 5.19 | 128.00 | 120.79 |
| 8 | N | 770 | HIS | CA-CB-CG | -5.19 | 108.61 | 113.80 |
| 8 | P | 331 | TYR | CA-C-N | 5.19 | 130.63 | 120.99 |
| 8 | P | 331 | TYR | C-N-CA | 5.19 | 130.63 | 120.99 |
| 8 | P | 1223 | ASN | N-CA-C | -5.19 | 106.81 | 112.72 |
| 2 | Z | 508 | PHE | CB-CG-CD1 | 5.19 | 129.52 | 120.70 |
| 12 | u | 553 | ILE | CA-C-O | -5.19 | 115.35 | 120.85 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | z | 655 | PHE | CA-C-N | 5.19 | 127.18 | 120.44 |
| 4 | z | 655 | PHE | C-N-CA | 5.19 | 127.18 | 120.44 |
| 6 | I | 388 | CYS | CA-C-O | -5.18 | 115.05 | 120.55 |
| 5 | K | 391 | GLU | CA-C-N | -5.18 | 115.57 | 122.72 |
| 5 | K | 391 | GLU | C-N-CA | -5.18 | 115.57 | 122.72 |
| 7 | O | 66 | VAL | CA-CB-CG1 | -5.18 | 101.59 | 110.40 |
| 7 | O | 1505 | HIS | O-C-N | 5.18 | 129.49 | 122.59 |
| 8 | P | 53 | GLU | CB-CG-CD | -5.18 | 103.78 | 112.60 |
| 8 | P | 204 | VAL | CB-CA-C | 5.18 | 115.40 | 110.16 |
| 8 | P | 989 | ASP | N-CA-CB | 5.18 | 118.84 | 110.65 |
| 9 | R | 820 | ILE | CA-C-N | 5.18 | 130.81 | 121.06 |
| 9 | R | 820 | ILE | C-N-CA | 5.18 | 130.81 | 121.06 |
| 9 | T | 730 | LYS | CA-C-O | -5.18 | 115.60 | 122.44 |
| 10 | U | 258 | TYR | CB-CA-C | 5.18 | 116.66 | 108.88 |
| 12 | v | 664 | ARG | CA-C-O | 5.18 | 125.92 | 120.42 |
| 21 | s | 15 | ASP | CA-C-N | -5.18 | 115.01 | 121.96 |
| 21 | s | 15 | ASP | C-N-CA | -5.18 | 115.01 | 121.96 |
| 1 | 0 | 1284 | ARG | NE-CZ-NH1 | -5.18 | 116.32 | 121.50 |
| 4 | G | 808 | ASP | N-CA-CB | 5.18 | 118.31 | 110.28 |
| 5 | K | 382 | LYS | N-CA-C | 5.18 | 116.93 | 111.28 |
| 7 | M | 641 | GLU | N-CA-C | 5.18 | 116.61 | 111.07 |
| 8 | N | 1490 | ARG | CD-NE-CZ | 5.18 | 131.66 | 124.40 |
| 7 | O | 1282 | ALA | N-CA-CB | 5.18 | 117.66 | 109.94 |
| 8 | P | 500 | LYS | N-CA-CB | 5.18 | 118.75 | 110.46 |
| 14 | a | 688 | PHE | CA-CB-CG | -5.18 | 108.62 | 113.80 |
| 1 | 0 | 1024 | LEU | N-CA-CB | 5.18 | 122.17 | 113.10 |
| 7 | M | 1523 | PHE | N-CA-C | 5.18 | 116.93 | 111.28 |
| 7 | O | 729 | MET | CA-C-N | 5.18 | 127.44 | 120.50 |
| 7 | O | 729 | MET | C-N-CA | 5.18 | 127.44 | 120.50 |
| 9 | Q | 814 | MET | CA-CB-CG | -5.18 | 103.74 | 114.10 |
| 9 | R | 334 | TRP | CG-CD2-CE3 | -5.18 | 128.72 | 133.90 |
| 1 | Y | 1000 | ASP | O-C-N | -5.18 | 114.71 | 123.00 |
| 12 | u | 335 | MET | CA-C-O | -5.18 | 115.91 | 121.56 |
| 12 | v | 177 | ALA | N-CA-C | -5.18 | 99.77 | 110.80 |
| 14 | h | 934 | GLU | CA-C-O | 5.18 | 126.85 | 121.15 |
| 14 | h | 1027 | LEU | N-CA-C | -5.18 | 99.84 | 108.34 |
| 2 | 1 | 1379 | VAL | N-CA-CB | -5.18 | 103.38 | 112.08 |
| 8 | N | 54 | SER | N-CA-CB | 5.18 | 119.24 | 110.49 |
| 7 | O | 1531 | THR | CA-C-O | -5.18 | 115.38 | 120.82 |
| 8 | P | 1412 | LEU | CA-C-O | -5.18 | 115.06 | 120.55 |
| 9 | Q | 735 | THR | CA-C-N | 5.18 | 127.17 | 120.44 |
| 9 | Q | 735 | THR | C-N-CA | 5.18 | 127.17 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | S | 663 | ASP | N-CA-CB | -5.18 | 102.51 | 110.12 |
| 1 | Y | 771 | TYR | CA-C-N | 5.18 | 125.70 | 120.00 |
| 1 | Y | 771 | TYR | C-N-CA | 5.18 | 125.70 | 120.00 |
| 19 | m | 305 | ASN | O-C-N | -5.18 | 115.22 | 122.37 |
| 18 | e | 140 | LEU | N-CA-C | -5.18 | 106.81 | 113.23 |
| 14 | a | 433 | ILE | N-CA-C | -5.18 | 100.66 | 108.12 |
| 9 | T | 740 | GLU | CA-C-O | -5.18 | 115.37 | 120.70 |
| 10 | W | 251 | HIS | N-CA-CB | 5.18 | 119.24 | 110.49 |
| 19 | m | 534 | SER | N-CA-CB | 5.18 | 117.52 | 110.01 |
| 18 | e | 73 | ALA | CB-CA-C | -5.18 | 101.26 | 109.80 |
| 2 | 1 | 434 | PHE | N-CA-CB | 5.18 | 119.07 | 110.63 |
| 6 | L | 297 | ASP | CA-C-O | 5.18 | 127.33 | 121.32 |
| 7 | M | 1185 | ILE | N-CA-C | -5.18 | 106.39 | 111.88 |
| 7 | M | 1585 | PRO | CB-CA-C | -5.18 | 104.83 | 113.06 |
| 8 | N | 54 | SER | N-CA-C | -5.18 | 99.77 | 110.80 |
| 8 | N | 344 | SER | N-CA-CB | 5.18 | 117.65 | 109.94 |
| 7 | O | 572 | PHE | O-C-N | -5.18 | 113.02 | 122.44 |
| 7 | O | 1534 | GLY | N-CA-C | -5.18 | 102.64 | 112.27 |
| 8 | P | 143 | SER | CB-CA-C | 5.18 | 119.43 | 110.84 |
| 9 | Q | 283 | LEU | CA-C-O | -5.18 | 115.06 | 120.55 |
| 9 | Q | 334 | TRP | CD2-CE2-CZ2 | -5.18 | 117.22 | 122.40 |
| 10 | U | 329 | GLN | N-CA-C | -5.18 | 106.20 | 112.88 |
| 1 | Y | 107 | TYR | CD1-CE1-CZ | 5.18 | 128.92 | 119.60 |
| 1 | Y | 835 | SER | O-C-N | 5.18 | 128.97 | 122.86 |
| 4 | z | 759 | SER | O-C-N | 5.18 | 127.47 | 122.09 |
| 16 | j | 442 | THR | N-CA-C | -5.18 | 100.80 | 109.24 |
| 20 | n | 504 | PHE | CA-C-O | -5.18 | 115.37 | 120.70 |
| 20 | n | 893 | ASP | N-CA-C | -5.18 | 106.77 | 114.64 |
| 20 | n | 904 | LYS | CA-C-N | 5.18 | 127.73 | 120.28 |
| 20 | n | 904 | LYS | C-N-CA | 5.18 | 127.73 | 120.28 |
| 16 | c | 513 | ARG | CB-CA-C | -5.18 | 102.05 | 110.85 |
| 17 | d | 139 | ILE | CA-CB-CG1 | 5.18 | 119.20 | 110.40 |
| 14 | a | 536 | ILE | O-C-N | 5.18 | 127.16 | 121.83 |
| 7 | M | 137 | ASN | CB-CG-ND2 | -5.17 | 108.64 | 116.40 |
| 8 | N | 320 | MET | CB-CA-C | -5.17 | 100.69 | 109.38 |
| 7 | O | 948 | LEU | N-CA-CB | 5.17 | 117.51 | 110.01 |
| 9 | Q | 320 | TRP | CE2-CD2-CE3 | 5.17 | 123.97 | 118.80 |
| 9 | Q | 615 | ASP | N-CA-CB | 5.17 | 119.24 | 110.49 |
| 9 | Q | 678 | ASP | CA-CB-CG | 5.17 | 117.78 | 112.60 |
| 9 | T | 534 | PHE | CA-C-N | 5.17 | 128.18 | 120.31 |
| 9 | T | 534 | PHE | C-N-CA | 5.17 | 128.18 | 120.31 |
| 9 | T | 785 | MET | O-C-N | -5.17 | 116.63 | 122.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 1169 | ILE | CA-CB-CG1 | 5.17 | 119.20 | 110.40 |
| 12 | u | 101 | GLU | N-CA-C | -5.17 | 106.93 | 114.12 |
| 12 | u | 115 | SER | N-CA-C | -5.17 | 100.87 | 108.99 |
| 12 | u | 381 | ILE | CA-CB-CG2 | -5.17 | 101.70 | 110.50 |
| 12 | v | 706 | GLN | N-CA-C | 5.17 | 116.92 | 111.28 |
| 13 | w | 1310 | VAL | CB-CA-C | -5.17 | 105.15 | 112.14 |
| 14 | h | 456 | ALA | N-CA-CB | 5.17 | 119.23 | 110.49 |
| 15 | i | 74 | LEU | N-CA-CB | 5.17 | 118.41 | 110.70 |
| 15 | i | 550 | HIS | CG-CD2-NE2 | 5.17 | 112.37 | 107.20 |
| 15 | b | 52 | THR | N-CA-C | -5.17 | 101.21 | 109.23 |
| 1 | 0 | 315 | THR | CA-CB-OG1 | 5.17 | 117.36 | 109.60 |
| 1 | 0 | 838 | CYS | CA-C-N | 5.17 | 127.77 | 120.42 |
| 1 | 0 | 838 | CYS | C-N-CA | 5.17 | 127.77 | 120.42 |
| 2 | 1 | 1323 | TYR | CA-C-N | 5.17 | 128.83 | 120.55 |
| 2 | 1 | 1323 | TYR | C-N-CA | 5.17 | 128.83 | 120.55 |
| 12 | v | 372 | LYS | CA-C-N | -5.17 | 114.55 | 122.62 |
| 12 | v | 372 | LYS | C-N-CA | -5.17 | 114.55 | 122.62 |
| 4 | y | 757 | SER | N-CA-C | 5.17 | 116.92 | 111.28 |
| 19 | f | 678 | LEU | N-CA-C | -5.17 | 99.78 | 110.80 |
| 1 | 0 | 840 | GLU | CB-CA-C | -5.17 | 100.74 | 110.67 |
| 1 | 0 | 1207 | ARG | NE-CZ-NH2 | -5.17 | 114.55 | 119.20 |
| 2 | 1 | 178 | ASN | N-CA-CB | 5.17 | 119.23 | 110.49 |
| 2 | 1 | 801 | LEU | O-C-N | 5.17 | 128.63 | 122.27 |
| 8 | N | 1011 | GLU | N-CA-CB | 5.17 | 117.70 | 110.56 |
| 9 | R | 229 | ASN | OD1-CG-ND2 | -5.17 | 117.43 | 122.60 |
| 2 | Z | 281 | VAL | CA-CB-CG2 | -5.17 | 101.61 | 110.40 |
| 2 | Z | 1252 | ASP | N-CA-C | 5.17 | 116.77 | 110.41 |
| 12 | v | 46 | TYR | CA-C-N | 5.17 | 131.42 | 121.54 |
| 12 | v | 46 | TYR | C-N-CA | 5.17 | 131.42 | 121.54 |
| 4 | z | 794 | ILE | CA-C-N | 5.17 | 127.16 | 120.44 |
| 4 | z | 794 | ILE | C-N-CA | 5.17 | 127.16 | 120.44 |
| 14 | h | 173 | PHE | CB-CG-CD1 | -5.17 | 111.91 | 120.70 |
| 15 | i | 407 | PRO | N-CA-CB | 5.17 | 109.16 | 103.26 |
| 16 | j | 177 | THR | CA-C-N | 5.17 | 127.63 | 120.29 |
| 16 | j | 177 | THR | C-N-CA | 5.17 | 127.63 | 120.29 |
| 19 | m | 723 | THR | N-CA-C | -5.17 | 105.65 | 112.94 |
| 20 | n | 619 | SER | N-CA-C | 5.17 | 116.60 | 111.07 |
| 19 | f | 411 | LYS | CA-C-O | -5.17 | 114.02 | 119.97 |
| 19 | f | 720 | ARG | NH1-CZ-NH2 | 5.17 | 126.02 | 119.30 |
| 14 | a | 650 | HIS | CA-CB-CG | -5.17 | 108.63 | 113.80 |
| 14 | a | 985 | ILE | CB-CA-C | 5.17 | 118.32 | 111.70 |
| 1 | 0 | 1359 | ASP | CA-CB-CG | 5.17 | 117.77 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 226 | THR | CA-C-N | 5.17 | 127.52 | 120.54 |
| 2 | 1 | 226 | THR | C-N-CA | 5.17 | 127.52 | 120.54 |
| 6 | F | 274 | ARG | CA-C-O | -5.17 | 115.38 | 120.70 |
| 8 | N | 863 | GLY | CA-C-N | 5.17 | 129.56 | 122.84 |
| 8 | N | 863 | GLY | C-N-CA | 5.17 | 129.56 | 122.84 |
| 7 | O | 227 | ASP | CA-C-N | 5.17 | 130.30 | 122.08 |
| 7 | O | 227 | ASP | C-N-CA | 5.17 | 130.30 | 122.08 |
| 9 | Q | 94 | GLN | CA-C-N | 5.17 | 127.21 | 120.28 |
| 9 | Q | 94 | GLN | C-N-CA | 5.17 | 127.21 | 120.28 |
| 9 | S | 683 | THR | CA-C-N | 5.17 | 131.23 | 122.65 |
| 9 | S | 683 | THR | C-N-CA | 5.17 | 131.23 | 122.65 |
| 14 | h | 267 | PRO | CA-C-N | 5.17 | 129.90 | 122.35 |
| 14 | h | 267 | PRO | C-N-CA | 5.17 | 129.90 | 122.35 |
| 16 | c | 177 | THR | N-CA-CB | 5.17 | 117.64 | 109.83 |
| 16 | c | 498 | ASN | CA-CB-CG | 5.17 | 117.77 | 112.60 |
| 14 | a | 846 | SER | N-CA-C | -5.17 | 106.23 | 112.54 |
| 7 | M | 237 | PHE | N-CA-C | 5.17 | 116.91 | 111.28 |
| 8 | N | 1174 | ASN | N-CA-CB | 5.17 | 118.82 | 110.40 |
| 7 | O | 980 | ASP | CB-CA-C | -5.17 | 101.89 | 110.68 |
| 8 | P | 1187 | ILE | CA-C-N | 5.17 | 127.16 | 120.44 |
| 8 | P | 1187 | ILE | C-N-CA | 5.17 | 127.16 | 120.44 |
| 9 | Q | 702 | ILE | CA-C-N | 5.17 | 128.17 | 120.31 |
| 9 | Q | 702 | ILE | C-N-CA | 5.17 | 128.17 | 120.31 |
| 14 | h | 210 | ARG | N-CA-C | -5.17 | 106.66 | 113.17 |
| 14 | h | 488 | THR | CA-CB-OG1 | 5.17 | 117.35 | 109.60 |
| 16 | j | 410 | PHE | N-CA-CB | 5.17 | 119.19 | 110.77 |
| 20 | n | 961 | SER | N-CA-CB | 5.17 | 117.72 | 110.12 |
| 21 | t | 69 | VAL | CA-C-N | 5.17 | 130.93 | 122.81 |
| 21 | t | 69 | VAL | C-N-CA | 5.17 | 130.93 | 122.81 |
| 1 | 0 | 157 | PRO | N-CA-CB | 5.17 | 107.84 | 103.35 |
| 1 | 0 | 171 | THR | N-CA-C | -5.17 | 99.99 | 108.41 |
| 2 | 1 | 419 | ASP | CA-CB-CG | 5.17 | 117.77 | 112.60 |
| 6 | F | 337 | LYS | N-CA-C | 5.17 | 116.91 | 111.28 |
| 7 | O | 174 | LEU | CA-C-N | 5.17 | 127.20 | 120.28 |
| 7 | O | 174 | LEU | C-N-CA | 5.17 | 127.20 | 120.28 |
| 7 | O | 247 | LEU | CA-C-N | 5.17 | 125.14 | 120.03 |
| 7 | O | 247 | LEU | C-N-CA | 5.17 | 125.14 | 120.03 |
| 7 | O | 1518 | PHE | CA-CB-CG | -5.17 | 108.63 | 113.80 |
| 8 | P | 598 | VAL | O-C-N | -5.17 | 116.68 | 121.90 |
| 8 | P | 1254 | ARG | N-CA-C | -5.17 | 106.48 | 112.89 |
| 9 | Q | 280 | GLN | CG-CD-OE1 | -5.17 | 110.47 | 120.80 |
| 9 | R | 223 | ASN | CB-CG-ND2 | -5.17 | 108.65 | 116.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | R | 614 | ARG | NE-CZ-NH2 | -5.17 | 114.55 | 119.20 |
| 9 | S | 738 | GLN | OE1-CD-NE2 | 5.17 | 127.77 | 122.60 |
| 1 | Y | 1208 | SER | CA-C-N | 5.17 | 131.41 | 121.54 |
| 1 | Y | 1208 | SER | C-N-CA | 5.17 | 131.41 | 121.54 |
| 12 | u | 283 | GLY | O-C-N | -5.17 | 116.60 | 121.77 |
| 12 | v | 294 | LEU | N-CA-C | -5.17 | 100.75 | 109.07 |
| 15 | i | 58 | ILE | N-CA-C | -5.17 | 100.32 | 108.90 |
| 17 | k | 71 | ALA | CA-C-O | -5.17 | 116.00 | 121.94 |
| 19 | m | 336 | PRO | CA-C-N | 5.17 | 127.20 | 120.28 |
| 19 | m | 336 | PRO | C-N-CA | 5.17 | 127.20 | 120.28 |
| 20 | n | 626 | ASN | CA-C-N | 5.17 | 129.60 | 120.87 |
| 20 | n | 626 | ASN | C-N-CA | 5.17 | 129.60 | 120.87 |
| 2 | 1 | 449 | ASP | N-CA-C | -5.17 | 107.04 | 113.55 |
| 4 | A | 697 | LEU | CB-CA-C | -5.17 | 102.22 | 110.79 |
| 6 | I | 378 | HIS | CA-C-N | 5.17 | 127.16 | 120.44 |
| 6 | I | 378 | HIS | C-N-CA | 5.17 | 127.16 | 120.44 |
| 8 | P | 222 | GLU | N-CA-C | -5.17 | 106.11 | 112.72 |
| 9 | T | 135 | ASP | CA-C-N | 5.17 | 127.15 | 120.44 |
| 9 | T | 135 | ASP | C-N-CA | 5.17 | 127.15 | 120.44 |
| 18 | l | 133 | ILE | N-CA-C | -5.17 | 100.63 | 108.17 |
| 2 | 1 | 979 | GLN | CA-C-N | 5.16 | 127.15 | 120.44 |
| 2 | 1 | 979 | GLN | C-N-CA | 5.16 | 127.15 | 120.44 |
| 7 | M | 643 | THR | CA-C-N | 5.16 | 127.20 | 120.28 |
| 7 | M | 643 | THR | C-N-CA | 5.16 | 127.20 | 120.28 |
| 8 | N | 1080 | GLU | CA-C-O | -5.16 | 115.05 | 120.63 |
| 8 | N | 1215 | VAL | N-CA-CB | 5.16 | 118.32 | 110.58 |
| 8 | P | 1426 | SER | N-CA-C | -5.16 | 106.82 | 113.02 |
| 9 | T | 577 | ARG | CD-NE-CZ | -5.16 | 117.17 | 124.40 |
| 11 | V | 373 | ASN | CA-CB-CG | 5.16 | 117.76 | 112.60 |
| 14 | h | 498 | HIS | N-CA-C | -5.16 | 106.22 | 112.88 |
| 14 | h | 558 | LEU | N-CA-C | 5.16 | 117.52 | 109.52 |
| 15 | i | 214 | ARG | NE-CZ-NH1 | 5.16 | 126.66 | 121.50 |
| 18 | l | 223 | SER | CA-C-N | 5.16 | 129.97 | 123.10 |
| 18 | l | 223 | SER | C-N-CA | 5.16 | 129.97 | 123.10 |
| 20 | n | 397 | PRO | N-CA-CB | 5.16 | 107.66 | 103.32 |
| 21 | s | 14 | SER | CA-C-N | 5.16 | 131.32 | 121.87 |
| 21 | s | 14 | SER | C-N-CA | 5.16 | 131.32 | 121.87 |
| 16 | c | 252 | ASN | CA-CB-CG | -5.16 | 107.44 | 112.60 |
| 20 | g | 368 | PHE | O-C-N | 5.16 | 129.14 | 122.43 |
| 20 | g | 613 | ILE | CA-C-N | 5.16 | 127.20 | 120.28 |
| 20 | g | 613 | ILE | C-N-CA | 5.16 | 127.20 | 120.28 |
| 20 | g | 1014 | SER | N-CA-C | -5.16 | 99.55 | 108.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | a | 695 | TYR | CA-C-N | 5.16 | 125.67 | 119.94 |
| 14 | a | 695 | TYR | C-N-CA | 5.16 | 125.67 | 119.94 |
| 2 | 1 | 1058 | CYS | CA-C-N | 5.16 | 127.62 | 120.29 |
| 2 | 1 | 1058 | CYS | C-N-CA | 5.16 | 127.62 | 120.29 |
| 2 | 1 | 1105 | GLU | CA-C-N | 5.16 | 131.40 | 121.54 |
| 2 | 1 | 1105 | GLU | C-N-CA | 5.16 | 131.40 | 121.54 |
| 5 | H | 506 | ILE | CB-CA-C | 5.16 | 121.92 | 111.60 |
| 7 | O | 182 | ARG | N-CA-C | -5.16 | 106.67 | 113.12 |
| 8 | P | 439 | LEU | N-CA-CB | -5.16 | 101.72 | 110.50 |
| 9 | T | 812 | GLN | N-CA-C | 5.16 | 119.33 | 113.19 |
| 2 | 1 | 715 | LEU | N-CA-C | 5.16 | 116.91 | 111.28 |
| 8 | P | 781 | ASP | N-CA-C | -5.16 | 106.67 | 113.17 |
| 9 | Q | 322 | ILE | O-C-N | -5.16 | 117.31 | 123.04 |
| 9 | S | 773 | ASN | N-CA-CB | 5.16 | 118.09 | 110.56 |
| 1 | Y | 121 | LEU | N-CA-C | 5.16 | 117.52 | 110.24 |
| 1 | Y | 585 | ILE | N-CA-CB | 5.16 | 118.32 | 110.58 |
| 12 | u | 49 | LEU | N-CA-CB | 5.16 | 119.21 | 110.49 |
| 14 | h | 265 | SER | O-C-N | 5.16 | 129.45 | 122.59 |
| 15 | i | 422 | MET | CG-SD-CE | 5.16 | 112.25 | 100.90 |
| 16 | c | 329 | ASP | CA-C-N | 5.16 | 125.99 | 120.47 |
| 16 | c | 329 | ASP | C-N-CA | 5.16 | 125.99 | 120.47 |
| 20 | g | 1138 | GLY | O-C-N | -5.16 | 116.86 | 122.84 |
| 14 | a | 832 | PHE | N-CA-C | -5.16 | 105.74 | 111.36 |
| 5 | E | 338 | ALA | N-CA-C | 5.16 | 116.90 | 111.28 |
| 5 | H | 287 | GLN | CA-C-O | 5.16 | 129.57 | 120.80 |
| 7 | M | 919 | ASN | OD1-CG-ND2 | 5.16 | 127.76 | 122.60 |
| 8 | N | 1028 | THR | N-CA-CB | 5.16 | 119.21 | 110.49 |
| 7 | O | 179 | ILE | CA-CB-CG2 | -5.16 | 101.73 | 110.50 |
| 9 | Q | 459 | LEU | N-CA-C | -5.16 | 106.23 | 112.88 |
| 9 | S | 738 | GLN | N-CA-CB | 5.16 | 118.19 | 110.19 |
| 9 | S | 821 | GLN | N-CA-CB | 5.16 | 118.29 | 110.14 |
| 9 | T | 507 | ALA | CB-CA-C | -5.16 | 102.78 | 110.88 |
| 11 | X | 386 | PRO | N-CA-C | 5.16 | 119.33 | 111.34 |
| 1 | Y | 1115 | VAL | N-CA-CB | 5.16 | 118.84 | 111.82 |
| 2 | Z | 750 | PRO | N-CA-C | -5.16 | 109.31 | 114.68 |
| 2 | Z | 1303 | ALA | CA-C-O | 5.16 | 127.29 | 121.51 |
| 13 | x | 1404 | GLU | CA-C-N | 5.16 | 127.15 | 120.44 |
| 13 | x | 1404 | GLU | C-N-CA | 5.16 | 127.15 | 120.44 |
| 14 | h | 929 | HIS | CE1-NE2-CD2 | -5.16 | 103.84 | 109.00 |
| 15 | i | 392 | GLN | O-C-N | -5.16 | 115.39 | 121.32 |
| 16 | j | 372 | LEU | N-CA-CB | 5.16 | 118.39 | 110.70 |
| 19 | m | 60 | SER | N-CA-C | 5.16 | 116.59 | 111.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | m | 458 | ARG | NE-CZ-NH2 | -5.16 | 114.56 | 119.20 |
| 19 | m | 460 | LYS | CA-CB-CG | 5.16 | 124.42 | 114.10 |
| 15 | b | 341 | GLY | CA-C-O | -5.16 | 112.84 | 119.13 |
| 16 | c | 653 | GLU | N-CA-C | -5.16 | 106.67 | 113.17 |
| 14 | a | 524 | VAL | N-CA-CB | 5.16 | 117.17 | 110.57 |
| 14 | a | 640 | PHE | CA-CB-CG | -5.16 | 108.64 | 113.80 |
| 1 | 0 | 113 | HIS | ND1-CE1-NE2 | 5.16 | 113.56 | 108.40 |
| 1 | 0 | 316 | LYS | N-CA-C | -5.16 | 106.23 | 112.88 |
| 7 | M | 47 | SER | CA-C-N | 5.16 | 127.19 | 120.28 |
| 7 | M | 47 | SER | C-N-CA | 5.16 | 127.19 | 120.28 |
| 7 | M | 48 | ARG | NE-CZ-NH1 | -5.16 | 116.34 | 121.50 |
| 8 | P | 1600 | ALA | O-C-N | 5.16 | 127.66 | 122.09 |
| 9 | R | 64 | LYS | CA-C-O | 5.16 | 126.75 | 121.23 |
| 9 | T | 732 | TRP | CA-C-N | 5.16 | 131.74 | 122.46 |
| 9 | T | 732 | TRP | C-N-CA | 5.16 | 131.74 | 122.46 |
| 14 | h | 864 | PHE | CA-C-O | 5.16 | 125.92 | 119.78 |
| 17 | d | 229 | ARG | NH1-CZ-NH2 | -5.16 | 112.60 | 119.30 |
| 20 | g | 806 | GLU | CB-CA-C | -5.16 | 102.78 | 110.88 |
| 6 | I | 455 | GLU | CB-CA-C | -5.16 | 102.75 | 110.90 |
| 7 | M | 1050 | ASP | CA-C-N | 5.16 | 127.64 | 120.63 |
| 7 | M | 1050 | ASP | C-N-CA | 5.16 | 127.64 | 120.63 |
| 8 | N | 420 | THR | CA-CB-CG2 | 5.16 | 119.27 | 110.50 |
| 7 | O | 1508 | ILE | N-CA-C | -5.16 | 98.62 | 109.34 |
| 8 | P | 457 | LEU | N-CA-CB | 5.16 | 119.20 | 110.49 |
| 8 | P | 618 | LEU | CA-C-N | 5.16 | 130.98 | 121.70 |
| 8 | P | 618 | LEU | C-N-CA | 5.16 | 130.98 | 121.70 |
| 1 | Y | 1100 | LYS | CA-C-O | -5.16 | 112.36 | 119.12 |
| 2 | Z | 441 | ARG | N-CA-C | -5.16 | 100.67 | 108.46 |
| 12 | u | 657 | TYR | CA-C-O | 5.16 | 125.70 | 119.31 |
| 14 | h | 623 | LEU | CA-C-O | -5.16 | 113.86 | 120.31 |
| 14 | h | 680 | LEU | O-C-N | -5.16 | 116.52 | 122.09 |
| 15 | i | 557 | ALA | CA-C-O | -5.16 | 115.38 | 120.90 |
| 15 | i | 625 | ALA | CA-C-N | 5.16 | 124.95 | 119.28 |
| 15 | i | 625 | ALA | C-N-CA | 5.16 | 124.95 | 119.28 |
| 19 | m | 256 | LEU | CA-C-N | 5.16 | 127.56 | 120.39 |
| 19 | m | 256 | LEU | C-N-CA | 5.16 | 127.56 | 120.39 |
| 19 | m | 589 | HIS | CG-CD2-NE2 | 5.16 | 112.36 | 107.20 |
| 19 | f | 463 | GLU | CA-C-N | 5.16 | 127.61 | 120.29 |
| 19 | f | 463 | GLU | C-N-CA | 5.16 | 127.61 | 120.29 |
| 14 | a | 411 | LEU | CA-C-N | 5.16 | 127.19 | 120.28 |
| 14 | a | 411 | LEU | C-N-CA | 5.16 | 127.19 | 120.28 |
| 4 | A | 766 | ILE | N-CA-CB | 5.15 | 117.55 | 110.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 906 | GLN | CA-C-O | -5.15 | 115.41 | 120.82 |
| 15 | i | 105 | SER | CA-C-N | 5.15 | 127.61 | 120.29 |
| 15 | i | 105 | SER | C-N-CA | 5.15 | 127.61 | 120.29 |
| 19 | f | 320 | HIS | CB-CA-C | -5.15 | 100.16 | 110.42 |
| 2 | 1 | 242 | HIS | CB-CG-CD2 | 5.15 | 137.90 | 131.20 |
| 8 | N | 366 | SER | CA-C-N | 5.15 | 127.19 | 120.28 |
| 8 | N | 366 | SER | C-N-CA | 5.15 | 127.19 | 120.28 |
| 7 | O | 1674 | CYS | CB-CA-C | -5.15 | 102.79 | 110.88 |
| 2 | Z | 109 | PRO | CA-C-N | 5.15 | 128.07 | 120.91 |
| 2 | Z | 109 | PRO | C-N-CA | 5.15 | 128.07 | 120.91 |
| 13 | x | 1387 | LYS | CA-C-N | 5.15 | 127.18 | 120.28 |
| 13 | x | 1387 | LYS | C-N-CA | 5.15 | 127.18 | 120.28 |
| 4 | z | 792 | GLN | CA-C-N | 5.15 | 127.61 | 120.29 |
| 4 | z | 792 | GLN | C-N-CA | 5.15 | 127.61 | 120.29 |
| 16 | j | 616 | VAL | CB-CA-C | 5.15 | 118.79 | 112.04 |
| 20 | n | 668 | ASN | CA-CB-CG | -5.15 | 107.45 | 112.60 |
| 21 | o | 25 | LEU | CA-C-N | 5.15 | 127.14 | 120.44 |
| 21 | o | 25 | LEU | C-N-CA | 5.15 | 127.14 | 120.44 |
| 19 | f | 37 | ASN | CA-C-N | 5.15 | 127.52 | 120.46 |
| 19 | f | 37 | ASN | C-N-CA | 5.15 | 127.52 | 120.46 |
| 19 | f | 482 | ARG | NE-CZ-NH1 | 5.15 | 126.65 | 121.50 |
| 14 | a | 422 | ARG | N-CA-C | -5.15 | 102.69 | 110.06 |
| 1 | 0 | 1011 | ARG | N-CA-CB | 5.15 | 117.61 | 110.04 |
| 1 | 0 | 1365 | ASN | CB-CA-C | -5.15 | 102.73 | 110.92 |
| 7 | M | 256 | HIS | CA-C-N | 5.15 | 127.14 | 120.44 |
| 7 | M | 256 | HIS | C-N-CA | 5.15 | 127.14 | 120.44 |
| 7 | O | 263 | LEU | N-CA-C | 5.15 | 117.29 | 111.11 |
| 7 | O | 1452 | SER | N-CA-CB | 5.15 | 117.61 | 109.94 |
| 7 | O | 1510 | ASP | N-CA-CB | 5.15 | 119.02 | 110.52 |
| 9 | Q | 481 | THR | N-CA-CB | 5.15 | 118.26 | 110.28 |
| 9 | Q | 696 | TYR | CB-CA-C | -5.15 | 99.23 | 109.79 |
| 11 | V | 368 | ARG | CA-C-N | 5.15 | 131.38 | 121.18 |
| 11 | V | 368 | ARG | C-N-CA | 5.15 | 131.38 | 121.18 |
| 1 | Y | 618 | THR | N-CA-C | -5.15 | 102.44 | 110.42 |
| 2 | Z | 1164 | PHE | CA-CB-CG | 5.15 | 118.95 | 113.80 |
| 17 | k | 28 | SER | CA-C-O | 5.15 | 126.21 | 120.80 |
| 6 | C | 453 | ILE | N-CA-CB | 5.15 | 116.22 | 110.51 |
| 5 | E | 351 | GLN | O-C-N | -5.15 | 116.48 | 122.81 |
| 7 | M | 1123 | ASN | CA-C-O | 5.15 | 127.87 | 120.51 |
| 7 | O | 50 | GLN | CB-CA-C | -5.15 | 102.24 | 110.79 |
| 7 | O | 218 | HIS | CA-CB-CG | -5.15 | 108.65 | 113.80 |
| 19 | m | 52 | ASP | CA-CB-CG | 5.15 | 117.75 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 21 | o | 11 | VAL | CA-C-O | 5.15 | 126.72 | 120.85 |
| 20 | g | 1134 | HIS | ND1-CE1-NE2 | 5.15 | 113.55 | 108.40 |
| 14 | a | 152 | LEU | CA-C-N | 5.15 | 130.96 | 121.85 |
| 14 | a | 152 | LEU | C-N-CA | 5.15 | 130.96 | 121.85 |
| 14 | a | 770 | PHE | CA-C-O | 5.15 | 125.02 | 119.15 |
| 1 | 0 | 715 | PRO | N-CA-C | 5.15 | 119.32 | 111.34 |
| 2 | 1 | 1196 | ASN | CB-CG-ND2 | -5.15 | 108.68 | 116.40 |
| 5 | E | 512 | ILE | N-CA-C | 5.15 | 115.36 | 110.42 |
| 4 | G | 789 | GLU | CA-CB-CG | 5.15 | 124.39 | 114.10 |
| 6 | I | 457 | ILE | CA-C-N | 5.15 | 128.13 | 120.31 |
| 6 | I | 457 | ILE | C-N-CA | 5.15 | 128.13 | 120.31 |
| 8 | N | 830 | THR | CA-C-O | 5.15 | 126.55 | 121.20 |
| 8 | N | 1597 | ARG | NE-CZ-NH2 | -5.15 | 114.57 | 119.20 |
| 7 | O | 185 | PHE | N-CA-C | -5.15 | 105.32 | 111.03 |
| 7 | O | 1657 | ASP | CA-C-N | 5.15 | 124.76 | 119.05 |
| 7 | O | 1657 | ASP | C-N-CA | 5.15 | 124.76 | 119.05 |
| 8 | P | 875 | LYS | N-CA-CB | 5.15 | 119.19 | 110.49 |
| 9 | Q | 745 | LEU | CA-C-O | -5.15 | 113.86 | 120.04 |
| 9 | T | 261 | GLU | CA-C-N | 5.15 | 127.69 | 120.28 |
| 9 | T | 261 | GLU | C-N-CA | 5.15 | 127.69 | 120.28 |
| 11 | V | 271 | ILE | N-CA-C | -5.15 | 100.79 | 108.46 |
| 2 | Z | 1204 | ASP | N-CA-C | -5.15 | 104.61 | 111.87 |
| 14 | h | 737 | ILE | CA-CB-CG2 | -5.15 | 101.75 | 110.50 |
| 15 | b | 360 | PHE | CA-CB-CG | 5.15 | 118.95 | 113.80 |
| 16 | c | 368 | GLY | N-CA-C | -5.15 | 104.78 | 111.52 |
| 1 | 0 | 276 | HIS | O-C-N | -5.15 | 116.67 | 123.21 |
| 1 | 0 | 1009 | HIS | CG-CD2-NE2 | 5.15 | 112.35 | 107.20 |
| 5 | K | 453 | LEU | N-CA-C | -5.15 | 105.84 | 112.68 |
| 7 | M | 645 | ILE | O-C-N | 5.15 | 128.92 | 122.59 |
| 9 | T | 536 | ASN | CA-C-O | -5.15 | 115.40 | 120.70 |
| 11 | V | 390 | ASN | CA-CB-CG | 5.15 | 117.75 | 112.60 |
| 12 | v | 321 | ASP | CA-CB-CG | 5.15 | 117.75 | 112.60 |
| 18 | l | 141 | GLU | CB-CG-CD | -5.15 | 103.85 | 112.60 |
| 19 | m | 688 | LEU | N-CA-CB | -5.15 | 103.78 | 110.88 |
| 16 | c | 480 | GLN | CA-C-N | 5.15 | 128.13 | 120.31 |
| 16 | c | 480 | GLN | C-N-CA | 5.15 | 128.13 | 120.31 |
| 7 | M | 204 | GLY | N-CA-C | -5.14 | 105.15 | 114.46 |
| 7 | M | 1236 | ILE | CA-CB-CG1 | 5.14 | 119.14 | 110.40 |
| 8 | N | 277 | THR | N-CA-CB | 5.14 | 119.18 | 110.49 |
| 8 | P | 199 | ILE | N-CA-CB | 5.14 | 118.15 | 111.67 |
| 8 | P | 687 | LYS | CG-CD-CE | 5.14 | 123.13 | 111.30 |
| 9 | Q | 83 | VAL | CA-C-N | 5.14 | 131.37 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | Q | 83 | VAL | C-N-CA | 5.14 | 131.37 | 121.54 |
| 9 | Q | 465 | ILE | CA-CB-CG2 | -5.14 | 101.76 | 110.50 |
| 12 | u | 285 | PHE | CA-C-O | 5.14 | 126.85 | 121.19 |
| 4 | z | 764 | SER | CA-C-N | 5.14 | 127.13 | 120.44 |
| 4 | z | 764 | SER | C-N-CA | 5.14 | 127.13 | 120.44 |
| 14 | h | 878 | HIS | CB-CG-ND1 | 5.14 | 130.42 | 122.70 |
| 16 | j | 129 | ASN | OD1-CG-ND2 | 5.14 | 127.74 | 122.60 |
| 16 | c | 416 | ASP | N-CA-C | -5.14 | 103.21 | 110.31 |
| 19 | f | 377 | ASN | CA-CB-CG | 5.14 | 117.74 | 112.60 |
| 1 | 0 | 1147 | GLU | CB-CG-CD | -5.14 | 103.86 | 112.60 |
| 2 | 1 | 355 | HIS | ND1-CE1-NE2 | 5.14 | 113.54 | 108.40 |
| 7 | M | 496 | SER | N-CA-C | -5.14 | 105.80 | 111.71 |
| 7 | O | 313 | ALA | N-CA-C | 5.14 | 117.62 | 111.71 |
| 9 | R | 67 | THR | CA-C-N | 5.14 | 127.12 | 120.44 |
| 9 | R | 67 | THR | C-N-CA | 5.14 | 127.12 | 120.44 |
| 9 | T | 415 | ILE | N-CA-C | -5.14 | 108.26 | 113.20 |
| 9 | T | 551 | ARG | CB-CA-C | -5.14 | 102.81 | 110.88 |
| 12 | v | 69 | PHE | N-CA-CB | 5.14 | 118.25 | 109.87 |
| 13 | w | 1305 | GLN | CA-C-N | 5.14 | 127.04 | 120.56 |
| 13 | w | 1305 | GLN | C-N-CA | 5.14 | 127.04 | 120.56 |
| 13 | x | 1392 | ARG | CA-C-O | -5.14 | 115.10 | 120.55 |
| 14 | h | 852 | SER | CA-C-N | 5.14 | 131.16 | 122.26 |
| 14 | h | 852 | SER | C-N-CA | 5.14 | 131.16 | 122.26 |
| 18 | l | 212 | LYS | CA-C-N | 5.14 | 132.10 | 122.74 |
| 18 | l | 212 | LYS | C-N-CA | 5.14 | 132.10 | 122.74 |
| 18 | l | 229 | GLN | OE1-CD-NE2 | -5.14 | 117.46 | 122.60 |
| 21 | r | 65 | PHE | N-CA-CB | 5.14 | 120.44 | 111.13 |
| 20 | g | 821 | LEU | CA-C-O | 5.14 | 124.86 | 118.43 |
| 9 | R | 334 | TRP | CD2-CE2-CZ2 | -5.14 | 117.26 | 122.40 |
| 2 | Z | 412 | ILE | CA-CB-CG1 | 5.14 | 119.14 | 110.40 |
| 12 | v | 35 | ILE | CA-C-N | 5.14 | 129.73 | 123.10 |
| 12 | v | 35 | ILE | C-N-CA | 5.14 | 129.73 | 123.10 |
| 13 | x | 1393 | ASP | CA-C-N | 5.14 | 125.65 | 119.94 |
| 13 | x | 1393 | ASP | C-N-CA | 5.14 | 125.65 | 119.94 |
| 16 | j | 169 | GLY | O-C-N | -5.14 | 115.51 | 122.35 |
| 18 | l | 239 | ARG | NE-CZ-NH2 | -5.14 | 114.57 | 119.20 |
| 15 | b | 596 | SER | N-CA-C | -5.14 | 104.34 | 110.41 |
| 19 | f | 408 | ASP | N-CA-CB | 5.14 | 117.77 | 110.16 |
| 20 | g | 647 | LYS | O-C-N | -5.14 | 115.95 | 122.27 |
| 14 | a | 370 | ASP | N-CA-CB | 5.14 | 119.38 | 111.46 |
| 1 | 0 | 770 | PHE | CA-CB-CG | 5.14 | 118.94 | 113.80 |
| 5 | E | 532 | ALA | O-C-N | 5.14 | 127.57 | 122.12 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 90 | GLU | N-CA-CB | 5.14 | 117.92 | 110.47 |
| 8 | P | 776 | TYR | CA-CB-CG | 5.14 | 123.15 | 113.90 |
| 9 | Q | 369 | THR | N-CA-C | -5.14 | 106.41 | 113.30 |
| 1 | Y | 1469 | ASN | CA-C-N | 5.14 | 127.17 | 120.28 |
| 1 | Y | 1469 | ASN | C-N-CA | 5.14 | 127.17 | 120.28 |
| 12 | u | 536 | LEU | CA-C-O | -5.14 | 115.10 | 120.55 |
| 15 | i | 338 | VAL | O-C-N | 5.14 | 127.25 | 121.90 |
| 18 | l | 196 | ARG | CA-C-O | -5.14 | 115.54 | 121.19 |
| 19 | m | 449 | LEU | CA-C-N | 5.14 | 128.64 | 121.24 |
| 19 | m | 449 | LEU | C-N-CA | 5.14 | 128.64 | 121.24 |
| 19 | m | 462 | ILE | N-CA-CB | 5.14 | 116.56 | 110.55 |
| 16 | c | 485 | GLN | N-CA-CB | 5.14 | 120.53 | 112.46 |
| 20 | g | 549 | MET | CA-C-O | -5.14 | 113.42 | 119.48 |
| 5 | B | 354 | GLY | CA-C-O | -5.14 | 118.13 | 122.29 |
| 5 | E | 441 | GLN | CA-C-O | -5.14 | 115.10 | 120.55 |
| 6 | L | 346 | ASP | CA-C-O | -5.14 | 115.10 | 120.55 |
| 7 | O | 27 | GLU | CA-C-N | 5.14 | 131.22 | 121.97 |
| 7 | O | 27 | GLU | C-N-CA | 5.14 | 131.22 | 121.97 |
| 7 | O | 1498 | LEU | CA-C-O | -5.14 | 115.10 | 120.80 |
| 2 | Z | 395 | ASN | N-CA-CB | 5.14 | 117.50 | 109.85 |
| 12 | v | 701 | LEU | CA-C-O | -5.14 | 115.10 | 120.55 |
| 15 | i | 403 | HIS | CG-CD2-NE2 | 5.14 | 112.34 | 107.20 |
| 17 | k | 52 | HIS | CB-CG-ND1 | 5.14 | 130.41 | 122.70 |
| 19 | m | 477 | ARG | NE-CZ-NH1 | 5.14 | 126.64 | 121.50 |
| 20 | n | 313 | TYR | CB-CG-CD2 | 5.14 | 128.51 | 120.80 |
| 15 | b | 388 | ASN | OD1-CG-ND2 | -5.14 | 117.46 | 122.60 |
| 20 | g | 270 | LEU | N-CA-CB | 5.14 | 120.24 | 111.66 |
| 1 | 0 | 456 | ASN | CA-C-O | 5.14 | 127.02 | 121.06 |
| 1 | 0 | 1473 | HIS | CE1-NE2-CD2 | -5.14 | 103.86 | 109.00 |
| 2 | 1 | 593 | GLN | OE1-CD-NE2 | 5.14 | 127.74 | 122.60 |
| 2 | 1 | 1011 | ILE | CA-C-O | 5.14 | 123.60 | 119.29 |
| 4 | J | 697 | LEU | O-C-N | 5.14 | 128.67 | 122.35 |
| 7 | M | 1443 | ASN | CA-C-N | 5.14 | 130.30 | 122.29 |
| 7 | M | 1443 | ASN | C-N-CA | 5.14 | 130.30 | 122.29 |
| 8 | P | 463 | PHE | O-C-N | -5.14 | 117.09 | 123.36 |
| 8 | P | 1443 | THR | CA-CB-OG1 | 5.14 | 117.30 | 109.60 |
| 9 | Q | 357 | LYS | N-CA-CB | 5.14 | 118.77 | 110.65 |
| 9 | Q | 621 | HIS | N-CA-CB | 5.14 | 117.67 | 110.12 |
| 9 | R | 605 | GLU | CB-CG-CD | -5.14 | 103.87 | 112.60 |
| 9 | T | 655 | THR | N-CA-CB | 5.14 | 117.59 | 109.94 |
| 14 | h | 246 | TRP | CB-CG-CD2 | -5.14 | 119.61 | 126.80 |
| 14 | h | 650 | HIS | CE1-NE2-CD2 | -5.14 | 103.86 | 109.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | i | 640 | GLU | N-CA-C | 5.14 | 116.88 | 109.07 |
| 16 | j | 244 | VAL | CA-C-N | 5.14 | 128.16 | 120.87 |
| 16 | j | 244 | VAL | C-N-CA | 5.14 | 128.16 | 120.87 |
| 17 | k | 206 | TRP | CB-CG-CD1 | 5.14 | 134.60 | 126.90 |
| 20 | n | 241 | GLN | CA-C-N | 5.14 | 130.45 | 122.49 |
| 20 | n | 241 | GLN | C-N-CA | 5.14 | 130.45 | 122.49 |
| 20 | n | 1134 | HIS | CB-CG-CD2 | 5.14 | 137.88 | 131.20 |
| 15 | b | 214 | ARG | N-CA-C | 5.14 | 118.58 | 112.72 |
| 16 | c | 219 | ASP | N-CA-C | -5.14 | 106.97 | 113.18 |
| 17 | d | 25 | ALA | N-CA-CB | 5.14 | 119.14 | 110.77 |
| 17 | d | 175 | THR | N-CA-C | -5.14 | 101.56 | 109.52 |
| 18 | e | 67 | GLU | CA-C-N | -5.14 | 115.00 | 122.86 |
| 18 | e | 67 | GLU | C-N-CA | -5.14 | 115.00 | 122.86 |
| 2 | 1 | 820 | ASP | CA-CB-CG | 5.13 | 117.73 | 112.60 |
| 5 | H | 528 | GLU | N-CA-CB | 5.13 | 117.67 | 110.12 |
| 7 | O | 58 | LEU | N-CA-CB | 5.13 | 118.41 | 110.60 |
| 7 | O | 437 | ASP | CA-CB-CG | 5.13 | 117.73 | 112.60 |
| 7 | O | 1161 | LEU | O-C-N | -5.13 | 116.21 | 122.22 |
| 8 | P | 641 | ILE | N-CA-C | -5.13 | 106.09 | 113.07 |
| 9 | Q | 275 | LYS | CA-C-N | 5.13 | 127.16 | 120.28 |
| 9 | Q | 275 | LYS | C-N-CA | 5.13 | 127.16 | 120.28 |
| 9 | S | 457 | TYR | N-CA-CB | 5.13 | 119.77 | 110.83 |
| 9 | S | 617 | LYS | CA-C-N | 5.13 | 129.41 | 120.68 |
| 9 | S | 617 | LYS | C-N-CA | 5.13 | 129.41 | 120.68 |
| 9 | T | 656 | LEU | CA-C-N | 5.13 | 127.03 | 120.56 |
| 9 | T | 656 | LEU | C-N-CA | 5.13 | 127.03 | 120.56 |
| 2 | Z | 236 | SER | N-CA-C | -5.13 | 100.33 | 109.06 |
| 2 | Z | 876 | ALA | N-CA-CB | 5.13 | 119.44 | 110.81 |
| 12 | v | 64 | VAL | N-CA-C | -5.13 | 100.92 | 108.11 |
| 19 | m | 194 | ASP | CA-C-N | 5.13 | 127.16 | 120.28 |
| 19 | m | 194 | ASP | C-N-CA | 5.13 | 127.16 | 120.28 |
| 21 | r | 38 | GLU | O-C-N | 5.13 | 127.56 | 122.12 |
| 16 | c | 481 | LEU | O-C-N | -5.13 | 115.95 | 122.27 |
| 17 | d | 116 | LEU | CA-C-O | -5.13 | 115.96 | 121.56 |
| 14 | a | 169 | VAL | N-CA-C | -5.13 | 106.79 | 111.67 |
| 2 | 1 | 1379 | VAL | CA-CB-CG2 | 5.13 | 119.12 | 110.40 |
| 6 | F | 313 | ALA | CB-CA-C | -5.13 | 100.81 | 110.67 |
| 6 | F | 332 | LYS | CA-CB-CG | -5.13 | 103.83 | 114.10 |
| 7 | O | 553 | ILE | CA-CB-CG1 | 5.13 | 119.13 | 110.40 |
| 9 | Q | 65 | ASP | CB-CA-C | -5.13 | 100.20 | 110.42 |
| 9 | R | 227 | GLN | N-CA-CB | 5.13 | 117.45 | 110.01 |
| 2 | Z | 179 | LYS | CB-CA-C | -5.13 | 100.20 | 110.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | i | 169 | VAL | CA-CB-CG1 | -5.13 | 101.67 | 110.40 |
| 19 | m | 58 | ASP | CA-CB-CG | 5.13 | 117.73 | 112.60 |
| 21 | p | 40 | ASP | CA-C-N | 5.13 | 127.03 | 120.56 |
| 21 | p | 40 | ASP | C-N-CA | 5.13 | 127.03 | 120.56 |
| 15 | b | 554 | GLU | CA-C-O | 5.13 | 127.26 | 121.51 |
| 4 | D | 659 | THR | N-CA-CB | 5.13 | 117.45 | 110.01 |
| 7 | M | 27 | GLU | N-CA-C | -5.13 | 107.69 | 114.31 |
| 8 | N | 1426 | SER | N-CA-CB | 5.13 | 117.45 | 110.01 |
| 8 | P | 218 | ASN | CA-C-O | 5.13 | 125.36 | 118.38 |
| 9 | S | 648 | GLU | CB-CA-C | 5.13 | 118.73 | 111.86 |
| 10 | W | 317 | THR | CA-C-O | -5.13 | 114.81 | 120.30 |
| 19 | m | 322 | LEU | CA-C-N | 5.13 | 128.50 | 120.75 |
| 19 | m | 322 | LEU | C-N-CA | 5.13 | 128.50 | 120.75 |
| 21 | r | 38 | GLU | CA-C-N | 5.13 | 127.16 | 120.28 |
| 21 | r | 38 | GLU | C-N-CA | 5.13 | 127.16 | 120.28 |
| 8 | N | 212 | TRP | N-CA-CB | 5.13 | 118.76 | 110.40 |
| 9 | R | 696 | TYR | CB-CA-C | 5.13 | 118.60 | 110.19 |
| 9 | S | 126 | GLU | N-CA-CB | 5.13 | 117.75 | 110.16 |
| 1 | Y | 832 | VAL | O-C-N | 5.13 | 128.98 | 122.57 |
| 19 | m | 649 | TYR | CB-CA-C | 5.13 | 118.22 | 109.24 |
| 15 | b | 507 | LEU | CA-C-N | 5.13 | 126.17 | 120.06 |
| 15 | b | 507 | LEU | C-N-CA | 5.13 | 126.17 | 120.06 |
| 17 | d | 238 | ASN | N-CA-C | -5.13 | 101.04 | 109.40 |
| 1 | 0 | 1386 | PRO | CA-N-CD | -5.13 | 104.82 | 112.00 |
| 7 | M | 1087 | CYS | CA-C-N | 5.13 | 127.67 | 120.28 |
| 7 | M | 1087 | CYS | C-N-CA | 5.13 | 127.67 | 120.28 |
| 8 | N | 1083 | ALA | N-CA-C | 5.13 | 117.61 | 111.71 |
| 8 | P | 1098 | ASN | CA-C-N | 5.13 | 130.86 | 122.65 |
| 8 | P | 1098 | ASN | C-N-CA | 5.13 | 130.86 | 122.65 |
| 8 | P | 1403 | ASN | CA-CB-CG | 5.13 | 117.73 | 112.60 |
| 13 | x | 1353 | SER | CA-C-N | 5.13 | 127.11 | 120.44 |
| 13 | x | 1353 | SER | C-N-CA | 5.13 | 127.11 | 120.44 |
| 19 | m | 409 | LYS | CA-C-O | -5.13 | 114.98 | 120.42 |
| 20 | n | 831 | LEU | N-CA-C | -5.13 | 106.84 | 114.64 |
| 20 | n | 882 | TYR | CB-CA-C | -5.13 | 101.23 | 110.36 |
| 20 | n | 1135 | SER | N-CA-C | 5.13 | 119.39 | 113.18 |
| 15 | b | 744 | MET | CA-CB-CG | 5.13 | 124.36 | 114.10 |
| 14 | a | 416 | GLY | CA-C-N | 5.13 | 127.57 | 120.29 |
| 14 | a | 416 | GLY | C-N-CA | 5.13 | 127.57 | 120.29 |
| 14 | a | 807 | ILE | CA-C-O | 5.13 | 123.60 | 118.98 |
| 1 | 0 | 141 | GLY | O-C-N | -5.13 | 118.71 | 122.71 |
| 2 | 1 | 494 | ASN | CA-CB-CG | 5.13 | 117.73 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 790 | SER | CA-C-N | 5.13 | 131.33 | 121.54 |
| 7 | M | 790 | SER | C-N-CA | 5.13 | 131.33 | 121.54 |
| 7 | O | 489 | TYR | CA-C-O | 5.13 | 125.87 | 119.97 |
| 7 | O | 1299 | ASN | CA-C-O | -5.13 | 115.44 | 120.82 |
| 9 | S | 575 | ALA | CA-C-N | 5.13 | 127.15 | 120.28 |
| 9 | S | 575 | ALA | C-N-CA | 5.13 | 127.15 | 120.28 |
| 11 | V | 347 | TYR | O-C-N | -5.13 | 115.42 | 121.32 |
| 2 | Z | 568 | LYS | N-CA-C | -5.13 | 106.16 | 112.72 |
| 12 | u | 125 | SER | N-CA-C | -5.13 | 101.50 | 109.24 |
| 12 | u | 341 | ASN | N-CA-CB | 5.13 | 119.15 | 110.49 |
| 12 | v | 181 | ASP | CA-C-N | 5.13 | 131.20 | 121.97 |
| 12 | v | 181 | ASP | C-N-CA | 5.13 | 131.20 | 121.97 |
| 12 | v | 403 | ASN | CA-C-O | -5.13 | 113.14 | 120.16 |
| 14 | h | 982 | TYR | N-CA-CB | 5.13 | 117.75 | 110.06 |
| 16 | c | 254 | GLN | N-CA-C | -5.13 | 107.41 | 113.97 |
| 20 | g | 872 | ILE | O-C-N | 5.13 | 127.59 | 121.80 |
| 2 | 1 | 1005 | TYR | N-CA-C | 5.12 | 116.95 | 111.36 |
| 7 | M | 1346 | ASN | CA-C-N | 5.12 | 128.71 | 120.30 |
| 7 | M | 1346 | ASN | C-N-CA | 5.12 | 128.71 | 120.30 |
| 7 | M | 1593 | ASN | O-C-N | 5.12 | 127.55 | 122.12 |
| 8 | N | 759 | ASN | CA-CB-CG | 5.12 | 117.72 | 112.60 |
| 14 | h | 774 | TYR | CA-CB-CG | 5.12 | 123.12 | 113.90 |
| 19 | m | 69 | GLU | N-CA-C | 5.12 | 116.87 | 111.28 |
| 17 | d | 10 | GLU | N-CA-C | -5.12 | 105.04 | 113.50 |
| 2 | 1 | 670 | PRO | CA-C-O | 5.12 | 127.50 | 121.56 |
| 5 | B | 328 | GLY | CA-C-O | -5.12 | 112.53 | 122.27 |
| 4 | J | 798 | ASN | CA-C-O | -5.12 | 115.44 | 120.82 |
| 5 | K | 356 | GLU | CA-C-N | 5.12 | 125.67 | 119.98 |
| 5 | K | 356 | GLU | C-N-CA | 5.12 | 125.67 | 119.98 |
| 7 | M | 114 | LEU | CB-CA-C | -5.12 | 99.28 | 109.99 |
| 8 | N | 276 | ASN | OD1-CG-ND2 | 5.12 | 127.72 | 122.60 |
| 9 | Q | 655 | THR | N-CA-C | 5.12 | 116.86 | 111.28 |
| 9 | R | 658 | ASN | OD1-CG-ND2 | -5.12 | 117.48 | 122.60 |
| 9 | R | 671 | ASP | N-CA-CB | 5.12 | 119.15 | 110.49 |
| 2 | Z | 1351 | TYR | O-C-N | 5.12 | 127.53 | 122.10 |
| 12 | v | 401 | ASP | CA-CB-CG | 5.12 | 117.72 | 112.60 |
| 14 | h | 537 | THR | N-CA-C | -5.12 | 105.78 | 112.23 |
| 16 | c | 334 | ASP | CA-CB-CG | -5.12 | 107.48 | 112.60 |
| 18 | e | 134 | LEU | N-CA-CB | 5.12 | 117.98 | 110.35 |
| 18 | e | 160 | PRO | CA-C-O | -5.12 | 113.13 | 120.56 |
| 18 | e | 300 | HIS | O-C-N | -5.12 | 116.97 | 123.17 |
| 19 | f | 113 | ASN | N-CA-CB | 5.12 | 118.59 | 110.55 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 700 | GLU | O-C-N | -5.12 | 116.69 | 122.12 |
| 1 | 0 | 1056 | SER | N-CA-C | 5.12 | 116.86 | 111.28 |
| 2 | 1 | 1185 | GLU | CB-CG-CD | -5.12 | 103.89 | 112.60 |
| 6 | I | 301 | HIS | N-CA-C | -5.12 | 106.27 | 112.88 |
| 6 | I | 308 | ILE | O-C-N | -5.12 | 115.26 | 121.10 |
| 7 | M | 131 | TYR | O-C-N | 5.12 | 129.19 | 122.33 |
| 7 | M | 927 | GLY | N-CA-C | 5.12 | 118.84 | 112.64 |
| 8 | N | 750 | PHE | CB-CG-CD1 | -5.12 | 111.99 | 120.70 |
| 7 | O | 255 | LEU | CA-C-N | 5.12 | 127.10 | 120.44 |
| 7 | O | 255 | LEU | C-N-CA | 5.12 | 127.10 | 120.44 |
| 7 | O | 553 | ILE | N-CA-C | -5.12 | 101.28 | 109.17 |
| 9 | Q | 244 | SER | N-CA-CB | 5.12 | 118.07 | 110.49 |
| 9 | R | 71 | TYR | CA-C-N | 5.12 | 127.10 | 120.44 |
| 9 | R | 71 | TYR | C-N-CA | 5.12 | 127.10 | 120.44 |
| 9 | S | 77 | GLY | N-CA-C | -5.12 | 102.78 | 112.10 |
| 9 | S | 478 | TYR | CA-C-N | 5.12 | 127.14 | 120.28 |
| 9 | S | 478 | TYR | C-N-CA | 5.12 | 127.14 | 120.28 |
| 2 | Z | 127 | ASP | N-CA-C | -5.12 | 102.71 | 110.24 |
| 12 | u | 116 | ILE | N-CA-C | 5.12 | 117.49 | 111.09 |
| 14 | h | 481 | HIS | CA-CB-CG | -5.12 | 108.68 | 113.80 |
| 14 | h | 495 | TYR | CB-CG-CD1 | 5.12 | 128.48 | 120.80 |
| 18 | l | 325 | ASP | O-C-N | -5.12 | 116.69 | 122.12 |
| 19 | m | 237 | ILE | CA-CB-CG2 | -5.12 | 101.79 | 110.50 |
| 20 | n | 471 | GLN | OE1-CD-NE2 | 5.12 | 127.72 | 122.60 |
| 17 | d | 204 | SER | N-CA-C | -5.12 | 105.93 | 113.61 |
| 20 | g | 708 | TRP | CA-C-N | -5.12 | 111.76 | 121.54 |
| 20 | g | 708 | TRP | C-N-CA | -5.12 | 111.76 | 121.54 |
| 14 | a | 10 | ASN | CA-C-N | 5.12 | 130.59 | 122.60 |
| 14 | a | 10 | ASN | C-N-CA | 5.12 | 130.59 | 122.60 |
| 14 | a | 485 | LYS | N-CA-C | 5.12 | 116.77 | 109.14 |
| 1 | 0 | 903 | ILE | CA-C-O | 5.12 | 126.28 | 120.95 |
| 1 | 0 | 1415 | ILE | N-CA-C | 5.12 | 119.52 | 113.22 |
| 2 | 1 | 993 | PRO | CA-C-O | -5.12 | 115.83 | 122.13 |
| 12 | u | 141 | CYS | O-C-N | -5.12 | 117.25 | 123.29 |
| 14 | a | 377 | GLU | N-CA-C | -5.12 | 95.75 | 107.48 |
| 1 | 0 | 166 | THR | CA-CB-OG1 | 5.12 | 117.28 | 109.60 |
| 6 | F | 373 | PHE | CA-C-O | -5.12 | 115.12 | 120.55 |
| 4 | J | 769 | ILE | CB-CA-C | -5.12 | 105.23 | 112.14 |
| 5 | K | 300 | ASP | CA-C-N | 5.12 | 125.19 | 119.87 |
| 5 | K | 300 | ASP | C-N-CA | 5.12 | 125.19 | 119.87 |
| 6 | L | 281 | ASP | N-CA-C | -5.12 | 105.59 | 111.07 |
| 7 | M | 1335 | ILE | CA-C-O | -5.12 | 115.75 | 121.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 574 | HIS | CB-CG-CD2 | -5.12 | 124.55 | 131.20 |
| 8 | N | 1556 | LEU | O-C-N | -5.12 | 116.69 | 122.12 |
| 8 | P | 817 | PRO | CA-N-CD | -5.12 | 104.83 | 112.00 |
| 11 | V | 385 | ILE | CA-C-N | 5.12 | 125.40 | 119.92 |
| 11 | V | 385 | ILE | C-N-CA | 5.12 | 125.40 | 119.92 |
| 2 | Z | 768 | ILE | N-CA-C | -5.12 | 107.76 | 112.83 |
| 12 | v | 147 | GLU | CB-CG-CD | -5.12 | 103.90 | 112.60 |
| 13 | w | 1349 | LEU | N-CA-CB | 5.12 | 117.73 | 110.16 |
| 13 | x | 1121 | GLY | N-CA-C | -5.12 | 101.05 | 113.18 |
| 21 | s | 19 | LYS | O-C-N | 5.12 | 127.34 | 122.07 |
| 20 | g | 508 | ASN | OD1-CG-ND2 | 5.12 | 127.72 | 122.60 |
| 4 | G | 680 | TYR | N-CA-C | 5.12 | 116.86 | 111.28 |
| 7 | M | 117 | VAL | N-CA-CB | 5.12 | 119.11 | 110.56 |
| 7 | O | 724 | ASN | N-CA-C | 5.12 | 117.51 | 110.35 |
| 9 | S | 461 | ASP | O-C-N | -5.12 | 116.56 | 122.09 |
| 13 | w | 1387 | LYS | N-CA-C | 5.12 | 116.94 | 111.36 |
| 16 | j | 140 | LYS | N-CA-C | -5.12 | 107.17 | 113.41 |
| 19 | m | 243 | TRP | O-C-N | -5.12 | 116.70 | 122.12 |
| 14 | a | 980 | VAL | N-CA-CB | 5.12 | 117.84 | 112.21 |
| 14 | a | 1029 | ASP | N-CA-C | -5.12 | 106.99 | 113.18 |
| 1 | 0 | 1208 | SER | CA-C-N | 5.12 | 128.93 | 121.31 |
| 1 | 0 | 1208 | SER | C-N-CA | 5.12 | 128.93 | 121.31 |
| 7 | M | 266 | ASP | CA-CB-CG | -5.12 | 107.48 | 112.60 |
| 9 | S | 249 | ARG | NE-CZ-NH2 | 5.12 | 123.80 | 119.20 |
| 9 | S | 693 | ALA | N-CA-C | -5.12 | 106.05 | 113.21 |
| 12 | u | 336 | SER | N-CA-C | -5.12 | 101.51 | 109.24 |
| 14 | h | 304 | LEU | CA-C-N | 5.12 | 130.91 | 121.70 |
| 14 | h | 304 | LEU | C-N-CA | 5.12 | 130.91 | 121.70 |
| 16 | j | 552 | TYR | N-CA-C | 5.12 | 116.54 | 111.07 |
| 19 | m | 456 | GLN | OE1-CD-NE2 | 5.12 | 127.72 | 122.60 |
| 19 | m | 518 | ILE | CA-C-O | 5.12 | 123.40 | 118.90 |
| 20 | n | 140 | LEU | CA-C-O | -5.12 | 115.29 | 120.71 |
| 20 | n | 829 | VAL | N-CA-C | -5.12 | 101.11 | 108.42 |
| 21 | q | 89 | PHE | CA-CB-CG | 5.12 | 118.92 | 113.80 |
| 15 | b | 164 | ASP | CA-CB-CG | -5.12 | 107.48 | 112.60 |
| 19 | f | 391 | HIS | CB-CA-C | -5.12 | 102.30 | 110.79 |
| 2 | 1 | 505 | GLY | CA-C-N | -5.11 | 115.98 | 122.37 |
| 2 | 1 | 505 | GLY | C-N-CA | -5.11 | 115.98 | 122.37 |
| 2 | 1 | 704 | VAL | CA-C-N | 5.11 | 128.11 | 120.90 |
| 2 | 1 | 704 | VAL | C-N-CA | 5.11 | 128.11 | 120.90 |
| 5 | K | 313 | TYR | CB-CG-CD2 | -5.11 | 113.13 | 120.80 |
| 7 | M | 76 | SER | N-CA-CB | 5.11 | 117.73 | 110.16 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 293 | GLU | CA-C-N | 5.11 | 127.90 | 120.79 |
| 8 | N | 293 | GLU | C-N-CA | 5.11 | 127.90 | 120.79 |
| 8 | N | 409 | GLU | O-C-N | 5.11 | 129.39 | 122.59 |
| 7 | O | 99 | ALA | N-CA-C | -5.11 | 106.63 | 112.92 |
| 7 | O | 119 | PHE | CA-CB-CG | 5.11 | 118.91 | 113.80 |
| 7 | O | 564 | ASP | N-CA-CB | 5.11 | 117.38 | 109.91 |
| 7 | O | 692 | TYR | CA-C-N | 5.11 | 128.78 | 120.60 |
| 7 | O | 692 | TYR | C-N-CA | 5.11 | 128.78 | 120.60 |
| 7 | O | 1591 | ASP | CA-C-O | 5.11 | 125.97 | 120.55 |
| 9 | Q | 88 | LYS | N-CA-C | 5.11 | 116.54 | 111.07 |
| 9 | R | 247 | GLY | CA-C-O | -5.11 | 115.74 | 121.31 |
| 9 | R | 267 | ASP | CB-CA-C | 5.11 | 119.99 | 111.30 |
| 9 | R | 556 | TYR | CB-CG-CD2 | -5.11 | 113.13 | 120.80 |
| 9 | S | 25 | LEU | N-CA-CB | 5.11 | 117.73 | 110.16 |
| 9 | S | 645 | GLN | OE1-CD-NE2 | -5.11 | 117.49 | 122.60 |
| 1 | Y | 1090 | GLU | CA-C-N | 5.11 | 128.60 | 121.24 |
| 1 | Y | 1090 | GLU | C-N-CA | 5.11 | 128.60 | 121.24 |
| 2 | Z | 1381 | ASP | N-CA-CB | 5.11 | 117.43 | 110.42 |
| 13 | x | 1441 | LEU | CA-C-N | 5.11 | 127.09 | 120.44 |
| 13 | x | 1441 | LEU | C-N-CA | 5.11 | 127.09 | 120.44 |
| 15 | i | 244 | TYR | CB-CG-CD1 | 5.11 | 128.47 | 120.80 |
| 17 | k | 212 | TRP | CZ3-CH2-CZ2 | -5.11 | 114.85 | 121.50 |
| 21 | p | 84 | LEU | CB-CA-C | -5.11 | 101.68 | 110.22 |
| 19 | f | 104 | LEU | CA-C-N | 5.11 | 127.13 | 120.28 |
| 19 | f | 104 | LEU | C-N-CA | 5.11 | 127.13 | 120.28 |
| 19 | f | 421 | LYS | N-CA-C | 5.11 | 116.85 | 111.28 |
| 20 | g | 394 | LYS | N-CA-CB | 5.11 | 119.82 | 111.74 |
| 14 | a | 71 | HIS | ND1-CE1-NE2 | 5.11 | 113.51 | 108.40 |
| 14 | a | 474 | ASN | CA-CB-CG | -5.11 | 107.49 | 112.60 |
| 14 | a | 740 | PHE | N-CA-C | -5.11 | 106.89 | 112.72 |
| 5 | H | 313 | TYR | CB-CG-CD2 | -5.11 | 113.13 | 120.80 |
| 8 | P | 348 | LYS | N-CA-CB | -5.11 | 102.61 | 110.12 |
| 8 | P | 576 | TYR | CA-CB-CG | 5.11 | 123.10 | 113.90 |
| 8 | P | 981 | LYS | N-CA-CB | 5.11 | 118.58 | 110.55 |
| 10 | W | 352 | GLN | CA-C-N | 5.11 | 130.57 | 122.60 |
| 10 | W | 352 | GLN | C-N-CA | 5.11 | 130.57 | 122.60 |
| 13 | w | 1232 | ILE | CB-CA-C | -5.11 | 105.43 | 111.97 |
| 19 | m | 604 | VAL | CB-CA-C | 5.11 | 118.37 | 110.50 |
| 20 | g | 127 | ASP | O-C-N | -5.11 | 116.83 | 122.86 |
| 20 | g | 868 | HIS | CB-CG-CD2 | -5.11 | 124.55 | 131.20 |
| 20 | g | 1139 | SER | CA-C-N | -5.11 | 112.77 | 121.97 |
| 20 | g | 1139 | SER | C-N-CA | -5.11 | 112.77 | 121.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 590 | GLY | O-C-N | 5.11 | 127.22 | 122.57 |
| 2 | 1 | 1170 | GLN | CA-C-N | 5.11 | 129.26 | 120.72 |
| 2 | 1 | 1170 | GLN | C-N-CA | 5.11 | 129.26 | 120.72 |
| 7 | O | 285 | PHE | CA-C-N | 5.11 | 127.00 | 120.56 |
| 7 | O | 285 | PHE | C-N-CA | 5.11 | 127.00 | 120.56 |
| 8 | P | 680 | ASP | CA-CB-CG | -5.11 | 107.49 | 112.60 |
| 9 | T | 70 | HIS | CA-C-O | -5.11 | 115.45 | 120.82 |
| 9 | T | 698 | ASP | O-C-N | -5.11 | 115.95 | 122.34 |
| 11 | V | 380 | SER | CA-C-N | 5.11 | 130.60 | 122.94 |
| 11 | V | 380 | SER | C-N-CA | 5.11 | 130.60 | 122.94 |
| 2 | Z | 182 | LEU | CA-C-N | 5.11 | 132.04 | 122.74 |
| 2 | Z | 182 | LEU | C-N-CA | 5.11 | 132.04 | 122.74 |
| 12 | v | 227 | LEU | O-C-N | 5.11 | 127.54 | 122.12 |
| 12 | v | 638 | ILE | CA-C-O | -5.11 | 115.64 | 120.95 |
| 15 | i | 150 | ALA | CA-C-N | 5.11 | 127.00 | 120.56 |
| 15 | i | 150 | ALA | C-N-CA | 5.11 | 127.00 | 120.56 |
| 16 | j | 357 | ILE | N-CA-CB | 5.11 | 116.53 | 110.55 |
| 20 | n | 839 | PHE | N-CA-CB | 5.11 | 117.87 | 109.90 |
| 21 | s | 23 | ASP | CA-C-N | 5.11 | 127.46 | 120.46 |
| 21 | s | 23 | ASP | C-N-CA | 5.11 | 127.46 | 120.46 |
| 19 | f | 252 | GLN | CB-CA-C | -5.11 | 104.81 | 111.40 |
| 20 | g | 731 | GLU | N-CA-C | -5.11 | 105.41 | 113.02 |
| 14 | a | 299 | GLN | N-CA-C | -5.11 | 100.12 | 108.76 |
| 4 | D | 685 | MET | CA-C-N | 5.11 | 127.55 | 120.29 |
| 4 | D | 685 | MET | C-N-CA | 5.11 | 127.55 | 120.29 |
| 7 | M | 1003 | LEU | CA-C-N | 5.11 | 127.08 | 120.44 |
| 7 | M | 1003 | LEU | C-N-CA | 5.11 | 127.08 | 120.44 |
| 8 | N | 1255 | ILE | O-C-N | 5.11 | 125.73 | 121.85 |
| 7 | O | 19 | GLU | CA-C-O | -5.11 | 115.79 | 121.51 |
| 8 | P | 55 | LEU | CA-C-N | 5.11 | 130.49 | 122.21 |
| 8 | P | 55 | LEU | C-N-CA | 5.11 | 130.49 | 122.21 |
| 8 | P | 302 | LEU | O-C-N | 5.11 | 128.55 | 122.27 |
| 8 | P | 973 | THR | N-CA-CB | 5.11 | 120.01 | 111.53 |
| 9 | Q | 439 | HIS | O-C-N | -5.11 | 115.60 | 122.19 |
| 14 | h | 142 | ALA | N-CA-C | 5.11 | 121.68 | 110.80 |
| 14 | h | 802 | TYR | O-C-N | 5.11 | 129.86 | 123.12 |
| 19 | m | 194 | ASP | N-CA-C | 5.11 | 116.93 | 111.36 |
| 14 | a | 731 | ASN | CA-CB-CG | -5.11 | 107.49 | 112.60 |
| 1 | 0 | 970 | ILE | CA-C-N | 5.11 | 127.46 | 120.46 |
| 1 | 0 | 970 | ILE | C-N-CA | 5.11 | 127.46 | 120.46 |
| 4 | J | 670 | VAL | CA-C-N | 5.11 | 127.08 | 120.44 |
| 4 | J | 670 | VAL | C-N-CA | 5.11 | 127.08 | 120.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | M | 863 | GLU | N-CA-C | 5.11 | 116.85 | 111.28 |
| 7 | M | 1390 | GLN | CB-CA-C | -5.11 | 99.54 | 110.32 |
| 8 | N | 1180 | GLN | CB-CA-C | -5.11 | 101.18 | 110.63 |
| 7 | O | 2 | LYS | N-CA-C | -5.11 | 99.92 | 110.80 |
| 7 | O | 77 | LEU | CB-CA-C | -5.11 | 102.31 | 110.79 |
| 7 | O | 987 | GLU | N-CA-C | 5.11 | 116.85 | 111.28 |
| 9 | T | 774 | LEU | N-CA-C | -5.11 | 105.62 | 111.14 |
| 1 | Y | 1168 | GLN | N-CA-CB | 5.11 | 119.12 | 110.49 |
| 1 | Y | 1181 | PHE | N-CA-C | -5.11 | 106.88 | 114.64 |
| 2 | Z | 127 | ASP | O-C-N | 5.11 | 129.19 | 123.06 |
| 2 | Z | 192 | HIS | CG-CD2-NE2 | 5.11 | 112.31 | 107.20 |
| 2 | Z | 841 | ARG | N-CA-C | 5.11 | 116.85 | 111.28 |
| 12 | u | 128 | LYS | N-CA-C | -5.11 | 107.02 | 114.12 |
| 15 | i | 66 | PRO | CA-C-N | 5.11 | 128.58 | 121.02 |
| 15 | i | 66 | PRO | C-N-CA | 5.11 | 128.58 | 121.02 |
| 20 | n | 256 | ILE | CB-CG1-CD1 | 5.11 | 124.52 | 113.80 |
| 14 | a | 544 | MET | CA-C-N | 5.11 | 131.50 | 122.67 |
| 14 | a | 544 | MET | C-N-CA | 5.11 | 131.50 | 122.67 |
| 1 | 0 | 1453 | HIS | CE1-NE2-CD2 | -5.11 | 103.89 | 109.00 |
| 2 | 1 | 192 | HIS | CE1-NE2-CD2 | -5.11 | 103.89 | 109.00 |
| 5 | B | 321 | ALA | CA-C-N | 5.11 | 127.67 | 120.42 |
| 5 | B | 321 | ALA | C-N-CA | 5.11 | 127.67 | 120.42 |
| 8 | N | 1026 | THR | N-CA-CB | 5.11 | 117.57 | 109.71 |
| 7 | O | 498 | THR | N-CA-C | -5.11 | 101.86 | 109.11 |
| 7 | O | 742 | GLN | N-CA-CB | 5.11 | 119.12 | 110.49 |
| 9 | T | 307 | SER | N-CA-C | -5.11 | 107.43 | 113.97 |
| 2 | Z | 618 | ASP | CA-C-N | 5.11 | 130.75 | 121.92 |
| 2 | Z | 618 | ASP | C-N-CA | 5.11 | 130.75 | 121.92 |
| 12 | u | 259 | LEU | N-CA-CB | 5.11 | 117.41 | 110.01 |
| 12 | v | 30 | GLN | CB-CG-CD | 5.11 | 121.28 | 112.60 |
| 13 | w | 1221 | VAL | N-CA-C | 5.11 | 115.32 | 110.42 |
| 14 | h | 583 | LEU | O-C-N | -5.11 | 115.49 | 122.33 |
| 16 | j | 541 | ALA | CB-CA-C | -5.11 | 100.44 | 109.02 |
| 21 | s | 47 | LYS | CA-C-N | 5.11 | 127.12 | 120.28 |
| 21 | s | 47 | LYS | C-N-CA | 5.11 | 127.12 | 120.28 |
| 21 | t | 40 | ASP | N-CA-C | 5.11 | 116.53 | 111.07 |
| 15 | b | 163 | LYS | CB-CA-C | -5.11 | 101.18 | 110.63 |
| 16 | c | 660 | VAL | N-CA-C | -5.11 | 106.17 | 111.58 |
| 20 | g | 160 | GLU | O-C-N | -5.11 | 117.40 | 123.22 |
| 14 | a | 547 | VAL | CA-C-N | 5.11 | 127.54 | 120.29 |
| 14 | a | 547 | VAL | C-N-CA | 5.11 | 127.54 | 120.29 |
| 14 | a | 995 | ARG | CA-C-N | 5.11 | 131.29 | 121.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | a | 995 | ARG | C-N-CA | 5.11 | 131.29 | 121.54 |
| 14 | a | 1005 | ASN | N-CA-C | -5.11 | 106.74 | 113.17 |
| 9 | Q | 782 | ILE | O-C-N | 5.10 | 127.09 | 121.83 |
| 9 | R | 599 | ARG | CA-C-O | 5.10 | 126.51 | 120.69 |
| 9 | S | 30 | ASP | CA-C-O | -5.10 | 112.12 | 120.80 |
| 15 | i | 90 | LEU | N-CA-C | -5.10 | 100.85 | 109.07 |
| 18 | l | 246 | THR | CA-C-N | 5.10 | 129.76 | 122.72 |
| 18 | l | 246 | THR | C-N-CA | 5.10 | 129.76 | 122.72 |
| 19 | m | 257 | ASP | CA-C-O | -5.10 | 114.86 | 120.17 |
| 2 | 1 | 486 | GLN | OE1-CD-NE2 | -5.10 | 117.50 | 122.60 |
| 5 | B | 456 | THR | OG1-CB-CG2 | 5.10 | 119.51 | 109.30 |
| 5 | E | 441 | GLN | N-CA-CB | 5.10 | 117.62 | 110.12 |
| 8 | N | 914 | ASP | CB-CA-C | 5.10 | 117.64 | 109.07 |
| 8 | N | 1312 | LEU | N-CA-C | 5.10 | 116.53 | 111.07 |
| 8 | P | 748 | HIS | CA-C-N | 5.10 | 129.06 | 120.29 |
| 8 | P | 748 | HIS | C-N-CA | 5.10 | 129.06 | 120.29 |
| 9 | T | 21 | LYS | CA-C-N | 5.10 | 127.12 | 120.28 |
| 9 | T | 21 | LYS | C-N-CA | 5.10 | 127.12 | 120.28 |
| 1 | Y | 162 | HIS | ND1-CE1-NE2 | 5.10 | 113.50 | 108.40 |
| 1 | Y | 892 | ALA | O-C-N | -5.10 | 116.58 | 122.09 |
| 2 | Z | 797 | ALA | CA-C-N | 5.10 | 128.06 | 120.31 |
| 2 | Z | 797 | ALA | C-N-CA | 5.10 | 128.06 | 120.31 |
| 13 | w | 1402 | LEU | CA-C-N | 5.10 | 127.12 | 120.28 |
| 13 | w | 1402 | LEU | C-N-CA | 5.10 | 127.12 | 120.28 |
| 14 | h | 241 | CYS | N-CA-CB | 5.10 | 119.11 | 110.49 |
| 20 | n | 500 | GLN | CB-CA-C | -5.10 | 102.07 | 110.08 |
| 18 | e | 5 | ASP | CA-CB-CG | 5.10 | 117.70 | 112.60 |
| 14 | a | 793 | PHE | O-C-N | -5.10 | 117.23 | 123.30 |
| 5 | B | 376 | LEU | N-CA-C | 5.10 | 116.53 | 111.07 |
| 6 | I | 329 | ASP | N-CA-CB | 5.10 | 117.41 | 110.01 |
| 5 | K | 342 | LYS | O-C-N | -5.10 | 115.47 | 121.23 |
| 9 | R | 502 | ASP | CA-C-N | 5.10 | 127.11 | 120.28 |
| 9 | R | 502 | ASP | C-N-CA | 5.10 | 127.11 | 120.28 |
| 9 | S | 488 | TYR | N-CA-C | 5.10 | 116.65 | 111.14 |
| 2 | Z | 426 | THR | CA-CB-CG2 | -5.10 | 101.83 | 110.50 |
| 20 | n | 438 | SER | O-C-N | 5.10 | 129.37 | 122.59 |
| 20 | n | 555 | GLN | N-CA-C | -5.10 | 106.30 | 112.88 |
| 2 | 1 | 953 | ILE | CB-CA-C | -5.10 | 106.41 | 111.30 |
| 7 | M | 1258 | HIS | CA-C-O | -5.10 | 112.13 | 120.80 |
| 7 | M | 1535 | ALA | N-CA-C | -5.10 | 106.47 | 113.30 |
| 8 | N | 1209 | ALA | CA-C-N | 5.10 | 127.11 | 120.28 |
| 8 | N | 1209 | ALA | C-N-CA | 5.10 | 127.11 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 1648 | GLN | CB-CG-CD | -5.10 | 103.93 | 112.60 |
| 7 | O | 198 | TYR | CB-CG-CD2 | -5.10 | 113.15 | 120.80 |
| 7 | O | 1438 | VAL | N-CA-C | 5.10 | 115.31 | 110.42 |
| 9 | S | 729 | ASN | O-C-N | 5.10 | 128.32 | 122.25 |
| 10 | W | 279 | ASP | CA-C-N | 5.10 | 128.01 | 120.82 |
| 10 | W | 279 | ASP | C-N-CA | 5.10 | 128.01 | 120.82 |
| 1 | Y | 278 | ARG | NH1-CZ-NH2 | -5.10 | 112.67 | 119.30 |
| 1 | Y | 1403 | PRO | N-CA-C | 5.10 | 122.98 | 112.47 |
| 15 | i | 517 | ASP | CA-CB-CG | 5.10 | 117.70 | 112.60 |
| 17 | d | 117 | LEU | CA-C-N | 5.10 | 129.68 | 123.10 |
| 17 | d | 117 | LEU | C-N-CA | 5.10 | 129.68 | 123.10 |
| 20 | g | 165 | ILE | CA-C-O | 5.10 | 125.99 | 120.53 |
| 20 | g | 873 | GLN | OE1-CD-NE2 | 5.10 | 127.70 | 122.60 |
| 14 | a | 442 | TYR | N-CA-CB | 5.10 | 117.47 | 110.07 |
| 14 | a | 692 | PHE | CA-C-O | 5.10 | 126.50 | 120.69 |
| 1 | 0 | 277 | GLU | CA-C-O | 5.10 | 124.90 | 119.34 |
| 4 | D | 813 | SER | CA-C-O | 5.10 | 125.83 | 119.97 |
| 7 | M | 185 | PHE | CA-C-N | 5.10 | 127.11 | 120.28 |
| 7 | M | 185 | PHE | C-N-CA | 5.10 | 127.11 | 120.28 |
| 8 | N | 390 | ILE | N-CA-CB | 5.10 | 115.69 | 110.23 |
| 8 | N | 446 | ALA | CA-C-O | 5.10 | 126.80 | 121.19 |
| 7 | O | 209 | ASN | CA-CB-CG | -5.10 | 107.50 | 112.60 |
| 7 | O | 1315 | THR | CA-C-O | 5.10 | 125.25 | 119.18 |
| 9 | Q | 226 | ARG | CA-C-N | 5.10 | 127.53 | 120.29 |
| 9 | Q | 226 | ARG | C-N-CA | 5.10 | 127.53 | 120.29 |
| 9 | S | 317 | ASP | N-CA-C | -5.10 | 100.69 | 107.88 |
| 15 | b | 132 | VAL | CA-C-N | 5.10 | 132.02 | 122.74 |
| 15 | b | 132 | VAL | C-N-CA | 5.10 | 132.02 | 122.74 |
| 16 | c | 425 | TYR | N-CA-C | -5.10 | 107.61 | 113.88 |
| 19 | f | 137 | LYS | CB-CA-C | 5.10 | 119.44 | 109.35 |
| 19 | f | 680 | ILE | O-C-N | -5.10 | 115.29 | 121.10 |
| 20 | g | 671 | ASN | N-CA-CB | 5.10 | 117.71 | 110.06 |
| 14 | a | 105 | ARG | CA-CB-CG | 5.10 | 124.30 | 114.10 |
| 4 | J | 661 | LYS | N-CA-CB | 5.10 | 117.46 | 110.07 |
| 10 | U | 340 | ILE | N-CA-C | -5.10 | 100.98 | 108.11 |
| 20 | n | 411 | ASN | CB-CG-ND2 | -5.10 | 108.76 | 116.40 |
| 14 | a | 263 | SER | CA-C-O | -5.10 | 115.83 | 121.33 |
| 14 | a | 676 | ALA | O-C-N | 5.10 | 127.32 | 122.07 |
| 6 | I | 402 | ASP | CA-CB-CG | -5.09 | 107.50 | 112.60 |
| 7 | M | 983 | ILE | CA-C-N | 5.09 | 127.11 | 120.28 |
| 7 | M | 983 | ILE | C-N-CA | 5.09 | 127.11 | 120.28 |
| 7 | O | 1002 | LEU | N-CA-C | -5.09 | 105.90 | 112.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | Q | 723 | ILE | N-CA-CB | 5.09 | 116.51 | 110.55 |
| 1 | Y | 1239 | ALA | N-CA-C | -5.09 | 106.31 | 112.88 |
| 12 | u | 689 | ILE | N-CA-C | 5.09 | 115.31 | 110.42 |
| 14 | h | 151 | HIS | ND1-CE1-NE2 | 5.09 | 113.50 | 108.40 |
| 15 | i | 337 | LEU | N-CA-C | 5.09 | 119.34 | 113.18 |
| 16 | j | 493 | VAL | CA-CB-CG1 | 5.09 | 119.06 | 110.40 |
| 20 | n | 897 | ALA | CB-CA-C | -5.09 | 103.05 | 110.95 |
| 19 | f | 274 | GLN | OE1-CD-NE2 | 5.09 | 127.69 | 122.60 |
| 1 | 0 | 446 | LEU | CA-C-N | 5.09 | 131.07 | 122.87 |
| 1 | 0 | 446 | LEU | C-N-CA | 5.09 | 131.07 | 122.87 |
| 5 | B | 515 | ASN | CA-CB-CG | 5.09 | 117.69 | 112.60 |
| 9 | Q | 811 | ARG | NE-CZ-NH2 | 5.09 | 123.78 | 119.20 |
| 2 | Z | 206 | LEU | O-C-N | -5.09 | 117.36 | 123.27 |
| 20 | n | 301 | ASN | CA-C-O | 5.09 | 124.42 | 118.77 |
| 7 | M | 1536 | SER | N-CA-C | 5.09 | 116.64 | 111.14 |
| 8 | N | 327 | PHE | N-CA-C | -5.09 | 106.16 | 112.93 |
| 8 | N | 600 | ASN | CA-CB-CG | -5.09 | 107.51 | 112.60 |
| 9 | R | 568 | ASP | CA-CB-CG | -5.09 | 107.51 | 112.60 |
| 1 | Y | 643 | THR | CA-CB-OG1 | 5.09 | 117.24 | 109.60 |
| 1 | Y | 837 | ASP | O-C-N | -5.09 | 116.72 | 122.12 |
| 1 | Y | 1357 | LYS | CB-CA-C | -5.09 | 102.00 | 110.81 |
| 16 | j | 544 | LEU | CA-C-N | 5.09 | 127.37 | 120.65 |
| 16 | j | 544 | LEU | C-N-CA | 5.09 | 127.37 | 120.65 |
| 19 | m | 200 | ALA | CA-C-N | 5.09 | 129.22 | 120.72 |
| 19 | m | 200 | ALA | C-N-CA | 5.09 | 129.22 | 120.72 |
| 15 | b | 222 | GLU | CA-C-O | 5.09 | 126.71 | 120.55 |
| 20 | g | 624 | THR | O-C-N | -5.09 | 117.21 | 122.96 |
| 20 | g | 690 | ARG | NE-CZ-NH1 | -5.09 | 116.41 | 121.50 |
| 14 | a | 117 | LEU | O-C-N | 5.09 | 129.28 | 123.02 |
| 14 | a | 367 | ASN | CA-C-O | -5.09 | 115.88 | 121.58 |
| 1 | 0 | 1473 | HIS | CG-CD2-NE2 | 5.09 | 112.29 | 107.20 |
| 5 | K | 362 | ASN | OD1-CG-ND2 | 5.09 | 127.69 | 122.60 |
| 8 | P | 190 | GLN | CA-C-N | 5.09 | 127.43 | 120.46 |
| 8 | P | 190 | GLN | C-N-CA | 5.09 | 127.43 | 120.46 |
| 8 | P | 273 | LEU | CA-C-N | 5.09 | 126.75 | 120.34 |
| 8 | P | 273 | LEU | C-N-CA | 5.09 | 126.75 | 120.34 |
| 8 | P | 461 | CYS | N-CA-CB | 5.09 | 120.41 | 111.55 |
| 8 | P | 849 | ASN | OD1-CG-ND2 | -5.09 | 117.51 | 122.60 |
| 9 | S | 154 | GLU | CA-C-N | 5.09 | 127.43 | 120.46 |
| 9 | S | 154 | GLU | C-N-CA | 5.09 | 127.43 | 120.46 |
| 9 | T | 252 | GLN | N-CA-CB | 5.09 | 117.60 | 110.12 |
| 9 | T | 636 | ARG | N-CA-C | -5.09 | 102.57 | 109.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | W | 282 | VAL | N-CA-CB | 5.09 | 119.63 | 111.23 |
| 1 | Y | 1373 | LYS | O-C-N | -5.09 | 116.83 | 122.07 |
| 2 | Z | 159 | ILE | CB-CA-C | 5.09 | 117.12 | 110.96 |
| 2 | Z | 874 | ASN | CA-CB-CG | -5.09 | 107.51 | 112.60 |
| 14 | h | 279 | TYR | N-CA-C | -5.09 | 108.10 | 114.56 |
| 20 | n | 347 | PHE | N-CA-C | -5.09 | 98.99 | 107.80 |
| 20 | n | 1088 | SER | N-CA-C | 5.09 | 117.72 | 111.82 |
| 15 | b | 710 | TYR | CA-C-N | 5.09 | 130.17 | 122.08 |
| 15 | b | 710 | TYR | C-N-CA | 5.09 | 130.17 | 122.08 |
| 16 | c | 360 | LEU | CA-C-O | 5.09 | 126.17 | 120.82 |
| 16 | c | 593 | LYS | CA-C-N | 5.09 | 127.10 | 120.28 |
| 16 | c | 593 | LYS | C-N-CA | 5.09 | 127.10 | 120.28 |
| 18 | e | 130 | ASN | CA-C-N | 5.09 | 129.33 | 120.68 |
| 18 | e | 130 | ASN | C-N-CA | 5.09 | 129.33 | 120.68 |
| 20 | g | 275 | ILE | CA-C-N | 5.09 | 127.94 | 120.71 |
| 20 | g | 275 | ILE | C-N-CA | 5.09 | 127.94 | 120.71 |
| 20 | g | 678 | TYR | CB-CA-C | 5.09 | 118.87 | 110.88 |
| 20 | g | 700 | GLU | CB-CA-C | -5.09 | 102.34 | 110.79 |
| 14 | a | 443 | LEU | CB-CA-C | -5.09 | 102.89 | 110.88 |
| 14 | a | 647 | PHE | CA-C-N | 5.09 | 125.63 | 119.98 |
| 14 | a | 647 | PHE | C-N-CA | 5.09 | 125.63 | 119.98 |
| 7 | M | 473 | SER | N-CA-C | 5.09 | 117.72 | 111.82 |
| 7 | M | 506 | ASN | N-CA-C | -5.09 | 106.09 | 113.21 |
| 7 | M | 1653 | LYS | N-CA-CB | 5.09 | 117.60 | 110.12 |
| 9 | T | 493 | ASP | CA-C-N | 5.09 | 127.86 | 120.79 |
| 9 | T | 493 | ASP | C-N-CA | 5.09 | 127.86 | 120.79 |
| 13 | x | 1104 | SER | CA-C-O | 5.09 | 127.11 | 121.56 |
| 19 | f | 509 | HIS | N-CA-C | -5.09 | 105.63 | 111.07 |
| 1 | 0 | 381 | VAL | N-CA-CB | 5.09 | 116.07 | 110.53 |
| 2 | 1 | 586 | TYR | O-C-N | 5.09 | 128.34 | 122.19 |
| 5 | B | 329 | HIS | ND1-CE1-NE2 | 5.09 | 113.49 | 108.40 |
| 6 | L | 374 | GLN | CG-CD-NE2 | 5.09 | 124.03 | 116.40 |
| 7 | M | 1299 | ASN | N-CA-CB | 5.09 | 117.52 | 109.94 |
| 7 | O | 561 | CYS | O-C-N | 5.09 | 127.31 | 122.07 |
| 1 | Y | 531 | PHE | CA-CB-CG | -5.09 | 108.71 | 113.80 |
| 1 | Y | 1443 | VAL | N-CA-C | 5.09 | 115.30 | 110.42 |
| 12 | v | 283 | GLY | N-CA-C | 5.09 | 122.72 | 112.34 |
| 16 | j | 157 | SER | O-C-N | 5.09 | 129.35 | 122.59 |
| 18 | l | 197 | GLY | N-CA-C | -5.09 | 105.33 | 112.60 |
| 18 | l | 237 | ASP | N-CA-C | -5.09 | 99.97 | 110.80 |
| 6 | F | 281 | ASP | CA-CB-CG | 5.08 | 117.69 | 112.60 |
| 8 | N | 554 | ILE | N-CA-CB | 5.08 | 118.30 | 112.15 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 844 | TYR | CB-CG-CD1 | 5.08 | 128.43 | 120.80 |
| 7 | O | 1287 | THR | CA-CB-OG1 | 5.08 | 117.23 | 109.60 |
| 1 | Y | 598 | PHE | CA-CB-CG | 5.08 | 118.89 | 113.80 |
| 1 | Y | 1071 | ALA | O-C-N | 5.08 | 127.31 | 122.07 |
| 1 | Y | 1157 | PHE | N-CA-CB | 5.08 | 117.90 | 110.88 |
| 2 | Z | 255 | VAL | CA-CB-CG2 | -5.08 | 101.76 | 110.40 |
| 12 | v | 221 | LYS | CA-C-N | 5.08 | 127.09 | 120.28 |
| 12 | v | 221 | LYS | C-N-CA | 5.08 | 127.09 | 120.28 |
| 14 | h | 386 | LEU | CA-C-O | -5.08 | 115.16 | 120.55 |
| 20 | n | 704 | SER | CA-C-N | 5.08 | 131.25 | 121.54 |
| 20 | n | 704 | SER | C-N-CA | 5.08 | 131.25 | 121.54 |
| 16 | c | 570 | MET | CA-C-N | 5.08 | 131.52 | 122.06 |
| 16 | c | 570 | MET | C-N-CA | 5.08 | 131.52 | 122.06 |
| 20 | g | 236 | SER | N-CA-C | -5.08 | 107.25 | 113.50 |
| 20 | g | 1000 | SER | CA-C-N | 5.08 | 128.04 | 120.31 |
| 20 | g | 1000 | SER | C-N-CA | 5.08 | 128.04 | 120.31 |
| 1 | 0 | 1346 | SER | N-CA-CB | 5.08 | 118.16 | 110.28 |
| 2 | 1 | 850 | HIS | CE1-NE2-CD2 | -5.08 | 103.92 | 109.00 |
| 4 | J | 683 | ALA | O-C-N | -5.08 | 116.73 | 122.12 |
| 5 | K | 397 | ARG | N-CA-C | 5.08 | 117.72 | 111.82 |
| 7 | M | 1480 | MET | CA-C-N | 5.08 | 127.51 | 120.29 |
| 7 | M | 1480 | MET | C-N-CA | 5.08 | 127.51 | 120.29 |
| 8 | N | 1459 | LYS | CB-CA-C | 5.08 | 119.77 | 110.11 |
| 7 | O | 1531 | THR | O-C-N | 5.08 | 127.31 | 122.07 |
| 9 | R | 280 | GLN | CA-C-O | -5.08 | 113.55 | 119.14 |
| 9 | S | 227 | GLN | OE1-CD-NE2 | -5.08 | 117.52 | 122.60 |
| 12 | u | 219 | ASN | N-CA-C | -5.08 | 101.59 | 109.72 |
| 12 | u | 433 | ASP | N-CA-CB | 5.08 | 119.08 | 110.49 |
| 13 | x | 1222 | GLU | N-CA-C | 5.08 | 116.82 | 111.28 |
| 13 | x | 1305 | GLN | O-C-N | 5.08 | 127.51 | 122.12 |
| 16 | j | 582 | LEU | CA-C-N | -5.08 | 114.67 | 122.60 |
| 16 | j | 582 | LEU | C-N-CA | -5.08 | 114.67 | 122.60 |
| 20 | g | 580 | SER | CA-C-N | 5.08 | 126.19 | 119.84 |
| 20 | g | 580 | SER | C-N-CA | 5.08 | 126.19 | 119.84 |
| 1 | 0 | 102 | ASP | CA-C-O | 5.08 | 125.81 | 120.42 |
| 1 | 0 | 165 | SER | N-CA-C | -5.08 | 106.77 | 113.17 |
| 6 | L | 293 | HIS | CB-CG-ND1 | 5.08 | 130.32 | 122.70 |
| 7 | M | 1166 | HIS | CE1-NE2-CD2 | -5.08 | 103.92 | 109.00 |
| 8 | N | 199 | ILE | N-CA-C | -5.08 | 105.92 | 113.39 |
| 8 | P | 414 | ASN | CA-C-N | 5.08 | 131.25 | 121.54 |
| 8 | P | 414 | ASN | C-N-CA | 5.08 | 131.25 | 121.54 |
| 8 | P | 1091 | ASP | CA-CB-CG | 5.08 | 117.68 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1130 | PHE | CA-C-N | 5.08 | 127.05 | 120.44 |
| 8 | P | 1130 | PHE | C-N-CA | 5.08 | 127.05 | 120.44 |
| 9 | Q | 542 | THR | CA-C-N | 5.08 | 129.32 | 120.68 |
| 9 | Q | 542 | THR | C-N-CA | 5.08 | 129.32 | 120.68 |
| 10 | W | 327 | ALA | CA-C-O | -5.08 | 113.46 | 119.05 |
| 1 | Y | 1092 | ASP | CA-C-N | 5.08 | 131.24 | 121.54 |
| 1 | Y | 1092 | ASP | C-N-CA | 5.08 | 131.24 | 121.54 |
| 1 | Y | 1438 | ASP | N-CA-C | -5.08 | 107.08 | 113.28 |
| 4 | z | 652 | ALA | CA-C-N | 5.08 | 127.05 | 120.44 |
| 4 | z | 652 | ALA | C-N-CA | 5.08 | 127.05 | 120.44 |
| 15 | i | 303 | PHE | CA-CB-CG | -5.08 | 108.72 | 113.80 |
| 15 | i | 308 | ASN | N-CA-CB | 5.08 | 118.16 | 110.28 |
| 18 | l | 88 | PRO | N-CA-C | -5.08 | 109.39 | 114.68 |
| 15 | b | 107 | TYR | CB-CA-C | 5.08 | 119.23 | 110.79 |
| 15 | b | 551 | ASN | CA-C-N | 5.08 | 127.64 | 120.42 |
| 15 | b | 551 | ASN | C-N-CA | 5.08 | 127.64 | 120.42 |
| 15 | b | 577 | GLU | CB-CG-CD | 5.08 | 121.24 | 112.60 |
| 16 | c | 315 | ASN | OD1-CG-ND2 | -5.08 | 117.52 | 122.60 |
| 16 | c | 566 | ASP | N-CA-C | -5.08 | 100.62 | 108.90 |
| 18 | e | 192 | ILE | CA-CB-CG2 | -5.08 | 101.86 | 110.50 |
| 6 | C | 385 | GLU | CA-C-O | 5.08 | 125.81 | 120.42 |
| 7 | M | 832 | PHE | O-C-N | 5.08 | 127.50 | 122.12 |
| 7 | M | 1086 | LEU | O-C-N | -5.08 | 116.74 | 122.12 |
| 7 | O | 459 | ASP | N-CA-CB | 5.08 | 117.92 | 110.35 |
| 9 | T | 706 | ILE | N-CA-C | -5.08 | 101.02 | 108.54 |
| 12 | v | 630 | TRP | CA-C-O | -5.08 | 115.17 | 120.55 |
| 20 | n | 417 | LEU | N-CA-CB | 5.08 | 118.69 | 110.41 |
| 15 | b | 186 | ARG | N-CA-C | 5.08 | 116.82 | 111.28 |
| 1 | 0 | 1310 | ASP | CA-CB-CG | 5.08 | 117.68 | 112.60 |
| 2 | 1 | 1013 | LYS | N-CA-C | 5.08 | 119.19 | 112.89 |
| 5 | E | 391 | GLU | N-CA-C | -5.08 | 108.35 | 114.75 |
| 4 | G | 792 | GLN | CA-C-N | 5.08 | 127.04 | 120.44 |
| 4 | G | 792 | GLN | C-N-CA | 5.08 | 127.04 | 120.44 |
| 8 | P | 61 | ASN | OD1-CG-ND2 | -5.08 | 117.52 | 122.60 |
| 9 | Q | 277 | TYR | CA-C-N | 5.08 | 127.59 | 120.28 |
| 9 | Q | 277 | TYR | C-N-CA | 5.08 | 127.59 | 120.28 |
| 9 | R | 476 | ASN | CB-CA-C | 5.08 | 120.53 | 110.42 |
| 9 | S | 139 | PHE | CA-C-O | 5.08 | 126.15 | 120.82 |
| 2 | Z | 128 | GLU | CA-C-N | -5.08 | 116.02 | 122.37 |
| 2 | Z | 128 | GLU | C-N-CA | -5.08 | 116.02 | 122.37 |
| 2 | Z | 380 | ASP | CA-C-N | 5.08 | 127.08 | 120.28 |
| 2 | Z | 380 | ASP | C-N-CA | 5.08 | 127.08 | 120.28 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 1002 | ILE | CA-C-N | 5.08 | 127.08 | 120.28 |
| 2 | Z | 1002 | ILE | C-N-CA | 5.08 | 127.08 | 120.28 |
| 18 | l | 62 | ASP | CA-C-O | -5.08 | 113.35 | 120.21 |
| 18 | l | 333 | ALA | N-CA-C | 5.08 | 117.80 | 110.28 |
| 18 | e | 118 | PRO | CA-C-O | -5.08 | 115.74 | 121.43 |
| 19 | f | 548 | GLN | OE1-CD-NE2 | 5.08 | 127.68 | 122.60 |
| 5 | H | 528 | GLU | N-CA-C | 5.08 | 116.81 | 111.28 |
| 7 | O | 1674 | CYS | CA-C-O | -5.08 | 115.49 | 120.82 |
| 8 | P | 477 | LEU | O-C-N | 5.08 | 127.50 | 122.12 |
| 9 | Q | 456 | ARG | CA-C-N | 5.08 | 128.91 | 120.94 |
| 9 | Q | 456 | ARG | C-N-CA | 5.08 | 128.91 | 120.94 |
| 9 | R | 260 | LEU | CA-C-N | 5.08 | 127.08 | 120.28 |
| 9 | R | 260 | LEU | C-N-CA | 5.08 | 127.08 | 120.28 |
| 2 | Z | 104 | ARG | CA-CB-CG | -5.08 | 103.95 | 114.10 |
| 18 | e | 173 | TRP | CA-C-N | 5.08 | 127.45 | 120.39 |
| 18 | e | 173 | TRP | C-N-CA | 5.08 | 127.45 | 120.39 |
| 20 | g | 873 | GLN | CA-C-N | 5.08 | 127.08 | 120.28 |
| 20 | g | 873 | GLN | C-N-CA | 5.08 | 127.08 | 120.28 |
| 2 | 1 | 496 | THR | CA-C-N | 5.08 | 128.06 | 120.90 |
| 2 | 1 | 496 | THR | C-N-CA | 5.08 | 128.06 | 120.90 |
| 8 | N | 861 | ILE | N-CA-C | -5.08 | 105.44 | 110.62 |
| 8 | N | 1446 | PHE | CA-C-O | -5.08 | 115.49 | 121.07 |
| 9 | Q | 51 | ARG | N-CA-CB | 5.08 | 118.19 | 110.42 |
| 2 | Z | 953 | ILE | CA-C-O | -5.08 | 114.44 | 120.78 |
| 2 | Z | 1321 | LEU | CA-C-O | 5.08 | 124.72 | 119.14 |
| 12 | u | 41 | ASN | N-CA-CB | 5.08 | 119.07 | 110.49 |
| 12 | u | 225 | LEU | O-C-N | 5.08 | 127.57 | 122.09 |
| 12 | v | 113 | HIS | N-CA-CB | 5.08 | 119.07 | 110.49 |
| 13 | w | 1142 | VAL | N-CA-CB | 5.08 | 119.61 | 111.23 |
| 4 | y | 662 | ILE | CA-C-N | 5.08 | 127.04 | 120.44 |
| 4 | y | 662 | ILE | C-N-CA | 5.08 | 127.04 | 120.44 |
| 19 | m | 220 | ASN | CA-C-N | 5.08 | 126.19 | 119.84 |
| 19 | m | 220 | ASN | C-N-CA | 5.08 | 126.19 | 119.84 |
| 21 | o | 9 | PRO | N-CA-C | 5.08 | 119.06 | 111.14 |
| 15 | b | 402 | ILE | N-CA-C | -5.08 | 98.78 | 109.34 |
| 17 | d | 107 | TRP | CZ3-CH2-CZ2 | 5.08 | 128.10 | 121.50 |
| 1 | 0 | 1203 | TYR | CA-C-O | 5.07 | 126.49 | 120.66 |
| 4 | G | 695 | GLN | N-CA-C | 5.07 | 117.70 | 111.82 |
| 8 | P | 163 | ASP | O-C-N | -5.07 | 116.05 | 122.19 |
| 8 | P | 410 | GLN | N-CA-CB | 5.07 | 118.28 | 110.21 |
| 9 | R | 222 | PHE | CA-C-N | 5.07 | 127.39 | 120.54 |
| 9 | R | 222 | PHE | C-N-CA | 5.07 | 127.39 | 120.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | T | 607 | ARG | NE-CZ-NH2 | 5.07 | 123.77 | 119.20 |
| 11 | X | 402 | ASN | CA-CB-CG | -5.07 | 107.53 | 112.60 |
| 12 | u | 228 | ASN | CB-CA-C | 5.07 | 119.48 | 110.85 |
| 4 | z | 647 | GLN | CA-C-N | 5.07 | 127.84 | 120.79 |
| 4 | z | 647 | GLN | C-N-CA | 5.07 | 127.84 | 120.79 |
| 14 | h | 694 | ASN | CA-CB-CG | 5.07 | 117.67 | 112.60 |
| 14 | h | 1007 | LEU | O-C-N | -5.07 | 115.78 | 122.42 |
| 16 | j | 480 | GLN | CA-CB-CG | 5.07 | 124.25 | 114.10 |
| 9 | Q | 346 | ILE | CA-C-N | 5.07 | 127.58 | 120.28 |
| 9 | Q | 346 | ILE | C-N-CA | 5.07 | 127.58 | 120.28 |
| 9 | Q | 725 | GLU | N-CA-CB | -5.07 | 102.72 | 110.07 |
| 16 | j | 280 | ILE | N-CA-CB | 5.07 | 116.48 | 110.55 |
| 16 | j | 343 | TRP | CH2-CZ2-CE2 | 5.07 | 124.09 | 117.50 |
| 20 | g | 396 | LYS | N-CA-CB | 5.07 | 119.40 | 110.37 |
| 20 | g | 1130 | GLU | O-C-N | -5.07 | 116.74 | 122.12 |
| 1 | 0 | 1413 | VAL | CG1-CB-CG2 | -5.07 | 99.64 | 110.80 |
| 4 | A | 686 | ALA | CB-CA-C | -5.07 | 102.37 | 110.79 |
| 6 | C | 348 | GLN | N-CA-C | 5.07 | 116.81 | 111.28 |
| 6 | C | 403 | THR | O-C-N | 5.07 | 129.46 | 122.46 |
| 5 | K | 524 | ASN | N-CA-C | -5.07 | 105.64 | 111.07 |
| 7 | M | 1236 | ILE | CA-CB-CG2 | -5.07 | 101.88 | 110.50 |
| 8 | N | 670 | HIS | CE1-NE2-CD2 | -5.07 | 103.93 | 109.00 |
| 8 | N | 703 | GLY | N-CA-C | -5.07 | 101.16 | 113.18 |
| 9 | R | 223 | ASN | CA-CB-CG | -5.07 | 107.53 | 112.60 |
| 9 | S | 299 | ALA | CA-C-N | 5.07 | 130.14 | 122.99 |
| 9 | S | 299 | ALA | C-N-CA | 5.07 | 130.14 | 122.99 |
| 9 | S | 786 | ILE | O-C-N | -5.07 | 116.95 | 121.87 |
| 9 | T | 223 | ASN | CA-CB-CG | -5.07 | 107.53 | 112.60 |
| 11 | V | 377 | PHE | N-CA-C | -5.07 | 100.00 | 110.80 |
| 2 | Z | 656 | HIS | ND1-CE1-NE2 | 5.07 | 113.47 | 108.40 |
| 12 | v | 273 | GLN | OE1-CD-NE2 | 5.07 | 127.67 | 122.60 |
| 14 | h | 983 | GLN | O-C-N | -5.07 | 115.78 | 122.42 |
| 16 | j | 593 | LYS | N-CA-CB | 5.07 | 117.57 | 110.12 |
| 19 | m | 353 | ASP | N-CA-CB | 5.07 | 119.62 | 111.91 |
| 20 | n | 722 | PHE | CG-CD1-CE1 | 5.07 | 129.32 | 120.70 |
| 15 | b | 679 | ASP | N-CA-C | -5.07 | 104.62 | 108.78 |
| 16 | c | 158 | MET | N-CA-C | -5.07 | 101.98 | 109.18 |
| 16 | c | 585 | ASN | O-C-N | -5.07 | 115.85 | 121.53 |
| 20 | g | 1078 | LEU | N-CA-C | -5.07 | 102.79 | 110.50 |
| 7 | M | 1661 | GLN | CA-C-N | 5.07 | 127.07 | 120.28 |
| 7 | M | 1661 | GLN | C-N-CA | 5.07 | 127.07 | 120.28 |
| 8 | P | 1385 | LEU | CA-C-N | 5.07 | 127.34 | 120.65 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | P | 1385 | LEU | C-N-CA | 5.07 | 127.34 | 120.65 |
| 2 | Z | 106 | ARG | NE-CZ-NH2 | 5.07 | 123.76 | 119.20 |
| 20 | n | 982 | GLU | CB-CG-CD | -5.07 | 103.98 | 112.60 |
| 5 | B | 528 | GLU | N-CA-C | 5.07 | 116.80 | 111.28 |
| 6 | F | 324 | GLN | O-C-N | 5.07 | 127.49 | 122.12 |
| 7 | O | 315 | GLU | N-CA-C | -5.07 | 106.34 | 112.88 |
| 8 | P | 634 | ILE | CA-C-O | -5.07 | 115.78 | 121.05 |
| 8 | P | 650 | ASP | CA-C-N | 5.07 | 127.78 | 120.38 |
| 8 | P | 650 | ASP | C-N-CA | 5.07 | 127.78 | 120.38 |
| 8 | P | 1122 | PHE | N-CA-C | -5.07 | 105.57 | 112.26 |
| 8 | P | 1595 | LYS | CA-C-O | -5.07 | 114.37 | 120.10 |
| 9 | S | 47 | ASN | N-CA-C | -5.07 | 100.45 | 109.06 |
| 1 | Y | 1471 | ILE | N-CA-C | 5.07 | 115.18 | 110.42 |
| 14 | h | 433 | ILE | O-C-N | -5.07 | 117.86 | 123.18 |
| 16 | j | 551 | ASN | OD1-CG-ND2 | -5.07 | 117.53 | 122.60 |
| 21 | p | 63 | LYS | N-CA-C | -5.07 | 106.01 | 113.61 |
| 16 | c | 417 | PRO | CA-C-N | 5.07 | 129.35 | 121.35 |
| 16 | c | 417 | PRO | C-N-CA | 5.07 | 129.35 | 121.35 |
| 14 | a | 444 | ALA | CA-C-O | -5.07 | 115.48 | 120.90 |
| 14 | a | 823 | ALA | CA-C-N | 5.07 | 127.58 | 120.28 |
| 14 | a | 823 | ALA | C-N-CA | 5.07 | 127.58 | 120.28 |
| 14 | a | 927 | ASN | CA-CB-CG | -5.07 | 107.53 | 112.60 |
| 1 | 0 | 1299 | GLY | N-CA-C | -5.07 | 107.61 | 115.67 |
| 2 | 1 | 1060 | TYR | CA-C-N | 5.07 | 129.29 | 120.68 |
| 2 | 1 | 1060 | TYR | C-N-CA | 5.07 | 129.29 | 120.68 |
| 8 | N | 1431 | ILE | N-CA-C | -5.07 | 107.91 | 113.43 |
| 7 | O | 624 | ASP | CA-C-O | 5.07 | 126.73 | 121.31 |
| 7 | O | 1351 | GLU | N-CA-CB | 5.07 | 117.36 | 110.01 |
| 8 | P | 68 | HIS | CE1-NE2-CD2 | -5.07 | 103.94 | 109.00 |
| 8 | P | 365 | LEU | CA-C-O | -5.07 | 115.18 | 120.55 |
| 8 | P | 913 | ASN | CA-CB-CG | -5.07 | 107.53 | 112.60 |
| 9 | R | 137 | ASP | CA-C-N | 5.07 | 127.03 | 120.44 |
| 9 | R | 137 | ASP | C-N-CA | 5.07 | 127.03 | 120.44 |
| 9 | S | 430 | LEU | N-CA-C | -5.07 | 106.24 | 114.09 |
| 9 | T | 155 | VAL | CA-C-N | 5.07 | 127.38 | 120.54 |
| 9 | T | 155 | VAL | C-N-CA | 5.07 | 127.38 | 120.54 |
| 1 | Y | 1385 | PHE | CA-C-N | 5.07 | 126.17 | 119.84 |
| 1 | Y | 1385 | PHE | C-N-CA | 5.07 | 126.17 | 119.84 |
| 2 | Z | 360 | LYS | N-CA-C | -5.07 | 107.10 | 113.28 |
| 12 | v | 50 | THR | O-C-N | -5.07 | 115.85 | 122.59 |
| 13 | w | 1235 | MET | CA-C-O | 5.07 | 126.14 | 120.82 |
| 14 | h | 771 | ASP | CA-C-N | 5.07 | 127.48 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 771 | ASP | C-N-CA | 5.07 | 127.48 | 120.29 |
| 15 | i | 284 | ALA | CA-C-O | 5.07 | 125.57 | 119.59 |
| 20 | n | 515 | ASN | CA-C-N | 5.07 | 127.05 | 120.26 |
| 20 | n | 515 | ASN | C-N-CA | 5.07 | 127.05 | 120.26 |
| 16 | c | 258 | ALA | N-CA-CB | 5.07 | 117.66 | 110.16 |
| 18 | e | 213 | SER | O-C-N | -5.07 | 116.64 | 123.23 |
| 19 | f | 430 | PRO | CB-CA-C | -5.07 | 104.95 | 112.55 |
| 20 | g | 620 | ASN | CA-C-N | 5.07 | 131.33 | 122.82 |
| 20 | g | 620 | ASN | C-N-CA | 5.07 | 131.33 | 122.82 |
| 14 | a | 802 | TYR | CB-CG-CD1 | 5.07 | 128.40 | 120.80 |
| 1 | 0 | 202 | GLN | CA-C-O | 5.06 | 127.36 | 121.44 |
| 8 | N | 682 | LEU | CA-C-N | 5.06 | 131.21 | 121.54 |
| 8 | N | 682 | LEU | C-N-CA | 5.06 | 131.21 | 121.54 |
| 8 | N | 1309 | ARG | NE-CZ-NH1 | -5.06 | 116.44 | 121.50 |
| 7 | O | 554 | SER | CA-C-N | 5.06 | 127.02 | 120.44 |
| 7 | O | 554 | SER | C-N-CA | 5.06 | 127.02 | 120.44 |
| 7 | O | 669 | THR | N-CA-C | 5.06 | 117.46 | 111.33 |
| 9 | R | 539 | ALA | CA-C-N | 5.06 | 127.57 | 120.28 |
| 9 | R | 539 | ALA | C-N-CA | 5.06 | 127.57 | 120.28 |
| 1 | Y | 454 | ARG | CD-NE-CZ | -5.06 | 117.31 | 124.40 |
| 1 | Y | 1205 | SER | CB-CA-C | -5.06 | 99.73 | 110.31 |
| 20 | n | 897 | ALA | N-CA-CB | 5.06 | 117.32 | 109.98 |
| 19 | f | 596 | GLU | N-CA-CB | 5.06 | 117.98 | 110.49 |
| 20 | g | 389 | SER | N-CA-C | -5.06 | 101.45 | 109.76 |
| 1 | 0 | 162 | HIS | CG-CD2-NE2 | 5.06 | 112.26 | 107.20 |
| 6 | F | 295 | LYS | N-CA-C | 5.06 | 117.53 | 111.71 |
| 7 | O | 1383 | GLN | CA-C-N | 5.06 | 127.37 | 120.54 |
| 7 | O | 1383 | GLN | C-N-CA | 5.06 | 127.37 | 120.54 |
| 8 | P | 1232 | HIS | ND1-CE1-NE2 | 5.06 | 113.46 | 108.40 |
| 9 | Q | 457 | TYR | CA-C-N | 5.06 | 128.40 | 120.75 |
| 9 | Q | 457 | TYR | C-N-CA | 5.06 | 128.40 | 120.75 |
| 9 | R | 761 | SER | CA-C-N | 5.06 | 130.16 | 122.87 |
| 9 | R | 761 | SER | C-N-CA | 5.06 | 130.16 | 122.87 |
| 9 | T | 834 | ASN | CB-CA-C | 5.06 | 120.33 | 111.06 |
| 2 | Z | 727 | ARG | NH1-CZ-NH2 | 5.06 | 125.88 | 119.30 |
| 2 | Z | 1008 | ILE | N-CA-CB | 5.06 | 117.05 | 110.57 |
| 14 | h | 167 | PHE | CA-CB-CG | -5.06 | 108.74 | 113.80 |
| 16 | j | 222 | ASP | N-CA-C | 5.06 | 116.80 | 111.28 |
| 18 | l | 51 | TRP | CA-C-N | 5.06 | 129.13 | 122.30 |
| 18 | l | 51 | TRP | C-N-CA | 5.06 | 129.13 | 122.30 |
| 20 | n | 512 | ILE | O-C-N | -5.06 | 117.68 | 123.10 |
| 20 | n | 915 | GLU | O-C-N | -5.06 | 115.86 | 122.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | f | 239 | LYS | N-CA-CB | 5.06 | 118.24 | 110.70 |
| 14 | a | 71 | HIS | CA-CB-CG | 5.06 | 118.86 | 113.80 |
| 7 | M | 814 | ASN | CA-C-N | 5.06 | 131.21 | 121.54 |
| 7 | M | 814 | ASN | C-N-CA | 5.06 | 131.21 | 121.54 |
| 7 | O | 1402 | ARG | CA-CB-CG | 5.06 | 124.22 | 114.10 |
| 9 | R | 726 | LEU | N-CA-C | 5.06 | 117.69 | 111.82 |
| 9 | S | 538 | LEU | N-CA-C | -5.06 | 106.27 | 112.90 |
| 11 | V | 358 | LEU | CA-C-O | 5.06 | 126.50 | 120.28 |
| 16 | j | 167 | LYS | CA-C-O | -5.06 | 114.15 | 119.97 |
| 20 | n | 413 | VAL | N-CA-C | -5.06 | 101.06 | 108.85 |
| 19 | f | 293 | ILE | O-C-N | 5.06 | 126.78 | 121.87 |
| 1 | 0 | 1410 | GLY | N-CA-C | 5.06 | 119.87 | 113.24 |
| 6 | L | 392 | SER | CA-C-O | -5.06 | 115.19 | 120.55 |
| 7 | M | 1400 | ALA | CA-C-O | 5.06 | 125.78 | 120.42 |
| 7 | M | 1499 | LEU | CA-C-N | 5.06 | 131.20 | 121.54 |
| 7 | M | 1499 | LEU | C-N-CA | 5.06 | 131.20 | 121.54 |
| 8 | N | 162 | HIS | CG-CD2-NE2 | 5.06 | 112.26 | 107.20 |
| 8 | N | 1394 | LYS | CA-C-N | 5.06 | 127.39 | 120.46 |
| 8 | N | 1394 | LYS | C-N-CA | 5.06 | 127.39 | 120.46 |
| 7 | O | 83 | LEU | N-CA-CB | 5.06 | 119.04 | 110.49 |
| 7 | O | 655 | LYS | CA-C-N | 5.06 | 127.13 | 120.60 |
| 7 | O | 655 | LYS | C-N-CA | 5.06 | 127.13 | 120.60 |
| 7 | O | 775 | ALA | N-CA-C | 5.06 | 116.80 | 111.28 |
| 9 | T | 787 | HIS | ND1-CE1-NE2 | 5.06 | 113.46 | 108.40 |
| 1 | Y | 368 | ILE | CA-C-O | 5.06 | 126.57 | 120.65 |
| 1 | Y | 780 | LEU | N-CA-CB | 5.06 | 117.51 | 109.82 |
| 2 | Z | 443 | ILE | N-CA-C | -5.06 | 101.20 | 108.89 |
| 12 | v | 418 | ALA | O-C-N | 5.06 | 129.14 | 123.27 |
| 13 | w | 1147 | THR | N-CA-C | -5.06 | 101.60 | 109.24 |
| 18 | l | 120 | HIS | ND1-CE1-NE2 | 5.06 | 113.46 | 108.40 |
| 16 | c | 262 | LYS | N-CA-CB | 5.06 | 118.12 | 110.28 |
| 20 | g | 300 | THR | CA-CB-OG1 | 5.06 | 117.19 | 109.60 |
| 1 | 0 | 859 | SER | N-CA-C | -5.06 | 106.36 | 112.88 |
| 1 | 0 | 1462 | PHE | CB-CG-CD1 | -5.06 | 112.10 | 120.70 |
| 2 | 1 | 709 | PHE | CA-C-N | 5.06 | 127.01 | 120.44 |
| 2 | 1 | 709 | PHE | C-N-CA | 5.06 | 127.01 | 120.44 |
| 2 | 1 | 982 | GLU | CA-C-N | 5.06 | 127.47 | 120.29 |
| 2 | 1 | 982 | GLU | C-N-CA | 5.06 | 127.47 | 120.29 |
| 2 | 1 | 1084 | LEU | N-CA-CB | 5.06 | 117.34 | 110.01 |
| 5 | B | 455 | LYS | CA-C-N | 5.06 | 127.51 | 120.63 |
| 5 | B | 455 | LYS | C-N-CA | 5.06 | 127.51 | 120.63 |
| 5 | E | 289 | GLN | CA-C-N | 5.06 | 129.99 | 121.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | E | 289 | GLN | C-N-CA | 5.06 | 129.99 | 121.14 |
| 7 | M | 132 | GLN | N-CA-C | 5.06 | 116.79 | 111.28 |
| 7 | O | 649 | LEU | N-CA-C | -5.06 | 106.36 | 112.88 |
| 7 | O | 892 | LYS | N-CA-C | -5.06 | 105.81 | 112.94 |
| 7 | O | 1494 | ASN | OD1-CG-ND2 | 5.06 | 127.66 | 122.60 |
| 8 | P | 1470 | LEU | CA-C-O | 5.06 | 125.60 | 119.38 |
| 1 | Y | 1318 | HIS | ND1-CE1-NE2 | 5.06 | 113.46 | 108.40 |
| 2 | Z | 805 | ILE | CA-CB-CG1 | 5.06 | 119.00 | 110.40 |
| 14 | h | 99 | ASN | N-CA-C | -5.06 | 101.86 | 109.85 |
| 14 | h | 937 | LEU | CA-C-N | 5.06 | 127.02 | 120.44 |
| 14 | h | 937 | LEU | C-N-CA | 5.06 | 127.02 | 120.44 |
| 18 | l | 95 | GLY | N-CA-C | -5.06 | 101.19 | 113.18 |
| 20 | n | 628 | HIS | CG-CD2-NE2 | 5.06 | 112.26 | 107.20 |
| 16 | c | 539 | PHE | CA-CB-CG | -5.06 | 108.74 | 113.80 |
| 7 | M | 218 | HIS | ND1-CE1-NE2 | 5.06 | 113.46 | 108.40 |
| 7 | M | 1213 | LEU | N-CA-CB | 5.06 | 119.03 | 110.49 |
| 8 | P | 373 | PRO | N-CD-CG | 5.06 | 110.78 | 103.20 |
| 9 | S | 372 | LYS | CA-C-O | -5.06 | 115.06 | 120.42 |
| 14 | h | 398 | VAL | CA-C-O | -5.06 | 114.46 | 120.78 |
| 20 | n | 452 | ASP | CA-CB-CG | 5.06 | 117.66 | 112.60 |
| 20 | n | 843 | PHE | N-CA-CB | -5.06 | 102.69 | 110.12 |
| 16 | c | 615 | ASN | CA-C-N | 5.06 | 127.39 | 120.46 |
| 16 | c | 615 | ASN | C-N-CA | 5.06 | 127.39 | 120.46 |
| 19 | f | 125 | TRP | N-CA-C | -5.06 | 99.17 | 108.02 |
| 14 | a | 400 | LYS | N-CA-CB | 5.06 | 118.73 | 111.65 |
| 8 | N | 463 | PHE | CA-C-O | -5.05 | 115.33 | 120.99 |
| 8 | N | 666 | PRO | N-CD-CG | 5.05 | 110.78 | 103.20 |
| 8 | N | 1072 | TYR | CA-C-O | -5.05 | 113.58 | 119.14 |
| 8 | P | 1490 | ARG | NH1-CZ-NH2 | -5.05 | 112.73 | 119.30 |
| 9 | Q | 603 | VAL | CA-C-N | 5.05 | 127.39 | 120.46 |
| 9 | Q | 603 | VAL | C-N-CA | 5.05 | 127.39 | 120.46 |
| 11 | X | 362 | SER | CA-C-O | -5.05 | 114.75 | 120.46 |
| 14 | h | 442 | TYR | CA-C-N | 5.05 | 127.01 | 120.44 |
| 14 | h | 442 | TYR | C-N-CA | 5.05 | 127.01 | 120.44 |
| 18 | l | 130 | ASN | OD1-CG-ND2 | 5.05 | 127.65 | 122.60 |
| 19 | m | 658 | LEU | CA-C-N | -5.05 | 112.12 | 122.58 |
| 19 | m | 658 | LEU | C-N-CA | -5.05 | 112.12 | 122.58 |
| 20 | n | 595 | ASN | O-C-N | -5.05 | 115.59 | 122.36 |
| 15 | b | 551 | ASN | CA-CB-CG | 5.05 | 117.65 | 112.60 |
| 16 | c | 524 | ASP | CA-CB-CG | 5.05 | 117.66 | 112.60 |
| 17 | d | 37 | GLU | CA-C-O | 5.05 | 127.77 | 121.81 |
| 20 | g | 1028 | LEU | O-C-N | 5.05 | 128.96 | 122.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | 1 | 1354 | ASP | CA-C-N | 5.05 | 128.52 | 121.24 |
| 2 | 1 | 1354 | ASP | C-N-CA | 5.05 | 128.52 | 121.24 |
| 4 | D | 819 | ASN | CB-CG-ND2 | 5.05 | 123.98 | 116.40 |
| 5 | H | 405 | ASN | CB-CG-OD1 | 5.05 | 130.91 | 120.80 |
| 8 | P | 1621 | LEU | CA-C-N | 5.05 | 127.01 | 120.44 |
| 8 | P | 1621 | LEU | C-N-CA | 5.05 | 127.01 | 120.44 |
| 13 | x | 1232 | ILE | CB-CA-C | -5.05 | 105.32 | 112.14 |
| 4 | y | 680 | TYR | CA-C-N | 5.05 | 127.31 | 120.44 |
| 4 | y | 680 | TYR | C-N-CA | 5.05 | 127.31 | 120.44 |
| 5 | B | 374 | ILE | CA-C-N | 5.05 | 127.59 | 120.42 |
| 5 | B | 374 | ILE | C-N-CA | 5.05 | 127.59 | 120.42 |
| 5 | B | 395 | ALA | CA-C-N | 5.05 | 127.46 | 120.29 |
| 5 | B | 395 | ALA | C-N-CA | 5.05 | 127.46 | 120.29 |
| 6 | I | 397 | ALA | CA-C-N | 5.05 | 126.93 | 120.56 |
| 6 | I | 397 | ALA | C-N-CA | 5.05 | 126.93 | 120.56 |
| 7 | M | 1445 | VAL | N-CA-CB | 5.05 | 117.04 | 110.57 |
| 7 | O | 233 | TYR | CA-C-O | 5.05 | 126.24 | 119.47 |
| 9 | R | 312 | LYS | CA-C-N | 5.05 | 131.19 | 121.54 |
| 9 | R | 312 | LYS | C-N-CA | 5.05 | 131.19 | 121.54 |
| 9 | R | 689 | ALA | N-CA-C | 5.05 | 116.48 | 111.07 |
| 9 | T | 787 | HIS | CA-C-O | -5.05 | 114.16 | 119.97 |
| 1 | Y | 128 | ASN | N-CA-CB | 5.05 | 119.66 | 111.27 |
| 13 | x | 1105 | ALA | CA-C-O | 5.05 | 127.35 | 121.44 |
| 16 | j | 273 | VAL | CB-CA-C | 5.05 | 118.96 | 112.14 |
| 20 | n | 997 | VAL | N-CA-C | -5.05 | 98.83 | 109.34 |
| 21 | q | 69 | VAL | CA-C-N | 5.05 | 128.02 | 120.95 |
| 21 | q | 69 | VAL | C-N-CA | 5.05 | 128.02 | 120.95 |
| 20 | g | 855 | LYS | CA-C-O | -5.05 | 116.05 | 121.56 |
| 14 | a | 230 | HIS | CE1-NE2-CD2 | -5.05 | 103.95 | 109.00 |
| 14 | a | 869 | HIS | CE1-NE2-CD2 | -5.05 | 103.95 | 109.00 |
| 7 | M | 340 | LEU | CA-C-O | 5.05 | 127.77 | 121.81 |
| 8 | N | 139 | GLY | CA-C-N | 5.05 | 127.99 | 120.31 |
| 8 | N | 139 | GLY | C-N-CA | 5.05 | 127.99 | 120.31 |
| 7 | O | 153 | THR | CA-CB-OG1 | 5.05 | 117.17 | 109.60 |
| 7 | O | 569 | ILE | CA-C-N | 5.05 | 128.68 | 120.60 |
| 7 | O | 569 | ILE | C-N-CA | 5.05 | 128.68 | 120.60 |
| 9 | R | 670 | LEU | O-C-N | 5.05 | 128.26 | 122.25 |
| 9 | R | 792 | SER | N-CA-C | -5.05 | 105.50 | 113.02 |
| 9 | S | 351 | GLN | CA-C-O | 5.05 | 125.77 | 120.42 |
| 9 | S | 487 | LEU | O-C-N | 5.05 | 128.90 | 122.84 |
| 9 | S | 830 | SER | N-CA-CB | 5.05 | 117.54 | 110.12 |
| 9 | T | 663 | ASP | N-CA-C | 5.05 | 116.47 | 110.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 440 | THR | CA-CB-OG1 | -5.05 | 102.03 | 109.60 |
| 4 | y | 696 | SER | N-CA-CB | 5.05 | 117.54 | 110.12 |
| 16 | j | 603 | PRO | O-C-N | 5.05 | 129.46 | 122.64 |
| 21 | r | 76 | PHE | CA-CB-CG | -5.05 | 108.75 | 113.80 |
| 20 | g | 539 | PHE | CA-C-O | 5.05 | 125.47 | 119.56 |
| 5 | E | 453 | LEU | CA-C-O | -5.05 | 113.67 | 119.78 |
| 7 | M | 1627 | LYS | CA-C-O | 5.05 | 125.77 | 120.42 |
| 8 | N | 588 | HIS | CB-CG-CD2 | 5.05 | 137.76 | 131.20 |
| 8 | P | 1441 | GLN | CG-CD-NE2 | -5.05 | 108.83 | 116.40 |
| 12 | v | 578 | ARG | CB-CA-C | -5.05 | 102.41 | 110.79 |
| 13 | w | 1270 | LEU | N-CA-C | 5.05 | 116.78 | 111.28 |
| 14 | h | 535 | ILE | CB-CA-C | 5.05 | 118.12 | 111.81 |
| 15 | i | 223 | TYR | N-CA-CB | 5.05 | 118.23 | 110.61 |
| 19 | f | 31 | ASN | N-CA-C | -5.05 | 102.70 | 110.32 |
| 14 | a | 539 | GLU | CA-C-N | 5.05 | 131.11 | 122.38 |
| 14 | a | 539 | GLU | C-N-CA | 5.05 | 131.11 | 122.38 |
| 2 | 1 | 842 | GLU | N-CA-C | 5.05 | 116.78 | 111.28 |
| 4 | A | 696 | SER | CA-C-N | 5.05 | 127.04 | 120.28 |
| 4 | A | 696 | SER | C-N-CA | 5.05 | 127.04 | 120.28 |
| 5 | B | 524 | ASN | N-CA-CB | 5.05 | 117.33 | 110.01 |
| 4 | G | 771 | ASN | CB-CA-C | -5.05 | 102.41 | 110.79 |
| 5 | H | 368 | ASN | N-CA-C | 5.05 | 116.86 | 111.36 |
| 7 | O | 178 | ASN | CA-CB-CG | 5.05 | 117.65 | 112.60 |
| 8 | P | 752 | SER | CA-C-N | 5.05 | 127.04 | 120.28 |
| 8 | P | 752 | SER | C-N-CA | 5.05 | 127.04 | 120.28 |
| 9 | R | 96 | LEU | N-CA-CB | 5.05 | 117.33 | 110.01 |
| 9 | S | 83 | VAL | N-CA-C | 5.05 | 119.84 | 109.34 |
| 9 | T | 344 | GLY | N-CA-C | -5.05 | 106.80 | 115.08 |
| 9 | T | 582 | GLU | N-CA-C | -5.05 | 105.43 | 111.03 |
| 2 | Z | 353 | VAL | CB-CA-C | -5.05 | 104.24 | 111.31 |
| 4 | y | 696 | SER | CA-C-N | 5.05 | 127.45 | 120.29 |
| 4 | y | 696 | SER | C-N-CA | 5.05 | 127.45 | 120.29 |
| 14 | h | 592 | LYS | CA-C-N | 5.05 | 126.16 | 120.66 |
| 14 | h | 592 | LYS | C-N-CA | 5.05 | 126.16 | 120.66 |
| 16 | j | 391 | TYR | CB-CG-CD2 | -5.05 | 113.23 | 120.80 |
| 17 | k | 171 | ARG | N-CA-C | -5.05 | 101.41 | 109.23 |
| 19 | m | 401 | PRO | CB-CA-C | -5.05 | 104.31 | 111.68 |
| 21 | q | 34 | LYS | N-CA-C | -5.05 | 107.11 | 114.12 |
| 15 | b | 179 | LEU | CA-C-O | 5.05 | 125.90 | 120.55 |
| 18 | e | 155 | LYS | CB-CA-C | -5.05 | 103.00 | 110.67 |
| 20 | g | 271 | ARG | N-CA-C | -5.05 | 99.76 | 108.69 |
| 14 | a | 663 | LEU | CB-CA-C | -5.05 | 102.41 | 110.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 859 | SER | CA-CB-OG | 5.04 | 121.19 | 111.10 |
| 4 | G | 703 | GLN | CA-C-O | 5.04 | 125.77 | 119.97 |
| 8 | N | 588 | HIS | CG-CD2-NE2 | 5.04 | 112.25 | 107.20 |
| 8 | N | 1208 | GLY | CA-C-N | 5.04 | 127.35 | 120.54 |
| 8 | N | 1208 | GLY | C-N-CA | 5.04 | 127.35 | 120.54 |
| 7 | O | 225 | SER | N-CA-C | -5.04 | 105.85 | 112.41 |
| 9 | S | 215 | TYR | N-CA-C | -5.04 | 105.86 | 111.36 |
| 1 | 0 | 374 | LYS | CA-C-N | 5.04 | 129.35 | 122.34 |
| 1 | 0 | 374 | LYS | C-N-CA | 5.04 | 129.35 | 122.34 |
| 2 | 1 | 184 | ASN | OD1-CG-ND2 | -5.04 | 117.56 | 122.60 |
| 6 | C | 342 | GLU | CA-C-N | 5.04 | 130.14 | 122.37 |
| 6 | C | 342 | GLU | C-N-CA | 5.04 | 130.14 | 122.37 |
| 7 | M | 172 | ASN | CB-CG-ND2 | -5.04 | 108.83 | 116.40 |
| 8 | N | 1288 | PHE | N-CA-CB | -5.04 | 102.50 | 110.06 |
| 8 | N | 1483 | ILE | N-CA-C | -5.04 | 98.77 | 107.24 |
| 7 | O | 868 | ALA | CB-CA-C | -5.04 | 102.74 | 110.81 |
| 7 | O | 1195 | PHE | N-CA-CB | 5.04 | 116.15 | 110.35 |
| 8 | P | 404 | ILE | CA-CB-CG1 | 5.04 | 118.98 | 110.40 |
| 8 | P | 1410 | SER | CB-CA-C | -5.04 | 102.96 | 110.88 |
| 8 | P | 1598 | LEU | CA-C-O | -5.04 | 113.84 | 119.79 |
| 9 | R | 213 | GLU | N-CA-C | 5.04 | 116.78 | 111.28 |
| 9 | R | 417 | ARG | NE-CZ-NH1 | 5.04 | 126.54 | 121.50 |
| 9 | R | 553 | ALA | CB-CA-C | -5.04 | 102.90 | 110.92 |
| 9 | R | 827 | GLU | CA-C-N | 5.04 | 127.00 | 120.44 |
| 9 | R | 827 | GLU | C-N-CA | 5.04 | 127.00 | 120.44 |
| 9 | T | 67 | THR | CA-C-N | 5.04 | 127.00 | 120.44 |
| 9 | T | 67 | THR | C-N-CA | 5.04 | 127.00 | 120.44 |
| 1 | Y | 578 | VAL | CA-C-O | -5.04 | 115.09 | 120.39 |
| 12 | u | 113 | HIS | CE1-NE2-CD2 | -5.04 | 103.96 | 109.00 |
| 15 | i | 416 | THR | O-C-N | 5.04 | 127.47 | 122.12 |
| 20 | n | 650 | LEU | N-CA-C | -5.04 | 105.87 | 112.23 |
| 21 | s | 20 | LEU | O-C-N | 5.04 | 127.90 | 122.15 |
| 17 | d | 176 | GLY | CA-C-O | -5.04 | 115.97 | 121.77 |
| 20 | g | 641 | VAL | CA-C-O | -5.04 | 113.77 | 119.42 |
| 20 | g | 1147 | THR | CB-CA-C | 5.04 | 120.00 | 110.62 |
| 14 | a | 135 | LEU | N-CA-CB | 5.04 | 117.33 | 110.42 |
| 1 | 0 | 673 | TYR | CB-CG-CD1 | 5.04 | 128.36 | 120.80 |
| 2 | 1 | 104 | ARG | CA-C-O | 5.04 | 125.56 | 119.11 |
| 6 | F | 461 | HIS | ND1-CE1-NE2 | 5.04 | 113.44 | 108.40 |
| 4 | J | 819 | ASN | CA-CB-CG | 5.04 | 117.64 | 112.60 |
| 7 | M | 122 | ASN | CA-C-O | -5.04 | 113.50 | 119.05 |
| 8 | N | 1222 | LEU | CA-C-O | 5.04 | 125.90 | 119.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | N | 1335 | GLN | N-CA-CB | 5.04 | 117.98 | 110.22 |
| 7 | O | 1455 | THR | CA-CB-OG1 | 5.04 | 117.16 | 109.60 |
| 9 | Q | 551 | ARG | N-CA-CB | 5.04 | 117.27 | 109.91 |
| 9 | R | 577 | ARG | N-CA-CB | 5.04 | 117.53 | 110.12 |
| 2 | Z | 549 | LYS | N-CA-C | -5.04 | 106.98 | 114.64 |
| 12 | v | 526 | GLU | CB-CA-C | -5.04 | 102.28 | 110.85 |
| 12 | v | 636 | ASN | N-CA-C | 5.04 | 117.67 | 111.82 |
| 19 | m | 341 | HIS | N-CA-C | -5.04 | 103.72 | 110.07 |
| 21 | r | 16 | ILE | CA-C-N | 5.04 | 128.03 | 120.87 |
| 21 | r | 16 | ILE | C-N-CA | 5.04 | 128.03 | 120.87 |
| 21 | t | 30 | ASP | CB-CA-C | -5.04 | 102.97 | 110.88 |
| 15 | b | 172 | PHE | CD1-CG-CD2 | -5.04 | 111.04 | 118.60 |
| 15 | b | 548 | SER | N-CA-C | -5.04 | 104.05 | 111.81 |
| 16 | c | 332 | ILE | CA-C-N | 5.04 | 127.29 | 120.38 |
| 16 | c | 332 | ILE | C-N-CA | 5.04 | 127.29 | 120.38 |
| 20 | g | 437 | TYR | CA-CB-CG | -5.04 | 104.83 | 113.90 |
| 14 | a | 403 | ASP | N-CA-CB | 5.04 | 119.01 | 110.49 |
| 4 | J | 648 | LEU | N-CA-CB | 5.04 | 117.32 | 110.01 |
| 9 | Q | 18 | ALA | N-CA-CB | 5.04 | 117.38 | 110.07 |
| 20 | n | 431 | SER | N-CA-CB | 5.04 | 119.90 | 111.53 |
| 16 | c | 205 | ASN | OD1-CG-ND2 | 5.04 | 127.64 | 122.60 |
| 18 | e | 298 | SER | N-CA-C | 5.04 | 117.61 | 110.10 |
| 2 | 1 | 1000 | LYS | CA-C-N | 5.04 | 126.99 | 120.44 |
| 2 | 1 | 1000 | LYS | C-N-CA | 5.04 | 126.99 | 120.44 |
| 2 | 1 | 1355 | SER | CA-C-N | 5.04 | 131.16 | 121.54 |
| 2 | 1 | 1355 | SER | C-N-CA | 5.04 | 131.16 | 121.54 |
| 7 | M | 1289 | ILE | CA-CB-CG1 | 5.04 | 118.97 | 110.40 |
| 7 | M | 1505 | HIS | O-C-N | 5.04 | 129.11 | 122.36 |
| 8 | N | 348 | LYS | N-CA-C | 5.04 | 116.77 | 111.28 |
| 8 | N | 699 | GLU | N-CA-C | -5.04 | 100.66 | 108.42 |
| 8 | N | 1445 | THR | N-CA-C | 5.04 | 116.77 | 111.28 |
| 7 | O | 145 | LEU | N-CA-CB | 5.04 | 117.62 | 110.16 |
| 7 | O | 820 | GLN | CB-CA-C | -5.04 | 102.63 | 110.94 |
| 9 | Q | 256 | SER | CA-C-N | 5.04 | 127.53 | 120.28 |
| 9 | Q | 256 | SER | C-N-CA | 5.04 | 127.53 | 120.28 |
| 9 | Q | 630 | ARG | NE-CZ-NH1 | -5.04 | 116.46 | 121.50 |
| 9 | T | 351 | GLN | N-CA-CB | 5.04 | 118.09 | 110.28 |
| 1 | Y | 651 | LYS | CA-CB-CG | 5.04 | 124.18 | 114.10 |
| 1 | Y | 942 | LYS | CA-C-O | -5.04 | 114.41 | 120.10 |
| 2 | Z | 583 | PRO | CA-C-N | 5.04 | 131.16 | 121.54 |
| 2 | Z | 583 | PRO | C-N-CA | 5.04 | 131.16 | 121.54 |
| 12 | v | 198 | ASN | CB-CG-ND2 | 5.04 | 123.96 | 116.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | z | 821 | ILE | CA-C-N | 5.04 | 127.34 | 120.54 |
| 4 | z | 821 | ILE | C-N-CA | 5.04 | 127.34 | 120.54 |
| 15 | i | 328 | LEU | N-CA-C | 5.04 | 116.77 | 111.28 |
| 19 | m | 149 | THR | N-CA-CB | 5.04 | 118.04 | 110.53 |
| 19 | m | 549 | PHE | O-C-N | -5.04 | 116.04 | 122.34 |
| 16 | c | 338 | LEU | CA-C-N | 5.04 | 127.03 | 120.28 |
| 16 | c | 338 | LEU | C-N-CA | 5.04 | 127.03 | 120.28 |
| 16 | c | 656 | ALA | CA-C-O | 5.04 | 125.17 | 119.27 |
| 19 | f | 259 | TYR | CA-CB-CG | -5.04 | 104.83 | 113.90 |
| 19 | f | 461 | GLN | O-C-N | 5.04 | 127.46 | 122.12 |
| 20 | g | 239 | LYS | O-C-N | -5.04 | 115.53 | 121.32 |
| 20 | g | 515 | ASN | CA-C-N | 5.04 | 127.01 | 120.26 |
| 20 | g | 515 | ASN | C-N-CA | 5.04 | 127.01 | 120.26 |
| 1 | 0 | 889 | GLU | CA-C-N | 5.04 | 127.30 | 120.65 |
| 1 | 0 | 889 | GLU | C-N-CA | 5.04 | 127.30 | 120.65 |
| 1 | 0 | 1114 | LYS | N-CA-C | -5.04 | 101.41 | 109.07 |
| 2 | 1 | 540 | VAL | CB-CA-C | 5.04 | 116.97 | 110.12 |
| 5 | E | 417 | THR | N-CA-C | -5.04 | 107.08 | 113.18 |
| 7 | M | 720 | HIS | CB-CG-CD2 | -5.04 | 124.65 | 131.20 |
| 1 | Y | 222 | ASN | CA-C-N | 5.04 | 128.36 | 120.75 |
| 1 | Y | 222 | ASN | C-N-CA | 5.04 | 128.36 | 120.75 |
| 1 | Y | 854 | ILE | CA-C-O | -5.04 | 113.42 | 119.36 |
| 1 | Y | 1266 | CYS | CA-C-N | 5.04 | 126.99 | 120.44 |
| 1 | Y | 1266 | CYS | C-N-CA | 5.04 | 126.99 | 120.44 |
| 2 | Z | 275 | THR | CA-C-O | -5.04 | 115.84 | 121.23 |
| 17 | d | 53 | GLU | CA-C-N | 5.04 | 129.78 | 121.87 |
| 17 | d | 53 | GLU | C-N-CA | 5.04 | 129.78 | 121.87 |
| 17 | d | 292 | ALA | N-CA-C | -5.04 | 101.41 | 109.07 |
| 1 | 0 | 1310 | ASP | N-CA-C | -5.04 | 101.25 | 108.60 |
| 2 | 1 | 990 | THR | CA-CB-CG2 | -5.04 | 101.94 | 110.50 |
| 4 | G | 677 | SER | CA-C-O | 5.04 | 125.83 | 120.24 |
| 7 | M | 777 | GLN | OE1-CD-NE2 | -5.04 | 117.56 | 122.60 |
| 7 | M | 1413 | LEU | N-CA-C | 5.04 | 117.50 | 111.71 |
| 8 | N | 557 | TYR | CB-CG-CD2 | -5.04 | 113.25 | 120.80 |
| 7 | O | 282 | PHE | CA-C-N | 5.04 | 127.29 | 120.44 |
| 7 | O | 282 | PHE | C-N-CA | 5.04 | 127.29 | 120.44 |
| 7 | O | 720 | HIS | CG-CD2-NE2 | 5.04 | 112.23 | 107.20 |
| 7 | O | 1169 | SER | O-C-N | -5.04 | 116.46 | 122.20 |
| 8 | P | 322 | HIS | CG-CD2-NE2 | 5.04 | 112.24 | 107.20 |
| 8 | P | 1417 | THR | N-CA-CB | 5.04 | 117.70 | 109.69 |
| 9 | Q | 608 | GLN | CA-C-O | -5.04 | 113.26 | 120.16 |
| 9 | R | 243 | SER | N-CA-C | -5.04 | 105.86 | 112.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | R | 510 | LEU | N-CA-C | -5.04 | 107.20 | 113.55 |
| 9 | S | 600 | ILE | CA-CB-CG2 | 5.04 | 119.06 | 110.50 |
| 2 | Z | 963 | THR | CA-CB-CG2 | -5.04 | 101.94 | 110.50 |
| 12 | v | 383 | GLN | CA-CB-CG | -5.04 | 104.03 | 114.10 |
| 15 | i | 256 | GLY | O-C-N | 5.04 | 128.34 | 122.45 |
| 18 | l | 45 | TRP | CA-C-O | -5.04 | 115.37 | 120.71 |
| 19 | m | 545 | ALA | N-CA-C | -5.04 | 105.61 | 112.26 |
| 19 | f | 694 | VAL | N-CA-C | -5.04 | 107.39 | 112.17 |
| 20 | g | 126 | SER | CA-C-N | 5.04 | 128.85 | 120.94 |
| 20 | g | 126 | SER | C-N-CA | 5.04 | 128.85 | 120.94 |
| 20 | g | 204 | GLY | N-CA-C | -5.04 | 106.11 | 112.65 |
| 20 | g | 259 | LYS | CA-C-O | 5.04 | 126.47 | 120.53 |
| 14 | a | 463 | ILE | N-CA-CB | 5.04 | 119.70 | 111.44 |
| 2 | 1 | 219 | GLU | CA-CB-CG | 5.03 | 124.17 | 114.10 |
| 6 | I | 309 | PRO | O-C-N | 5.03 | 129.07 | 122.27 |
| 7 | O | 558 | ILE | CA-C-N | 5.03 | 127.03 | 120.28 |
| 7 | O | 558 | ILE | C-N-CA | 5.03 | 127.03 | 120.28 |
| 7 | O | 1178 | LEU | O-C-N | 5.03 | 127.46 | 122.12 |
| 9 | Q | 300 | THR | N-CA-C | -5.03 | 101.50 | 109.96 |
| 9 | Q | 687 | LEU | CA-C-N | 5.03 | 127.96 | 120.31 |
| 9 | Q | 687 | LEU | C-N-CA | 5.03 | 127.96 | 120.31 |
| 9 | T | 69 | ALA | N-CA-C | 5.03 | 116.46 | 111.07 |
| 1 | Y | 610 | PRO | CA-C-N | 5.03 | 127.34 | 120.54 |
| 1 | Y | 610 | PRO | C-N-CA | 5.03 | 127.34 | 120.54 |
| 1 | Y | 938 | LEU | N-CA-C | -5.03 | 105.50 | 111.69 |
| 17 | k | 180 | ASN | N-CA-CB | 5.03 | 119.56 | 111.91 |
| 20 | n | 527 | ILE | N-CA-C | -5.03 | 101.06 | 108.11 |
| 20 | g | 665 | PHE | O-C-N | 5.03 | 127.89 | 122.15 |
| 1 | 0 | 1465 | ILE | CB-CA-C | 5.03 | 118.38 | 111.34 |
| 7 | M | 861 | GLN | CG-CD-NE2 | -5.03 | 108.85 | 116.40 |
| 8 | N | 1599 | SER | N-CA-CB | 5.03 | 117.31 | 110.01 |
| 7 | O | 900 | LEU | N-CA-C | -5.03 | 102.25 | 109.24 |
| 12 | u | 164 | ILE | N-CA-C | -5.03 | 101.07 | 108.11 |
| 18 | l | 145 | LEU | O-C-N | 5.03 | 128.52 | 121.83 |
| 20 | g | 180 | SER | N-CA-C | -5.03 | 101.04 | 109.24 |
| 14 | a | 121 | VAL | N-CA-C | -5.03 | 100.82 | 108.17 |
| 6 | F | 357 | LEU | N-CA-CB | -5.03 | 102.16 | 111.52 |
| 7 | M | 446 | CYS | N-CA-C | -5.03 | 106.98 | 112.72 |
| 7 | O | 695 | ALA | N-CA-C | -5.03 | 105.80 | 111.28 |
| 7 | O | 1346 | ASN | OD1-CG-ND2 | -5.03 | 117.57 | 122.60 |
| 9 | Q | 716 | LEU | N-CA-C | 5.03 | 116.57 | 111.14 |
| 9 | S | 267 | ASP | CA-CB-CG | -5.03 | 107.57 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | S | 268 | ILE | O-C-N | 5.03 | 126.82 | 121.89 |
| 9 | S | 355 | GLU | N-CA-C | -5.03 | 103.02 | 110.46 |
| 11 | V | 278 | GLU | N-CA-C | -5.03 | 105.62 | 112.26 |
| 11 | X | 353 | GLU | CB-CA-C | -5.03 | 101.10 | 109.55 |
| 13 | w | 1408 | ARG | CA-C-O | 5.03 | 125.75 | 120.42 |
| 14 | h | 365 | ILE | O-C-N | 5.03 | 127.91 | 123.03 |
| 15 | i | 415 | CYS | CA-C-O | -5.03 | 115.09 | 120.42 |
| 17 | k | 139 | ILE | CA-CB-CG2 | 5.03 | 119.05 | 110.50 |
| 18 | l | 174 | CYS | N-CA-C | -5.03 | 101.37 | 109.82 |
| 18 | l | 226 | ARG | CA-C-N | 5.03 | 130.39 | 122.49 |
| 18 | l | 226 | ARG | C-N-CA | 5.03 | 130.39 | 122.49 |
| 19 | m | 702 | TYR | CA-CB-CG | 5.03 | 122.95 | 113.90 |
| 21 | o | 34 | LYS | N-CA-C | -5.03 | 107.18 | 113.72 |
| 15 | b | 191 | ILE | CA-C-N | 5.03 | 129.94 | 121.14 |
| 15 | b | 191 | ILE | C-N-CA | 5.03 | 129.94 | 121.14 |
| 15 | b | 400 | GLY | CA-C-O | 5.03 | 124.31 | 118.98 |
| 16 | c | 391 | TYR | CB-CA-C | 5.03 | 119.17 | 111.02 |
| 20 | g | 343 | SER | N-CA-C | -5.03 | 100.08 | 110.80 |
| 14 | a | 269 | HIS | CE1-NE2-CD2 | -5.03 | 103.97 | 109.00 |
| 4 | G | 656 | GLU | O-C-N | -5.03 | 116.42 | 122.15 |
| 6 | L | 336 | PHE | CA-C-O | 5.03 | 125.72 | 119.79 |
| 7 | M | 232 | TYR | CB-CA-C | -5.03 | 103.33 | 111.28 |
| 8 | N | 302 | LEU | CA-C-O | -5.03 | 115.53 | 121.16 |
| 10 | U | 305 | TYR | CA-C-N | 5.03 | 126.13 | 119.84 |
| 10 | U | 305 | TYR | C-N-CA | 5.03 | 126.13 | 119.84 |
| 19 | m | 448 | ILE | CB-CA-C | -5.03 | 105.28 | 112.22 |
| 20 | n | 610 | LEU | O-C-N | 5.03 | 128.28 | 122.19 |
| 20 | g | 460 | TYR | CG-CD2-CE2 | 5.03 | 128.74 | 121.20 |
| 5 | E | 306 | THR | CA-CB-CG2 | -5.03 | 101.95 | 110.50 |
| 7 | O | 427 | THR | CA-C-O | 5.03 | 125.82 | 120.24 |
| 7 | O | 920 | ILE | N-CA-C | -5.03 | 98.02 | 108.88 |
| 9 | Q | 373 | ALA | CB-CA-C | -5.03 | 102.52 | 110.81 |
| 9 | R | 435 | TRP | CB-CG-CD1 | -5.03 | 119.36 | 126.90 |
| 9 | R | 704 | ARG | CB-CG-CD | 5.03 | 122.86 | 111.30 |
| 9 | T | 700 | ALA | CA-C-N | 5.03 | 125.52 | 119.94 |
| 9 | T | 700 | ALA | C-N-CA | 5.03 | 125.52 | 119.94 |
| 1 | Y | 209 | HIS | ND1-CE1-NE2 | 5.03 | 113.43 | 108.40 |
| 17 | k | 175 | THR | N-CA-CB | 5.03 | 119.34 | 111.20 |
| 20 | n | 751 | TYR | CA-C-N | 5.03 | 127.02 | 120.28 |
| 20 | n | 751 | TYR | C-N-CA | 5.03 | 127.02 | 120.28 |
| 18 | e | 233 | THR | CA-C-N | 5.03 | 125.44 | 120.31 |
| 18 | e | 233 | THR | C-N-CA | 5.03 | 125.44 | 120.31 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 19 | f | 471 | PRO | N-CA-CB | 5.03 | 108.53 | 103.25 |
| 20 | g | 1152 | THR | N-CA-CB | 5.03 | 119.12 | 111.18 |
| 14 | a | 349 | LEU | N-CA-C | -5.03 | 100.26 | 108.76 |
| 14 | a | 891 | LEU | CA-C-N | 5.03 | 131.27 | 121.41 |
| 14 | a | 891 | LEU | C-N-CA | 5.03 | 131.27 | 121.41 |
| 1 | 0 | 385 | LYS | N-CA-CB | 5.03 | 118.48 | 110.84 |
| 2 | 1 | 656 | HIS | N-CA-CB | -5.03 | 105.76 | 111.79 |
| 5 | H | 394 | THR | CA-C-N | 5.03 | 129.22 | 120.68 |
| 5 | H | 394 | THR | C-N-CA | 5.03 | 129.22 | 120.68 |
| 4 | J | 759 | SER | N-CA-C | -5.03 | 107.28 | 113.41 |
| 7 | M | 217 | LEU | O-C-N | 5.03 | 127.45 | 122.12 |
| 7 | M | 1660 | ASN | N-CA-C | -5.03 | 107.32 | 113.50 |
| 7 | O | 654 | PHE | CA-CB-CG | -5.03 | 108.78 | 113.80 |
| 7 | O | 862 | ALA | CA-C-N | 5.03 | 127.01 | 120.28 |
| 7 | O | 862 | ALA | C-N-CA | 5.03 | 127.01 | 120.28 |
| 8 | P | 661 | MET | N-CA-C | -5.03 | 107.13 | 114.12 |
| 8 | P | 1217 | ARG | CB-CG-CD | 5.03 | 122.86 | 111.30 |
| 9 | T | 432 | ILE | CA-CB-CG2 | -5.03 | 101.95 | 110.50 |
| 2 | Z | 396 | SER | CA-C-O | -5.03 | 116.08 | 120.60 |
| 2 | Z | 440 | ARG | NE-CZ-NH2 | -5.03 | 114.68 | 119.20 |
| 2 | Z | 1057 | TYR | N-CA-C | 5.03 | 116.57 | 111.14 |
| 15 | i | 271 | LEU | N-CA-CB | 5.03 | 119.31 | 110.37 |
| 19 | m | 116 | LEU | CA-C-O | -5.03 | 115.22 | 120.55 |
| 20 | n | 628 | HIS | CA-C-N | 5.03 | 128.83 | 120.94 |
| 20 | n | 628 | HIS | C-N-CA | 5.03 | 128.83 | 120.94 |
| 21 | s | 63 | LYS | N-CA-C | -5.03 | 106.40 | 112.88 |
| 15 | b | 719 | SER | N-CA-C | 5.03 | 117.59 | 110.10 |
| 19 | f | 220 | ASN | CA-CB-CG | 5.03 | 117.62 | 112.60 |
| 19 | f | 346 | LEU | CA-C-N | 5.03 | 127.02 | 120.28 |
| 19 | f | 346 | LEU | C-N-CA | 5.03 | 127.02 | 120.28 |
| 19 | f | 546 | LEU | N-CA-C | -5.03 | 104.78 | 111.87 |
| 20 | g | 1143 | GLU | N-CA-C | -5.03 | 106.74 | 112.92 |
| 14 | a | 602 | ILE | N-CA-CB | 5.03 | 117.50 | 110.56 |
| 2 | 1 | 342 | ILE | O-C-N | -5.02 | 117.31 | 122.63 |
| 6 | I | 293 | HIS | CE1-NE2-CD2 | -5.02 | 103.98 | 109.00 |
| 7 | M | 351 | HIS | CB-CG-CD2 | -5.02 | 124.67 | 131.20 |
| 8 | N | 57 | THR | N-CA-C | -5.02 | 107.14 | 114.12 |
| 7 | O | 133 | GLU | N-CA-C | 5.02 | 119.17 | 113.19 |
| 8 | P | 817 | PRO | CA-C-O | -5.02 | 111.30 | 118.89 |
| 9 | Q | 226 | ARG | O-C-N | -5.02 | 115.60 | 122.33 |
| 9 | Q | 833 | ILE | CA-CB-CG1 | 5.02 | 118.94 | 110.40 |
| 1 | Y | 124 | ARG | CA-C-O | 5.02 | 125.75 | 120.42 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | Z | 843 | TYR | CB-CG-CD2 | -5.02 | 113.27 | 120.80 |
| 13 | w | 1392 | ARG | O-C-N | 5.02 | 127.88 | 122.15 |
| 15 | b | 122 | ARG | CD-NE-CZ | -5.02 | 117.37 | 124.40 |
| 20 | g | 432 | LYS | CA-C-O | 5.02 | 124.43 | 118.90 |
| 4 | G | 645 | THR | O-C-N | 5.02 | 127.88 | 122.15 |
| 7 | M | 1241 | LYS | CA-C-N | 5.02 | 128.72 | 120.63 |
| 7 | M | 1241 | LYS | C-N-CA | 5.02 | 128.72 | 120.63 |
| 8 | N | 264 | LEU | CA-C-N | 5.02 | 126.97 | 120.44 |
| 8 | N | 264 | LEU | C-N-CA | 5.02 | 126.97 | 120.44 |
| 7 | O | 1442 | TRP | O-C-N | 5.02 | 127.45 | 122.08 |
| 8 | P | 524 | THR | CA-C-O | -5.02 | 115.14 | 120.92 |
| 8 | P | 708 | THR | O-C-N | -5.02 | 115.70 | 122.43 |
| 8 | P | 1637 | VAL | N-CA-CB | 5.02 | 118.95 | 110.56 |
| 9 | S | 705 | GLN | N-CA-CB | 5.02 | 117.29 | 110.01 |
| 12 | u | 230 | SER | CA-C-N | 5.02 | 127.27 | 120.44 |
| 12 | u | 230 | SER | C-N-CA | 5.02 | 127.27 | 120.44 |
| 4 | y | 702 | ARG | O-C-N | -5.02 | 116.80 | 122.12 |
| 14 | h | 159 | THR | O-C-N | -5.02 | 115.23 | 122.36 |
| 15 | i | 699 | TRP | CZ3-CH2-CZ2 | -5.02 | 114.97 | 121.50 |
| 16 | j | 331 | ARG | CB-CA-C | -5.02 | 103.00 | 110.88 |
| 15 | b | 730 | ASN | N-CA-CB | 5.02 | 117.59 | 110.16 |
| 16 | c | 607 | ARG | N-CA-CB | 5.02 | 118.98 | 110.49 |
| 17 | d | 289 | TRP | CA-CB-CG | -5.02 | 104.06 | 113.60 |
| 19 | f | 452 | LEU | N-CA-C | 5.02 | 121.50 | 110.80 |
| 20 | g | 149 | SER | CA-C-O | -5.02 | 113.47 | 118.34 |
| 14 | a | 380 | GLU | N-CA-C | -5.02 | 100.22 | 108.41 |
| 14 | a | 682 | ASP | CA-C-N | 5.02 | 128.34 | 120.75 |
| 14 | a | 682 | ASP | C-N-CA | 5.02 | 128.34 | 120.75 |
| 1 | 0 | 852 | PHE | CA-C-O | 5.02 | 125.74 | 120.42 |
| 9 | R | 670 | LEU | N-CA-C | -5.02 | 106.40 | 112.88 |
| 12 | u | 581 | PHE | N-CA-C | -5.02 | 107.81 | 114.04 |
| 14 | h | 541 | PRO | N-CA-C | 5.02 | 119.44 | 111.26 |
| 15 | b | 484 | VAL | N-CA-CB | 5.02 | 119.52 | 111.23 |
| 1 | 0 | 598 | PHE | N-CA-CB | 5.02 | 118.60 | 110.17 |
| 2 | 1 | 1096 | ASN | N-CA-C | -5.02 | 105.46 | 111.03 |
| 2 | 1 | 1241 | LEU | N-CA-C | 5.02 | 116.44 | 111.07 |
| 2 | 1 | 1318 | HIS | ND1-CE1-NE2 | 5.02 | 113.42 | 108.40 |
| 5 | H | 517 | GLN | N-CA-CB | 5.02 | 118.06 | 110.28 |
| 7 | M | 742 | GLN | CA-C-N | 5.02 | 129.14 | 121.51 |
| 7 | M | 742 | GLN | C-N-CA | 5.02 | 129.14 | 121.51 |
| 8 | N | 738 | ILE | N-CA-CB | 5.02 | 119.23 | 110.65 |
| 8 | N | 834 | ILE | N-CA-CB | 5.02 | 119.51 | 111.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | O | 1093 | SER | CB-CA-C | -5.02 | 102.46 | 110.79 |
| 9 | Q | 258 | LYS | N-CA-CB | 5.02 | 118.06 | 110.28 |
| 9 | R | 435 | TRP | CZ3-CH2-CZ2 | 5.02 | 128.03 | 121.50 |
| 9 | T | 246 | ASN | CA-CB-CG | -5.02 | 107.58 | 112.60 |
| 1 | Y | 1460 | ARG | CD-NE-CZ | -5.02 | 117.37 | 124.40 |
| 2 | Z | 116 | TYR | CA-C-O | 5.02 | 124.46 | 118.79 |
| 2 | Z | 215 | VAL | N-CA-C | -5.02 | 100.98 | 108.46 |
| 2 | Z | 816 | TYR | CA-C-N | 5.02 | 127.77 | 120.79 |
| 2 | Z | 816 | TYR | C-N-CA | 5.02 | 127.77 | 120.79 |
| 2 | Z | 1378 | PRO | CA-C-N | 5.02 | 129.57 | 122.09 |
| 2 | Z | 1378 | PRO | C-N-CA | 5.02 | 129.57 | 122.09 |
| 12 | v | 444 | THR | CB-CA-C | -5.02 | 100.83 | 109.86 |
| 13 | w | 1125 | ASP | O-C-N | 5.02 | 127.44 | 122.12 |
| 14 | h | 438 | GLU | O-C-N | 5.02 | 128.24 | 122.17 |
| 15 | i | 665 | LEU | N-CA-C | -5.02 | 104.46 | 110.88 |
| 20 | n | 728 | ALA | O-C-N | 5.02 | 127.87 | 122.15 |
| 2 | 1 | 758 | SER | CA-C-O | 5.02 | 125.53 | 119.31 |
| 2 | 1 | 1192 | THR | CA-C-N | 5.02 | 129.21 | 120.68 |
| 2 | 1 | 1192 | THR | C-N-CA | 5.02 | 129.21 | 120.68 |
| 7 | M | 12 | TYR | CB-CG-CD1 | 5.02 | 128.33 | 120.80 |
| 8 | N | 1226 | PHE | CA-C-N | 5.02 | 126.88 | 120.56 |
| 8 | N | 1226 | PHE | C-N-CA | 5.02 | 126.88 | 120.56 |
| 7 | O | 1285 | HIS | ND1-CE1-NE2 | 5.02 | 113.42 | 108.40 |
| 9 | S | 724 | ARG | CA-C-N | 5.02 | 127.41 | 120.29 |
| 9 | S | 724 | ARG | C-N-CA | 5.02 | 127.41 | 120.29 |
| 9 | T | 742 | LEU | CA-C-O | -5.02 | 115.10 | 120.42 |
| 12 | v | 693 | ILE | CA-C-N | 5.02 | 126.88 | 120.56 |
| 12 | v | 693 | ILE | C-N-CA | 5.02 | 126.88 | 120.56 |
| 4 | y | 650 | GLU | CA-C-O | 5.02 | 126.09 | 120.82 |
| 15 | i | 103 | GLU | CA-C-O | 5.02 | 125.74 | 120.42 |
| 15 | i | 547 | LEU | N-CA-C | 5.02 | 119.35 | 112.88 |
| 15 | i | 567 | LEU | CA-C-O | 5.02 | 125.15 | 119.18 |
| 16 | j | 455 | GLN | CG-CD-OE1 | 5.02 | 130.84 | 120.80 |
| 18 | l | 300 | HIS | CG-CD2-NE2 | 5.02 | 112.22 | 107.20 |
| 18 | l | 329 | ARG | NE-CZ-NH2 | -5.02 | 114.68 | 119.20 |
| 19 | m | 656 | ARG | CA-C-O | 5.02 | 126.09 | 120.82 |
| 20 | n | 234 | ARG | NE-CZ-NH2 | 5.02 | 123.72 | 119.20 |
| 21 | s | 9 | PRO | CA-C-O | -5.02 | 115.62 | 121.34 |
| 16 | c | 138 | ILE | CA-C-O | 5.02 | 126.17 | 120.85 |
| 17 | d | 71 | ALA | N-CA-CB | 5.02 | 117.61 | 110.44 |
| 17 | d | 232 | ILE | CA-C-N | -5.02 | 114.25 | 122.33 |
| 17 | d | 232 | ILE | C-N-CA | -5.02 | 114.25 | 122.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 20 | g | 371 | SER | N-CA-C | -5.02 | 102.14 | 109.81 |
| 20 | g | 785 | HIS | CE1-NE2-CD2 | -5.02 | 103.98 | 109.00 |
| 20 | g | 808 | TYR | CB-CA-C | 5.02 | 119.63 | 110.10 |
| 20 | g | 948 | GLN | CA-C-N | 5.02 | 127.51 | 120.28 |
| 20 | g | 948 | GLN | C-N-CA | 5.02 | 127.51 | 120.28 |
| 20 | g | 1118 | SER | N-CA-C | 5.02 | 119.11 | 112.89 |
| 14 | a | 500 | GLU | N-CA-C | -5.02 | 101.53 | 109.76 |
| 1 | 0 | 1101 | ARG | N-CA-CB | 5.02 | 118.00 | 110.53 |
| 9 | R | 147 | ASP | CA-C-O | -5.02 | 113.62 | 119.14 |
| 9 | S | 508 | ILE | CA-C-O | 5.02 | 126.49 | 121.17 |
| 17 | k | 69 | ILE | O-C-N | -5.02 | 117.88 | 123.20 |
| 15 | b | 144 | VAL | CA-CB-CG1 | 5.02 | 118.93 | 110.40 |
| 15 | b | 349 | TYR | O-C-N | 5.02 | 129.41 | 123.24 |
| 5 | B | 359 | ASN | CA-C-N | 5.01 | 127.00 | 120.28 |
| 5 | B | 359 | ASN | C-N-CA | 5.01 | 127.00 | 120.28 |
| 4 | G | 643 | LYS | N-CA-CB | -5.01 | 102.51 | 110.28 |
| 7 | M | 676 | ASP | CA-C-O | -5.01 | 115.23 | 120.55 |
| 8 | N | 948 | LEU | N-CA-CB | 5.01 | 118.97 | 110.49 |
| 8 | P | 416 | LEU | N-CA-CB | 5.01 | 118.97 | 110.49 |
| 9 | Q | 301 | ASN | CA-C-O | -5.01 | 114.20 | 119.97 |
| 9 | R | 332 | PRO | CB-CA-C | -5.01 | 103.29 | 111.56 |
| 9 | T | 101 | PRO | N-CA-C | -5.01 | 108.95 | 114.92 |
| 9 | T | 786 | ILE | N-CA-C | 5.01 | 115.24 | 110.53 |
| 10 | U | 325 | SER | CA-C-O | 5.01 | 125.86 | 120.55 |
| 1 | Y | 859 | SER | CA-C-N | 5.01 | 131.00 | 121.97 |
| 1 | Y | 859 | SER | C-N-CA | 5.01 | 131.00 | 121.97 |
| 12 | u | 703 | GLN | N-CA-C | 5.01 | 117.64 | 111.82 |
| 12 | v | 378 | ASP | CB-CA-C | 5.01 | 120.40 | 110.42 |
| 19 | m | 476 | LEU | N-CA-CB | 5.01 | 118.83 | 110.41 |
| 20 | n | 601 | ASN | N-CA-C | 5.01 | 117.48 | 111.71 |
| 20 | n | 842 | GLU | N-CA-C | -5.01 | 106.51 | 113.18 |
| 20 | n | 1076 | PHE | CB-CA-C | 5.01 | 117.00 | 109.63 |
| 21 | q | 45 | VAL | O-C-N | 5.01 | 127.11 | 121.90 |
| 15 | b | 550 | HIS | CG-CD2-NE2 | 5.01 | 112.21 | 107.20 |
| 19 | f | 460 | LYS | CB-CG-CD | 5.01 | 122.83 | 111.30 |
| 20 | g | 689 | ILE | CA-CB-CG1 | 5.01 | 118.93 | 110.40 |
| 2 | 1 | 161 | SER | N-CA-CB | 5.01 | 117.34 | 109.97 |
| 5 | K | 420 | ALA | N-CA-C | -5.01 | 106.85 | 113.17 |
| 6 | L | 276 | GLU | N-CA-CB | 5.01 | 117.58 | 110.16 |
| 7 | O | 437 | ASP | N-CA-CB | 5.01 | 117.58 | 110.16 |
| 9 | Q | 773 | ASN | CA-CB-CG | 5.01 | 117.61 | 112.60 |
| 2 | Z | 865 | GLU | N-CA-C | 5.01 | 118.17 | 111.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 14 | h | 743 | ASN | CB-CA-C | -5.01 | 104.92 | 112.09 |
| 16 | j | 558 | ASN | CA-CB-CG | -5.01 | 107.59 | 112.60 |
| 16 | c | 548 | TYR | CB-CG-CD1 | -5.01 | 113.28 | 120.80 |
| 20 | g | 365 | THR | N-CA-CB | 5.01 | 118.18 | 110.21 |
| 7 | M | 654 | PHE | CB-CG-CD2 | -5.01 | 112.18 | 120.70 |
| 7 | M | 980 | ASP | CA-C-N | 5.01 | 127.41 | 120.29 |
| 7 | M | 980 | ASP | C-N-CA | 5.01 | 127.41 | 120.29 |
| 8 | N | 1048 | LYS | N-CA-C | -5.01 | 102.06 | 109.83 |
| 8 | N | 1166 | VAL | CB-CA-C | 5.01 | 119.51 | 111.29 |
| 8 | N | 1437 | PRO | CB-CA-C | -5.01 | 103.29 | 111.56 |
| 7 | O | 1347 | ILE | CA-C-O | 5.01 | 125.88 | 120.47 |
| 7 | O | 1673 | LEU | O-C-N | 5.01 | 127.23 | 122.07 |
| 8 | P | 844 | TYR | N-CA-CB | 5.01 | 117.28 | 110.01 |
| 8 | P | 852 | PHE | CA-C-N | 5.01 | 127.00 | 120.28 |
| 8 | P | 852 | PHE | C-N-CA | 5.01 | 127.00 | 120.28 |
| 4 | z | 745 | TYR | CA-C-N | 5.01 | 127.93 | 120.31 |
| 4 | z | 745 | TYR | C-N-CA | 5.01 | 127.93 | 120.31 |
| 14 | h | 719 | PHE | CA-CB-CG | -5.01 | 108.79 | 113.80 |
| 19 | m | 204 | ASP | N-CA-C | 5.01 | 118.73 | 111.56 |
| 19 | m | 232 | ASN | OD1-CG-ND2 | -5.01 | 117.59 | 122.60 |
| 20 | n | 179 | ASN | N-CA-CB | 5.01 | 118.96 | 110.49 |
| 16 | c | 423 | GLN | N-CA-CB | 5.01 | 117.58 | 110.16 |
| 16 | c | 530 | LEU | N-CA-C | -5.01 | 100.12 | 110.80 |
| 14 | a | 294 | GLU | CB-CG-CD | -5.01 | 104.08 | 112.60 |
| 1 | 0 | 244 | ALA | CA-C-N | 5.01 | 129.70 | 123.14 |
| 1 | 0 | 244 | ALA | C-N-CA | 5.01 | 129.70 | 123.14 |
| 1 | 0 | 986 | THR | OG1-CB-CG2 | -5.01 | 99.28 | 109.30 |
| 1 | 0 | 1207 | ARG | NE-CZ-NH1 | 5.01 | 126.51 | 121.50 |
| 2 | 1 | 979 | GLN | N-CA-CB | 5.01 | 118.71 | 110.39 |
| 4 | G | 770 | ASN | O-C-N | 5.01 | 127.43 | 122.12 |
| 7 | O | 75 | ILE | CB-CA-C | -5.01 | 105.31 | 112.22 |
| 7 | O | 952 | SER | N-CA-CB | 5.01 | 118.79 | 110.52 |
| 7 | O | 1056 | LEU | CA-C-N | 5.01 | 126.95 | 120.44 |
| 7 | O | 1056 | LEU | C-N-CA | 5.01 | 126.95 | 120.44 |
| 7 | O | 1073 | MET | CB-CA-C | -5.01 | 102.33 | 110.85 |
| 9 | Q | 549 | ASP | N-CA-C | -5.01 | 98.74 | 109.81 |
| 9 | Q | 745 | LEU | CB-CA-C | 5.01 | 116.39 | 108.88 |
| 9 | T | 474 | PHE | CA-C-O | 5.01 | 125.49 | 119.43 |
| 1 | Y | 707 | ILE | N-CA-CB | 5.01 | 118.22 | 111.21 |
| 1 | Y | 1184 | PRO | N-CD-CG | 5.01 | 110.71 | 103.20 |
| 12 | v | 400 | SER | N-CA-CB | 5.01 | 118.96 | 110.49 |
| 14 | h | 893 | HIS | CB-CG-CD2 | -5.01 | 124.69 | 131.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 16 | j | 471 | ASP | N-CA-CB | 5.01 | 117.48 | 110.12 |
| 19 | m | 411 | LYS | CA-C-N | 5.01 | 126.99 | 120.28 |
| 19 | m | 411 | LYS | C-N-CA | 5.01 | 126.99 | 120.28 |
| 21 | t | 8 | THR | N-CA-C | -5.01 | 103.84 | 110.40 |
| 18 | e | 168 | ASP | CA-CB-CG | -5.01 | 107.59 | 112.60 |
| 19 | f | 360 | HIS | CA-CB-CG | -5.01 | 108.79 | 113.80 |
| 19 | f | 684 | ILE | CB-CA-C | 5.01 | 115.47 | 111.06 |
| 14 | a | 869 | HIS | CA-CB-CG | 5.01 | 118.81 | 113.80 |
| 2 | 1 | 434 | PHE | CA-CB-CG | -5.01 | 108.79 | 113.80 |
| 12 | u | 568 | CYS | CA-C-N | 5.01 | 126.99 | 120.28 |
| 12 | u | 568 | CYS | C-N-CA | 5.01 | 126.99 | 120.28 |
| 19 | m | 427 | GLU | CB-CA-C | 5.01 | 117.89 | 109.48 |
| 20 | n | 365 | THR | CA-CB-CG2 | -5.01 | 101.99 | 110.50 |
| 21 | q | 68 | TYR | CB-CG-CD2 | -5.01 | 113.29 | 120.80 |
| 15 | b | 372 | ALA | CB-CA-C | -5.01 | 101.36 | 110.63 |
| 19 | f | 594 | ILE | CB-CA-C | 5.01 | 119.13 | 112.22 |
| 5 | H | 456 | THR | O-C-N | 5.01 | 127.44 | 122.03 |
| 6 | I | 372 | PHE | N-CA-C | 5.01 | 117.63 | 111.82 |
| 7 | M | 490 | ALA | CA-C-N | 5.01 | 133.73 | 124.82 |
| 7 | M | 490 | ALA | C-N-CA | 5.01 | 133.73 | 124.82 |
| 7 | O | 882 | TYR | N-CA-C | 5.01 | 118.16 | 111.75 |
| 8 | P | 768 | ALA | O-C-N | 5.01 | 127.43 | 122.12 |
| 9 | Q | 420 | LEU | N-CA-C | -5.01 | 101.53 | 109.59 |
| 9 | R | 730 | LYS | N-CA-CB | 5.01 | 118.95 | 110.49 |
| 1 | Y | 625 | ALA | CA-C-O | 5.01 | 125.28 | 119.32 |
| 2 | Z | 541 | SER | CA-C-O | -5.01 | 114.12 | 120.28 |
| 2 | Z | 1278 | ASP | N-CA-C | -5.01 | 106.75 | 114.16 |
| 12 | u | 189 | LYS | CA-C-O | -5.01 | 113.37 | 119.43 |
| 12 | v | 395 | LYS | CA-C-O | -5.01 | 115.56 | 120.82 |
| 14 | h | 379 | ILE | N-CA-C | -5.01 | 98.83 | 107.24 |
| 14 | h | 451 | ARG | CG-CD-NE | -5.01 | 100.99 | 112.00 |
| 16 | j | 261 | LYS | O-C-N | -5.01 | 116.81 | 122.12 |
| 18 | l | 211 | HIS | CE1-NE2-CD2 | -5.01 | 103.99 | 109.00 |
| 19 | m | 245 | ARG | CB-CG-CD | 5.01 | 122.82 | 111.30 |
| 21 | o | 35 | TYR | CA-C-N | 5.01 | 130.32 | 122.11 |
| 21 | o | 35 | TYR | C-N-CA | 5.01 | 130.32 | 122.11 |
| 21 | o | 37 | LEU | CD1-CG-CD2 | 5.01 | 121.81 | 110.80 |
| 20 | g | 809 | LYS | N-CA-C | -5.01 | 107.21 | 113.72 |
| 14 | a | 661 | GLN | CA-C-N | 5.01 | 128.61 | 120.60 |
| 14 | a | 661 | GLN | C-N-CA | 5.01 | 128.61 | 120.60 |
| 4 | A | 775 | THR | CA-C-N | 5.00 | 129.08 | 120.72 |
| 4 | A | 775 | THR | C-N-CA | 5.00 | 129.08 | 120.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | E | 476 | GLN | CA-CB-CG | 5.00 | 124.11 | 114.10 |
| 7 | M | 1377 | VAL | N-CA-C | 5.00 | 115.61 | 110.36 |
| 9 | R | 131 | GLY | N-CA-C | 5.00 | 118.70 | 112.64 |
| 4 | y | 773 | SER | O-C-N | 5.00 | 127.22 | 122.07 |
| 20 | n | 144 | ALA | N-CA-C | 5.00 | 121.46 | 110.80 |
| 20 | n | 1024 | VAL | CA-C-O | -5.00 | 113.81 | 119.42 |
| 15 | b | 529 | TRP | N-CA-CB | 5.00 | 120.19 | 111.13 |
| 1 | 0 | 1146 | TYR | CB-CG-CD2 | 5.00 | 128.31 | 120.80 |
| 1 | 0 | 1317 | TYR | CA-C-O | 5.00 | 126.69 | 120.54 |
| 2 | 1 | 1067 | LYS | N-CA-C | 5.00 | 121.46 | 110.80 |
| 4 | G | 649 | THR | CA-C-O | 5.00 | 125.85 | 120.70 |
| 6 | L | 275 | GLN | N-CA-CB | 5.00 | 117.47 | 110.12 |
| 8 | N | 731 | SER | N-CA-CB | 5.00 | 117.42 | 110.26 |
| 8 | N | 1444 | LEU | N-CA-C | 5.00 | 116.54 | 111.14 |
| 7 | O | 1325 | SER | N-CA-C | 5.00 | 116.73 | 111.28 |
| 8 | P | 71 | LEU | N-CA-C | -5.00 | 105.89 | 112.94 |
| 8 | P | 391 | PRO | O-C-N | 5.00 | 129.09 | 123.03 |
| 8 | P | 564 | LEU | N-CA-CB | 5.00 | 117.56 | 110.16 |
| 8 | P | 774 | ILE | CA-CB-CG2 | -5.00 | 101.99 | 110.50 |
| 9 | Q | 616 | GLU | CA-C-N | 5.00 | 129.06 | 120.71 |
| 9 | Q | 616 | GLU | C-N-CA | 5.00 | 129.06 | 120.71 |
| 9 | S | 69 | ALA | N-CA-C | 5.00 | 116.54 | 111.14 |
| 9 | T | 713 | ILE | N-CA-CB | 5.00 | 116.98 | 110.57 |
| 1 | Y | 1486 | LYS | CB-CA-C | -5.00 | 103.03 | 110.88 |
| 2 | Z | 846 | ASP | N-CA-CB | 5.00 | 118.25 | 110.44 |
| 15 | i | 553 | ILE | CA-CB-CG2 | -5.00 | 101.99 | 110.50 |
| 17 | k | 204 | SER | N-CA-C | -5.00 | 107.03 | 114.64 |
| 19 | m | 474 | ASN | CB-CG-ND2 | -5.00 | 108.89 | 116.40 |
| 20 | n | 1026 | GLY | N-CA-C | -5.00 | 108.77 | 115.32 |
| 20 | g | 1080 | SER | N-CA-C | -5.00 | 101.30 | 108.60 |
| 2 | 1 | 174 | ILE | CA-CB-CG2 | -5.00 | 102.00 | 110.50 |
| 4 | A | 638 | ASP | CA-CB-CG | 5.00 | 117.60 | 112.60 |
| 4 | A | 768 | GLU | N-CA-CB | 5.00 | 117.26 | 110.01 |
| 4 | D | 660 | LYS | CG-CD-CE | 5.00 | 122.80 | 111.30 |
| 5 | E | 300 | ASP | O-C-N | 5.00 | 125.73 | 121.83 |
| 8 | N | 1131 | LYS | CA-C-O | 5.00 | 125.27 | 119.32 |
| 8 | N | 1217 | ARG | NH1-CZ-NH2 | -5.00 | 112.80 | 119.30 |
| 8 | P | 213 | PHE | N-CA-C | -5.00 | 105.29 | 113.19 |
| 8 | P | 453 | ALA | N-CA-C | 5.00 | 117.62 | 111.82 |
| 9 | R | 72 | LEU | CB-CA-C | -5.00 | 103.03 | 110.88 |
| 9 | S | 42 | ILE | CA-C-N | 5.00 | 128.79 | 120.94 |
| 9 | S | 42 | ILE | C-N-CA | 5.00 | 128.79 | 120.94 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | T | 221 | GLN | OE1-CD-NE2 | 5.00 | 127.60 | 122.60 |
| 9 | T | 696 | TYR | CA-C-O | -5.00 | 115.38 | 121.78 |
| 13 | x | 1270 | LEU | CB-CA-C | -5.00 | 102.39 | 110.79 |
| 13 | x | 1407 | SER | CA-C-N | 5.00 | 127.39 | 120.29 |
| 13 | x | 1407 | SER | C-N-CA | 5.00 | 127.39 | 120.29 |
| 14 | h | 390 | GLN | OE1-CD-NE2 | -5.00 | 117.60 | 122.60 |
| 16 | c | 364 | SER | N-CA-CB | 5.00 | 119.27 | 110.37 |
| 19 | f | 287 | HIS | ND1-CE1-NE2 | 5.00 | 113.40 | 108.40 |
| 20 | g | 622 | ASN | CA-CB-CG | 5.00 | 117.60 | 112.60 |
| 14 | a | 733 | SER | CA-C-O | -5.00 | 113.23 | 119.28 |

All (114) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 1 | 0 | 832 | VAL | CA |
| 1 | 0 | 1021 | TYR | CA |
| 1 | 0 | 1022 | ASP | CA |
| 1 | 0 | 1258 | LEU | CA |
| 2 | 1 | 308 | ASN | CA |
| 2 | 1 | 309 | LEU | CA |
| 2 | 1 | 678 | LYS | CA |
| 2 | 1 | 679 | SER | CA |
| 2 | 1 | 745 | ILE | CA |
| 2 | 1 | 915 | LYS | CA |
| 2 | 1 | 916 | PHE | CA |
| 2 | 1 | 921 | SER | CA |
| 2 | 1 | 922 | LYS | CA |
| 2 | 1 | 1039 | LEU | CA |
| 2 | 1 | 1300 | SER | CA |
| 2 | 1 | 1301 | SER | CA |
| 5 | B | 318 | GLU | CA |
| 5 | B | 319 | THR | CA |
| 5 | B | 323 | LEU | CA |
| 5 | B | 324 | TYR | CA |
| 6 | F | 369 | LEU | CA |
| 4 | G | 726 | VAL | CA |
| 4 | G | 727 | SER | CA |
| 5 | H | 323 | LEU | CA |
| 5 | H | 324 | TYR | CA |
| 6 | I | 370 | ASP | CA |
| 5 | K | 318 | GLU | CA |
| 5 | K | 319 | THR | CA |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 6 | L | 369 | LEU | CA |
| 6 | L | 370 | ASP | CA |
| 7 | M | 1137 | ASN | CA |
| 7 | M | 1138 | PHE | CA |
| 7 | M | 1188 | THR | CA |
| 7 | M | 1189 | MET | CA |
| 7 | M | 1273 | LYS | CA |
| 8 | N | 131 | ASP | CA |
| 8 | N | 132 | ASN | CA |
| 8 | N | 256 | THR | CA |
| 8 | N | 257 | LEU | CA |
| 8 | N | 551 | ASN | CA |
| 8 | N | 552 | LEU | CA |
| 8 | N | 576 | TYR | CA |
| 8 | N | 577 | MET | CA |
| 8 | N | 793 | LEU | CA |
| 8 | N | 794 | ILE | CA |
| 8 | N | 1059 | ASN | CA |
| 8 | N | 1060 | LEU | CA |
| 8 | N | 1094 | SER | CA |
| 8 | N | 1095 | GLU | CA |
| 7 | O | 602 | ASN | CA |
| 7 | O | 603 | GLU | CA |
| 7 | O | 1137 | ASN | CA |
| 7 | O | 1138 | PHE | CA |
| 7 | O | 1188 | THR | CA |
| 7 | O | 1189 | MET | CA |
| 8 | P | 256 | THR | CA |
| 8 | P | 257 | LEU | CA |
| 8 | P | 576 | TYR | CA |
| 8 | P | 577 | MET | CA |
| 8 | P | 1094 | SER | CA |
| 8 | P | 1095 | GLU | CA |
| 9 | Q | 753 | ALA | CA |
| 9 | Q | 754 | ARG | CA |
| 9 | R | 514 | LYS | CA |
| 9 | R | 515 | LEU | CA |
| 9 | T | 514 | LYS | CA |
| 9 | T | 515 | LEU | CA |
| 9 | T | 753 | ALA | CA |
| 9 | T | 754 | ARG | CA |
| 10 | U | 248 | TRP | CA |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 10 | U | 249 | ASP | CA |
| 10 | U | 283 | ILE | CA |
| 10 | U | 284 | LYS | CA |
| 11 | V | 301 | LEU | CA |
| 11 | V | 302 | ARG | CA |
| 11 | V | 402 | ASN | CA |
| 10 | W | 248 | TRP | CA |
| 10 | W | 249 | ASP | CA |
| 10 | W | 283 | ILE | CA |
| 10 | W | 284 | LYS | CA |
| 10 | W | 304 | LYS | CA |
| 10 | W | 305 | TYR | CA |
| 11 | X | 401 | ASP | CA |
| 11 | X | 402 | ASN | CA |
| 1 | Y | 831 | LYS | CA |
| 1 | Y | 832 | VAL | CA |
| 1 | Y | 1021 | TYR | CA |
| 1 | Y | 1022 | ASP | CA |
| 1 | Y | 1257 | GLN | CA |
| 1 | Y | 1258 | LEU | CA |
| 2 | Z | 456 | THR | CA |
| 2 | Z | 457 | SER | CA |
| 2 | Z | 678 | LYS | CA |
| 2 | Z | 679 | SER | CA |
| 2 | Z | 891 | ARG | CA |
| 2 | Z | 915 | LYS | CA |
| 2 | Z | 916 | PHE | CA |
| 2 | Z | 921 | SER | CA |
| 2 | Z | 922 | LYS | CA |
| 14 | h | 1011 | ASP | CA |
| 19 | m | 373 | THR | CA |
| 21 | o | 55 | ASN | CA |
| 21 | o | 56 | THR | CA |
| 21 | p | 55 | ASN | CA |
| 21 | p | 56 | THR | CA |
| 21 | q | 55 | ASN | CA |
| 21 | q | 56 | THR | CA |
| 21 | r | 55 | ASN | CA |
| 21 | r | 56 | THR | CA |
| 21 | s | 55 | ASN | CA |
| 21 | s | 56 | THR | CA |
| 21 | t | 55 | ASN | CA |

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| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 21 | t | 56 | THR | CA |
| 14 | a | 1011 | ASP | CA |

All (794) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | 0 | 1026 | TYR | Sidechain |
| 1 | 0 | 1045 | GLU | Peptide |
| 1 | 0 | 1060 | TYR | Peptide |
| 1 | 0 | 107 | TYR | Sidechain |
| 1 | 0 | 1142 | ARG | Sidechain |
| 1 | 0 | 1158 | HIS | Sidechain |
| 1 | 0 | 1204 | TYR | Sidechain |
| 1 | 0 | 1208 | SER | Peptide |
| 1 | 0 | 1211 | PHE | Sidechain |
| 1 | 0 | 1218 | TYR | Peptide |
| 1 | 0 | 1258 | LEU | Mainchain |
| 1 | 0 | 127 | TYR | Sidechain |
| 1 | 0 | 1280 | TYR | Sidechain |
| 1 | 0 | 133 | TYR | Sidechain |
| 1 | 0 | 1348 | ARG | Sidechain |
| 1 | 0 | 1428 | TYR | Sidechain |
| 1 | 0 | 1468 | TYR | Sidechain |
| 1 | 0 | 201 | TYR | Sidechain |
| 1 | 0 | 257 | PHE | Sidechain |
| 1 | 0 | 292 | ASN | Peptide |
| 1 | 0 | 298 | TYR | Sidechain |
| 1 | 0 | 369 | TYR | Sidechain |
| 1 | 0 | 419 | LYS | Mainchain |
| 1 | 0 | 445 | ARG | Sidechain |
| 1 | 0 | 523 | SER | Peptide |
| 1 | 0 | 531 | PHE | Sidechain |
| 1 | 0 | 592 | TYR | Sidechain |
| 1 | 0 | 659 | PHE | Sidechain |
| 1 | 0 | 673 | TYR | Sidechain |
| 1 | 0 | 771 | TYR | Sidechain |
| 1 | 0 | 779 | ARG | Sidechain |
| 1 | 0 | 782 | ARG | Peptide |
| 1 | 0 | 832 | VAL | Mainchain |
| 1 | 0 | 842 | TYR | Sidechain |
| 2 | 1 | 104 | ARG | Sidechain |
| 2 | 1 | 1074 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | 1 | 1098 | LEU | Peptide |
| 2 | 1 | 1101 | TYR | Sidechain |
| 2 | 1 | 1107 | HIS | Sidechain |
| 2 | 1 | 117 | TYR | Sidechain |
| 2 | 1 | 125 | PHE | Sidechain |
| 2 | 1 | 1301 | SER | Mainchain |
| 2 | 1 | 1351 | TYR | Sidechain |
| 2 | 1 | 1382 | TYR | Sidechain |
| 2 | 1 | 171 | TYR | Sidechain |
| 2 | 1 | 247 | PHE | Sidechain |
| 2 | 1 | 346 | GLU | Peptide |
| 2 | 1 | 386 | ARG | Sidechain |
| 2 | 1 | 431 | ARG | Sidechain |
| 2 | 1 | 433 | TYR | Sidechain |
| 2 | 1 | 507 | TYR | Sidechain |
| 2 | 1 | 512 | ARG | Sidechain |
| 2 | 1 | 579 | TYR | Sidechain |
| 2 | 1 | 631 | PHE | Sidechain |
| 2 | 1 | 635 | TYR | Sidechain |
| 2 | 1 | 720 | PHE | Sidechain |
| 2 | 1 | 729 | PHE | Sidechain |
| 2 | 1 | 770 | ARG | Sidechain |
| 2 | 1 | 815 | PHE | Sidechain |
| 2 | 1 | 843 | TYR | Sidechain |
| 2 | 1 | 849 | PHE | Sidechain |
| 2 | 1 | 883 | TYR | Sidechain |
| 2 | 1 | 916 | PHE | Sidechain |
| 2 | 1 | 948 | ARG | Sidechain |
| 4 | A | 699 | TYR | Sidechain |
| 5 | B | 309 | ARG | Sidechain |
| 5 | B | 440 | PHE | Sidechain |
| 5 | B | 446 | ARG | Sidechain |
| 5 | B | 462 | ARG | Sidechain |
| 6 | C | 283 | TYR | Sidechain |
| 6 | C | 314 | TYR | Sidechain |
| 4 | D | 658 | TYR | Sidechain |
| 4 | D | 745 | TYR | Sidechain |
| 4 | D | 805 | ARG | Sidechain |
| 5 | E | 309 | ARG | Sidechain |
| 5 | E | 313 | TYR | Sidechain |
| 5 | E | 385 | GLN | Peptide |
| 6 | F | 283 | TYR | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 6 | F | 310 | ARG | Sidechain |
| 6 | F | 350 | PHE | Sidechain |
| 4 | G | 658 | TYR | Sidechain |
| 4 | G | 680 | TYR | Sidechain |
| 4 | G | 745 | TYR | Sidechain |
| 5 | H | 378 | HIS | Sidechain |
| 5 | H | 469 | ARG | Sidechain |
| 5 | H | 507 | ASN | Peptide |
| 6 | I | 283 | TYR | Sidechain |
| 6 | I | 387 | TYR | Sidechain |
| 6 | I | 389 | ARG | Sidechain |
| 6 | I | 450 | PHE | Sidechain |
| 6 | I | 456 | ARG | Sidechain |
| 4 | J | 699 | TYR | Sidechain |
| 4 | J | 745 | TYR | Sidechain |
| 5 | K | 397 | ARG | Sidechain |
| 5 | K | 522 | TYR | Sidechain |
| 6 | L | 283 | TYR | Sidechain |
| 6 | L | 301 | HIS | Sidechain |
| 6 | L | 310 | ARG | Sidechain |
| 6 | L | 380 | TYR | Sidechain |
| 6 | L | 406 | PHE | Sidechain |
| 7 | M | 1013 | TYR | Sidechain |
| 7 | M | 106 | TYR | Sidechain |
| 7 | M | 1070 | TYR | Sidechain |
| 7 | M | 1097 | TYR | Sidechain |
| 7 | M | 1160 | TYR | Peptide |
| 7 | M | 1189 | MET | Mainchain |
| 7 | M | 1190 | TYR | Sidechain |
| 7 | M | 1219 | VAL | Peptide |
| 7 | M | 13 | ARG | Sidechain |
| 7 | M | 1345 | PHE | Sidechain |
| 7 | M | 1359 | PHE | Sidechain |
| 7 | M | 1361 | PHE | Peptide |
| 7 | M | 1394 | SER | Peptide |
| 7 | M | 1406 | TYR | Sidechain |
| 7 | M | 1490 | ARG | Sidechain |
| 7 | M | 1532 | ARG | Sidechain |
| 7 | M | 1534 | GLY | Peptide |
| 7 | M | 212 | PHE | Sidechain |
| 7 | M | 233 | TYR | Sidechain |
| 7 | M | 237 | PHE | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 7 | M | 245 | ARG | Sidechain |
| 7 | M | 269 | TYR | Sidechain |
| 7 | M | 342 | TYR | Sidechain |
| 7 | M | 418 | TYR | Sidechain |
| 7 | M | 486 | TYR | Sidechain |
| 7 | M | 488 | PHE | Sidechain |
| 7 | M | 489 | TYR | Sidechain |
| 7 | M | 508 | TYR | Sidechain |
| 7 | M | 527 | TYR | Sidechain |
| 7 | M | 546 | TYR | Sidechain |
| 7 | M | 565 | TYR | Sidechain |
| 7 | M | 620 | THR | Peptide |
| 7 | M | 736 | PHE | Sidechain |
| 7 | M | 744 | TYR | Sidechain |
| 7 | M | 745 | ARG | Sidechain |
| 7 | M | 752 | TYR | Sidechain |
| 7 | M | 771 | ARG | Sidechain |
| 7 | M | 774 | ARG | Sidechain |
| 7 | M | 8 | PHE | Sidechain |
| 7 | M | 827 | ILE | Peptide |
| 7 | M | 882 | TYR | Sidechain |
| 7 | M | 898 | TYR | Sidechain |
| 7 | M | 913 | TYR | Sidechain |
| 7 | M | 993 | ALA | Peptide |
| 8 | N | 1008 | THR | Peptide |
| 8 | N | 1033 | PHE | Sidechain |
| 8 | N | 1072 | TYR | Sidechain |
| 8 | N | 109 | ARG | Sidechain |
| 8 | N | 1196 | TYR | Sidechain |
| 8 | N | 1199 | TYR | Sidechain |
| 8 | N | 1217 | ARG | Sidechain |
| 8 | N | 1254 | ARG | Sidechain |
| 8 | N | 1263 | TYR | Sidechain |
| 8 | N | 1308 | TYR | Sidechain |
| 8 | N | 1349 | TYR | Sidechain |
| 8 | N | 1399 | ASN | Peptide |
| 8 | N | 1404 | PHE | Sidechain |
| 8 | N | 1429 | HIS | Sidechain |
| 8 | N | 1463 | SER | Peptide |
| 8 | N | 1525 | PHE | Sidechain |
| 8 | N | 1605 | PHE | Sidechain |
| 8 | N | 164 | TYR | Mainchain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 8 | N | 21 | PHE | Sidechain |
| 8 | N | 319 | PRO | Peptide |
| 8 | N | 330 | TYR | Sidechain |
| 8 | N | 331 | TYR | Sidechain |
| 8 | N | 341 | PHE | Sidechain |
| 8 | N | 369 | LEU | Peptide |
| 8 | N | 371 | PHE | Sidechain |
| 8 | N | 375 | TYR | Sidechain |
| 8 | N | 440 | ILE | Peptide |
| 8 | N | 463 | PHE | Sidechain |
| 8 | N | 552 | LEU | Mainchain |
| 8 | N | 59 | ARG | Sidechain |
| 8 | N | 727 | ASN | Peptide |
| 8 | N | 753 | TYR | Sidechain |
| 8 | N | 754 | TYR | Sidechain |
| 8 | N | 811 | ASP | Peptide |
| 8 | N | 835 | LEU | Peptide |
| 8 | N | 844 | TYR | Sidechain |
| 8 | N | 866 | ARG | Sidechain |
| 8 | N | 879 | ILE | Peptide |
| 8 | N | 88 | PHE | Sidechain |
| 8 | N | 884 | LEU | Peptide |
| 8 | N | 888 | TYR | Sidechain |
| 8 | N | 893 | TYR | Sidechain |
| 8 | N | 896 | PHE | Sidechain |
| 8 | N | 991 | LYS | Peptide |
| 7 | O | 106 | TYR | Sidechain |
| 7 | O | 1097 | TYR | Sidechain |
| 7 | O | 1108 | ARG | Sidechain |
| 7 | O | 1118 | ARG | Sidechain |
| 7 | O | 1138 | PHE | Mainchain |
| 7 | O | 1147 | PHE | Sidechain |
| 7 | O | 1156 | TYR | Sidechain |
| 7 | O | 1160 | TYR | Sidechain |
| 7 | O | 1180 | TYR | Sidechain |
| 7 | O | 1183 | TYR | Sidechain |
| 7 | O | 1189 | MET | Mainchain |
| 7 | O | 12 | TYR | Sidechain |
| 7 | O | 1237 | TYR | Sidechain |
| 7 | O | 1286 | PHE | Sidechain |
| 7 | O | 1292 | ARG | Sidechain |
| 7 | O | 1345 | PHE | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 7 | O | 1361 | PHE | Peptide |
| 7 | O | 1382 | TYR | Sidechain |
| 7 | O | 1394 | SER | Peptide |
| 7 | O | 1415 | ARG | Sidechain |
| 7 | O | 1431 | ARG | Sidechain |
| 7 | O | 1484 | ARG | Sidechain |
| 7 | O | 1518 | PHE | Sidechain |
| 7 | O | 171 | TYR | Sidechain |
| 7 | O | 188 | ARG | Sidechain |
| 7 | O | 232 | TYR | Sidechain |
| 7 | O | 233 | TYR | Sidechain |
| 7 | O | 295 | ARG | Sidechain |
| 7 | O | 430 | PHE | Sidechain |
| 7 | O | 431 | PHE | Sidechain |
| 7 | O | 510 | PHE | Sidechain |
| 7 | O | 547 | PHE | Sidechain |
| 7 | O | 619 | VAL | Peptide |
| 7 | O | 620 | THR | Peptide |
| 7 | O | 621 | TYR | Sidechain |
| 7 | O | 674 | PHE | Sidechain |
| 7 | O | 687 | TYR | Sidechain |
| 7 | O | 692 | TYR | Sidechain |
| 7 | O | 696 | PHE | Sidechain |
| 7 | O | 728 | TYR | Sidechain |
| 7 | O | 763 | HIS | Sidechain |
| 7 | O | 830 | TYR | Sidechain |
| 7 | O | 878 | TYR | Sidechain |
| 7 | O | 887 | PHE | Peptide |
| 7 | O | 898 | TYR | Sidechain |
| 7 | O | 904 | TYR | Sidechain |
| 7 | O | 910 | ARG | Sidechain |
| 7 | O | 929 | TYR | Peptide |
| 7 | O | 993 | ALA | Peptide |
| 8 | P | 1008 | THR | Peptide |
| 8 | P | 1009 | PRO | Peptide |
| 8 | P | 1022 | TYR | Sidechain |
| 8 | P | 111 | HIS | Sidechain |
| 8 | P | 1158 | TYR | Sidechain |
| 8 | P | 1199 | TYR | Sidechain |
| 8 | P | 1247 | PHE | Sidechain |
| 8 | P | 1254 | ARG | Sidechain |
| 8 | P | 1260 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 8 | P | 1309 | ARG | Sidechain |
| 8 | P | 1337 | LEU | Mainchain |
| 8 | P | 1392 | PHE | Sidechain |
| 8 | P | 1399 | ASN | Peptide |
| 8 | P | 1432 | ARG | Sidechain |
| 8 | P | 1463 | SER | Peptide |
| 8 | P | 1466 | TYR | Sidechain |
| 8 | P | 1524 | TYR | Sidechain |
| 8 | P | 216 | TYR | Sidechain |
| 8 | P | 282 | PHE | Sidechain |
| 8 | P | 411 | PHE | Sidechain |
| 8 | P | 432 | LEU | Peptide |
| 8 | P | 440 | ILE | Peptide |
| 8 | P | 475 | TYR | Sidechain |
| 8 | P | 527 | LYS | Peptide |
| 8 | P | 651 | TYR | Sidechain |
| 8 | P | 675 | TYR | Sidechain |
| 8 | P | 685 | TYR | Sidechain |
| 8 | P | 726 | LYS | Peptide |
| 8 | P | 727 | ASN | Peptide |
| 8 | P | 728 | ILE | Peptide |
| 8 | P | 775 | PHE | Sidechain |
| 8 | P | 780 | HIS | Sidechain |
| 8 | P | 810 | MET | Peptide |
| 8 | P | 811 | ASP | Peptide |
| 8 | P | 835 | LEU | Peptide |
| 8 | P | 842 | ASN | Mainchain |
| 8 | P | 866 | ARG | Sidechain |
| 8 | P | 888 | TYR | Sidechain |
| 8 | P | 894 | VAL | Peptide |
| 8 | P | 937 | SER | Peptide |
| 8 | P | 953 | TYR | Sidechain |
| 9 | Q | 277 | TYR | Sidechain |
| 9 | Q | 469 | TYR | Sidechain |
| 9 | Q | 474 | PHE | Sidechain |
| 9 | Q | 478 | TYR | Sidechain |
| 9 | Q | 496 | TYR | Sidechain |
| 9 | Q | 551 | ARG | Sidechain |
| 9 | Q | 607 | ARG | Sidechain |
| 9 | Q | 612 | HIS | Sidechain |
| 9 | Q | 630 | ARG | Sidechain |
| 9 | Q | 696 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 9 | Q | 704 | ARG | Sidechain |
| 9 | Q | 724 | ARG | Sidechain |
| 9 | Q | 727 | TYR | Sidechain |
| 9 | Q | 754 | ARG | Mainchain |
| 9 | Q | 816 | TYR | Sidechain |
| 9 | Q | 826 | ARG | Sidechain |
| 9 | R | 215 | TYR | Sidechain |
| 9 | R | 277 | TYR | Sidechain |
| 9 | R | 285 | TYR | Sidechain |
| 9 | R | 478 | TYR | Sidechain |
| 9 | R | 496 | TYR | Sidechain |
| 9 | R | 533 | ARG | Sidechain |
| 9 | R | 541 | TYR | Sidechain |
| 9 | R | 690 | ARG | Sidechain |
| 9 | R | 691 | ARG | Sidechain |
| 9 | R | 816 | TYR | Sidechain |
| 9 | R | 829 | TYR | Sidechain |
| 9 | S | 212 | PHE | Sidechain |
| 9 | S | 238 | PHE | Sidechain |
| 9 | S | 277 | TYR | Sidechain |
| 9 | S | 408 | ARG | Sidechain |
| 9 | S | 417 | ARG | Sidechain |
| 9 | S | 477 | TYR | Sidechain |
| 9 | S | 494 | TYR | Sidechain |
| 9 | S | 547 | TYR | Sidechain |
| 9 | S | 614 | ARG | Sidechain |
| 9 | S | 644 | TYR | Sidechain |
| 9 | S | 704 | ARG | Sidechain |
| 9 | S | 728 | PHE | Sidechain |
| 9 | S | 826 | ARG | Sidechain |
| 9 | S | 829 | TYR | Sidechain |
| 9 | T | 282 | PHE | Sidechain |
| 9 | T | 290 | TYR | Sidechain |
| 9 | T | 308 | PHE | Sidechain |
| 9 | T | 339 | TYR | Sidechain |
| 9 | T | 370 | TYR | Sidechain |
| 9 | T | 371 | PHE | Sidechain |
| 9 | T | 374 | TYR | Sidechain |
| 9 | T | 456 | ARG | Sidechain |
| 9 | T | 462 | PHE | Sidechain |
| 9 | T | 469 | TYR | Sidechain |
| 9 | T | 547 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 9 | T | 586 | PHE | Sidechain |
| 9 | T | 599 | ARG | Sidechain |
| 9 | T | 607 | ARG | Sidechain |
| 9 | T | 614 | ARG | Sidechain |
| 9 | T | 638 | TYR | Sidechain |
| 9 | T | 644 | TYR | Sidechain |
| 9 | T | 794 | TYR | Sidechain |
| 9 | T | 816 | TYR | Sidechain |
| 10 | U | 256 | PHE | Sidechain |
| 10 | U | 258 | TYR | Sidechain |
| 10 | U | 281 | ARG | Sidechain |
| 10 | U | 318 | TYR | Sidechain |
| 11 | V | 347 | TYR | Sidechain |
| 11 | V | 360 | TYR | Sidechain |
| 10 | W | 305 | TYR | Mainchain |
| 10 | W | 345 | TYR | Sidechain |
| 11 | X | 377 | PHE | Sidechain |
| 1 | Y | 1022 | ASP | Mainchain |
| 1 | Y | 1098 | TYR | Sidechain |
| 1 | Y | 1101 | ARG | Sidechain |
| 1 | Y | 1105 | TYR | Sidechain |
| 1 | Y | 1157 | PHE | Sidechain |
| 1 | Y | 1185 | TYR | Sidechain |
| 1 | Y | 1208 | SER | Peptide |
| 1 | Y | 1230 | PHE | Sidechain |
| 1 | Y | 1261 | ARG | Sidechain |
| 1 | Y | 1299 | GLY | Peptide |
| 1 | Y | 1331 | ARG | Sidechain |
| 1 | Y | 1427 | TYR | Sidechain |
| 1 | Y | 1444 | PHE | Sidechain |
| 1 | Y | 1447 | GLU | Peptide |
| 1 | Y | 1455 | TRP | Peptide |
| 1 | Y | 1460 | ARG | Sidechain |
| 1 | Y | 1468 | TYR | Sidechain |
| 1 | Y | 1477 | TYR | Sidechain |
| 1 | Y | 209 | HIS | Sidechain |
| 1 | Y | 241 | PHE | Sidechain |
| 1 | Y | 257 | PHE | Sidechain |
| 1 | Y | 260 | HIS | Sidechain |
| 1 | Y | 292 | ASN | Peptide |
| 1 | Y | 583 | TYR | Sidechain |
| 1 | Y | 659 | PHE | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | Y | 684 | PHE | Sidechain |
| 1 | Y | 696 | ARG | Sidechain |
| 1 | Y | 841 | TYR | Sidechain |
| 1 | Y | 949 | PHE | Sidechain |
| 1 | Y | 973 | ARG | Sidechain |
| 2 | Z | 1005 | TYR | Sidechain |
| 2 | Z | 1057 | TYR | Sidechain |
| 2 | Z | 1068 | ARG | Sidechain |
| 2 | Z | 1098 | LEU | Peptide |
| 2 | Z | 117 | TYR | Sidechain |
| 2 | Z | 1215 | TYR | Sidechain |
| 2 | Z | 1216 | TYR | Sidechain |
| 2 | Z | 1322 | TYR | Sidechain |
| 2 | Z | 1323 | TYR | Sidechain |
| 2 | Z | 1327 | ARG | Sidechain |
| 2 | Z | 171 | TYR | Sidechain |
| 2 | Z | 228 | PHE | Sidechain |
| 2 | Z | 231 | TYR | Sidechain |
| 2 | Z | 274 | PHE | Sidechain |
| 2 | Z | 288 | TYR | Sidechain |
| 2 | Z | 383 | HIS | Sidechain |
| 2 | Z | 431 | ARG | Sidechain |
| 2 | Z | 551 | TYR | Sidechain |
| 2 | Z | 594 | TYR | Sidechain |
| 2 | Z | 612 | TYR | Sidechain |
| 2 | Z | 614 | TYR | Sidechain |
| 2 | Z | 646 | TYR | Sidechain |
| 2 | Z | 883 | TYR | Sidechain |
| 2 | Z | 959 | TYR | Sidechain |
| 2 | Z | 994 | ARG | Sidechain |
| 14 | a | 1010 | PHE | Sidechain |
| 14 | a | 1035 | ARG | Peptide |
| 14 | a | 15 | TYR | Sidechain,Peptide |
| 14 | a | 202 | ASN | Peptide |
| 14 | a | 204 | TYR | Sidechain |
| 14 | a | 212 | PHE | Sidechain |
| 14 | a | 220 | TYR | Sidechain |
| 14 | a | 257 | TYR | Sidechain |
| 14 | a | 279 | TYR | Sidechain |
| 14 | a | 292 | PRO | Peptide |
| 14 | a | 294 | GLU | Peptide |
| 14 | a | 315 | PHE | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 14 | a | 348 | TYR | Sidechain |
| 14 | a | 436 | HIS | Sidechain |
| 14 | a | 451 | ARG | Sidechain |
| 14 | a | 484 | TYR | Sidechain |
| 14 | a | 492 | ASN | Peptide |
| 14 | a | 509 | TYR | Sidechain |
| 14 | a | 511 | ARG | Sidechain |
| 14 | a | 56 | TYR | Sidechain |
| 14 | a | 561 | GLN | Peptide |
| 14 | a | 660 | LYS | Peptide |
| 14 | a | 668 | TYR | Sidechain |
| 14 | a | 674 | LEU | Peptide |
| 14 | a | 686 | PHE | Sidechain |
| 14 | a | 695 | TYR | Sidechain |
| 14 | a | 71 | HIS | Sidechain |
| 14 | a | 744 | VAL | Peptide |
| 14 | a | 749 | TYR | Peptide |
| 14 | a | 782 | TYR | Peptide |
| 14 | a | 793 | PHE | Peptide |
| 14 | a | 802 | TYR | Sidechain |
| 14 | a | 803 | HIS | Sidechain |
| 14 | a | 806 | SER | Peptide |
| 14 | a | 819 | TYR | Peptide |
| 14 | a | 821 | HIS | Peptide |
| 14 | a | 826 | TYR | Sidechain |
| 14 | a | 832 | PHE | Sidechain |
| 14 | a | 847 | LYS | Peptide |
| 14 | a | 851 | TYR | Peptide |
| 14 | a | 862 | GLN | Peptide |
| 14 | a | 864 | PHE | Sidechain |
| 14 | a | 872 | TYR | Sidechain |
| 14 | a | 880 | ARG | Sidechain |
| 14 | a | 882 | PHE | Sidechain |
| 14 | a | 889 | LEU | Peptide |
| 14 | a | 892 | GLY | Peptide |
| 14 | a | 916 | ARG | Sidechain |
| 14 | a | 924 | ARG | Sidechain |
| 14 | a | 929 | HIS | Peptide |
| 14 | a | 936 | TYR | Sidechain |
| 14 | a | 945 | VAL | Peptide |
| 14 | a | 957 | ASP | Peptide |
| 14 | a | 958 | TRP | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 14 | a | 964 | LEU | Peptide |
| 14 | a | 965 | TYR | Sidechain |
| 15 | b | 107 | TYR | Sidechain |
| 15 | b | 112 | PHE | Sidechain |
| 15 | b | 122 | ARG | Sidechain |
| 15 | b | 140 | HIS | Sidechain |
| 15 | b | 189 | TYR | Sidechain |
| 15 | b | 244 | TYR | Sidechain |
| 15 | b | 256 | GLY | Peptide |
| 15 | b | 267 | ARG | Sidechain |
| 15 | b | 271 | LEU | Peptide |
| 15 | b | 273 | TYR | Sidechain |
| 15 | b | 331 | TYR | Sidechain |
| 15 | b | 419 | PHE | Sidechain |
| 15 | b | 469 | PHE | Sidechain |
| 15 | b | 482 | TRP | Peptide |
| 15 | b | 530 | ARG | Sidechain |
| 15 | b | 54 | ASN | Peptide |
| 15 | b | 655 | PHE | Peptide |
| 15 | b | 659 | PRO | Peptide |
| 15 | b | 662 | TYR | Sidechain |
| 15 | b | 681 | LYS | Peptide |
| 15 | b | 69 | PHE | Sidechain |
| 15 | b | 91 | TYR | Sidechain |
| 15 | b | 97 | ARG | Sidechain |
| 16 | c | 142 | ARG | Sidechain |
| 16 | c | 189 | TYR | Sidechain |
| 16 | c | 223 | TYR | Sidechain |
| 16 | c | 246 | TYR | Sidechain |
| 16 | c | 248 | TYR | Sidechain |
| 16 | c | 267 | ARG | Sidechain |
| 16 | c | 297 | TYR | Sidechain |
| 16 | c | 333 | ARG | Sidechain |
| 16 | c | 358 | TYR | Sidechain |
| 16 | c | 379 | PHE | Sidechain |
| 16 | c | 441 | ARG | Sidechain |
| 16 | c | 446 | ASP | Peptide |
| 16 | c | 456 | THR | Peptide |
| 16 | c | 477 | PHE | Sidechain |
| 16 | c | 509 | ARG | Sidechain |
| 16 | c | 513 | ARG | Sidechain |
| 16 | c | 519 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 16 | c | 548 | TYR | Sidechain |
| 16 | c | 617 | PHE | Sidechain |
| 16 | c | 634 | ILE | Peptide |
| 16 | c | 650 | HIS | Peptide |
| 17 | d | 131 | LYS | Peptide |
| 17 | d | 173 | PHE | Sidechain |
| 17 | d | 237 | ASP | Peptide |
| 17 | d | 259 | ARG | Sidechain |
| 17 | d | 36 | PHE | Sidechain |
| 17 | d | 58 | ARG | Sidechain |
| 17 | d | 62 | ALA | Peptide |
| 17 | d | 88 | ARG | Sidechain |
| 17 | d | 98 | HIS | Peptide |
| 18 | e | 113 | SER | Peptide |
| 18 | e | 116 | PHE | Sidechain |
| 18 | e | 177 | ARG | Sidechain |
| 18 | e | 228 | TYR | Sidechain |
| 18 | e | 303 | HIS | Sidechain |
| 18 | e | 305 | GLY | Peptide |
| 18 | e | 324 | ASP | Peptide |
| 18 | e | 332 | LYS | Peptide |
| 18 | e | 68 | TYR | Sidechain |
| 18 | e | 70 | ARG | Sidechain |
| 19 | f | 117 | TYR | Sidechain |
| 19 | f | 245 | ARG | Sidechain |
| 19 | f | 248 | TYR | Sidechain |
| 19 | f | 279 | TYR | Sidechain |
| 19 | f | 334 | ARG | Peptide |
| 19 | f | 384 | TYR | Sidechain |
| 19 | f | 387 | ARG | Sidechain |
| 19 | f | 42 | PHE | Sidechain |
| 19 | f | 426 | TYR | Sidechain |
| 19 | f | 482 | ARG | Peptide |
| 19 | f | 536 | ARG | Sidechain |
| 19 | f | 552 | ARG | Sidechain |
| 19 | f | 580 | PHE | Sidechain |
| 19 | f | 587 | TYR | Sidechain |
| 19 | f | 649 | TYR | Sidechain |
| 19 | f | 659 | TYR | Sidechain |
| 19 | f | 662 | PHE | Sidechain |
| 19 | f | 676 | LYS | Peptide |
| 19 | f | 683 | PHE | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 19 | f | 685 | SER | Peptide |
| 19 | f | 692 | SER | Peptide |
| 20 | g | 1006 | TYR | Sidechain |
| 20 | g | 1020 | ARG | Sidechain |
| 20 | g | 1031 | PHE | Sidechain |
| 20 | g | 1110 | ARG | Sidechain |
| 20 | g | 119 | TYR | Sidechain |
| 20 | g | 175 | TYR | Sidechain |
| 20 | g | 252 | PHE | Sidechain |
| 20 | g | 292 | PHE | Sidechain |
| 20 | g | 303 | HIS | Sidechain |
| 20 | g | 351 | ILE | Mainchain |
| 20 | g | 378 | PHE | Peptide |
| 20 | g | 380 | THR | Peptide |
| 20 | g | 400 | PHE | Sidechain |
| 20 | g | 450 | ARG | Sidechain |
| 20 | g | 460 | TYR | Sidechain |
| 20 | g | 466 | TYR | Sidechain |
| 20 | g | 503 | TYR | Sidechain |
| 20 | g | 529 | HIS | Sidechain |
| 20 | g | 541 | SER | Peptide |
| 20 | g | 547 | PRO | Peptide |
| 20 | g | 563 | PHE | Peptide |
| 20 | g | 574 | ASN | Peptide |
| 20 | g | 621 | TYR | Sidechain |
| 20 | g | 628 | HIS | Peptide |
| 20 | g | 66 | ARG | Sidechain |
| 20 | g | 750 | TYR | Sidechain |
| 20 | g | 77 | SER | Peptide |
| 20 | g | 790 | HIS | Sidechain |
| 20 | g | 80 | PHE | Peptide |
| 20 | g | 803 | GLN | Peptide |
| 20 | g | 839 | PHE | Sidechain |
| 20 | g | 881 | LYS | Peptide |
| 20 | g | 907 | THR | Peptide |
| 20 | g | 945 | ARG | Sidechain |
| 20 | g | 949 | TYR | Sidechain |
| 20 | g | 981 | ARG | Sidechain |
| 20 | g | 984 | PHE | Sidechain |
| 14 | h | 1023 | LYS | Peptide |
| 14 | h | 1035 | ARG | Peptide |
| 14 | h | 14 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 14 | h | 15 | TYR | Peptide |
| 14 | h | 168 | TYR | Sidechain |
| 14 | h | 194 | TYR | Sidechain |
| 14 | h | 229 | PHE | Sidechain |
| 14 | h | 27 | TYR | Sidechain |
| 14 | h | 279 | TYR | Sidechain |
| 14 | h | 338 | ARG | Sidechain |
| 14 | h | 392 | GLU | Peptide |
| 14 | h | 451 | ARG | Sidechain |
| 14 | h | 494 | PHE | Sidechain |
| 14 | h | 516 | PHE | Peptide |
| 14 | h | 561 | GLN | Peptide |
| 14 | h | 591 | MET | Peptide |
| 14 | h | 627 | TYR | Sidechain |
| 14 | h | 647 | PHE | Sidechain |
| 14 | h | 668 | TYR | Sidechain |
| 14 | h | 67 | TYR | Sidechain |
| 14 | h | 695 | TYR | Sidechain |
| 14 | h | 70 | TYR | Sidechain |
| 14 | h | 720 | PHE | Peptide |
| 14 | h | 738 | ARG | Sidechain |
| 14 | h | 749 | TYR | Sidechain |
| 14 | h | 770 | PHE | Sidechain |
| 14 | h | 782 | TYR | Peptide |
| 14 | h | 793 | PHE | Peptide |
| 14 | h | 806 | SER | Peptide |
| 14 | h | 821 | HIS | Peptide |
| 14 | h | 834 | ARG | Sidechain |
| 14 | h | 846 | SER | Peptide |
| 14 | h | 847 | LYS | Peptide |
| 14 | h | 851 | TYR | Sidechain |
| 14 | h | 862 | GLN | Peptide |
| 14 | h | 885 | VAL | Peptide |
| 14 | h | 888 | VAL | Peptide |
| 14 | h | 889 | LEU | Peptide |
| 14 | h | 892 | GLY | Peptide |
| 14 | h | 901 | ARG | Sidechain |
| 14 | h | 924 | ARG | Sidechain |
| 14 | h | 938 | ARG | Sidechain |
| 14 | h | 941 | ASP | Peptide |
| 14 | h | 945 | VAL | Peptide |
| 14 | h | 954 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 14 | h | 957 | ASP | Peptide |
| 14 | h | 958 | TRP | Peptide |
| 14 | h | 964 | LEU | Peptide |
| 14 | h | 968 | ARG | Sidechain |
| 15 | i | 173 | TYR | Sidechain |
| 15 | i | 186 | ARG | Sidechain |
| 15 | i | 190 | PHE | Sidechain |
| 15 | i | 223 | TYR | Sidechain |
| 15 | i | 244 | TYR | Sidechain |
| 15 | i | 255 | ARG | Sidechain |
| 15 | i | 265 | ILE | Peptide |
| 15 | i | 271 | LEU | Peptide |
| 15 | i | 273 | TYR | Sidechain |
| 15 | i | 343 | GLN | Peptide |
| 15 | i | 362 | LEU | Peptide |
| 15 | i | 464 | TYR | Sidechain |
| 15 | i | 497 | ARG | Sidechain |
| 15 | i | 511 | TYR | Peptide |
| 15 | i | 52 | THR | Mainchain |
| 15 | i | 528 | GLU | Peptide |
| 15 | i | 550 | HIS | Sidechain |
| 15 | i | 593 | ALA | Peptide |
| 15 | i | 625 | ALA | Peptide |
| 15 | i | 642 | TRP | Peptide |
| 15 | i | 647 | ARG | Sidechain |
| 15 | i | 657 | TYR | Sidechain |
| 15 | i | 658 | LEU | Peptide |
| 15 | i | 662 | TYR | Sidechain |
| 15 | i | 710 | TYR | Sidechain |
| 15 | i | 717 | ASP | Peptide |
| 15 | i | 76 | TYR | Sidechain,Peptide |
| 15 | i | 87 | LYS | Peptide |
| 15 | i | 91 | TYR | Sidechain |
| 15 | i | 97 | ARG | Sidechain |
| 16 | j | 207 | TYR | Sidechain |
| 16 | j | 223 | TYR | Sidechain |
| 16 | j | 248 | TYR | Sidechain |
| 16 | j | 285 | ARG | Sidechain |
| 16 | j | 295 | PHE | Sidechain |
| 16 | j | 297 | TYR | Sidechain |
| 16 | j | 324 | TYR | Sidechain |
| 16 | j | 358 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 16 | j | 425 | TYR | Sidechain |
| 16 | j | 446 | ASP | Peptide |
| 16 | j | 452 | TYR | Sidechain |
| 16 | j | 475 | PHE | Sidechain |
| 16 | j | 489 | HIS | Sidechain |
| 16 | j | 529 | ARG | Sidechain |
| 16 | j | 552 | TYR | Sidechain |
| 16 | j | 596 | ARG | Sidechain |
| 16 | j | 602 | PHE | Sidechain |
| 16 | j | 615 | ASN | Peptide |
| 16 | j | 620 | TYR | Sidechain |
| 16 | j | 648 | TYR | Sidechain,Peptide |
| 16 | j | 650 | HIS | Peptide |
| 17 | k | 19 | TYR | Sidechain |
| 17 | k | 20 | TYR | Sidechain |
| 17 | k | 88 | ARG | Sidechain |
| 18 | l | 114 | VAL | Peptide |
| 18 | l | 13 | HIS | Sidechain |
| 18 | l | 137 | TYR | Sidechain |
| 18 | l | 146 | ARG | Sidechain |
| 18 | l | 20 | TYR | Sidechain |
| 18 | l | 309 | SER | Peptide |
| 18 | l | 335 | TYR | Sidechain |
| 18 | l | 39 | ASP | Peptide |
| 18 | l | 52 | ARG | Sidechain |
| 18 | l | 97 | ARG | Sidechain |
| 19 | m | 15 | PHE | Sidechain |
| 19 | m | 279 | TYR | Sidechain |
| 19 | m | 330 | ARG | Sidechain |
| 19 | m | 334 | ARG | Peptide |
| 19 | m | 40 | ARG | Sidechain |
| 19 | m | 416 | TYR | Sidechain |
| 19 | m | 509 | HIS | Sidechain |
| 19 | m | 597 | TYR | Sidechain |
| 19 | m | 653 | TYR | Sidechain |
| 19 | m | 685 | SER | Peptide |
| 19 | m | 686 | GLU | Peptide |
| 19 | m | 73 | ARG | Sidechain |
| 20 | n | 112 | SER | Peptide |
| 20 | n | 118 | PRO | Peptide |
| 20 | n | 120 | ILE | Peptide |
| 20 | n | 137 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 20 | n | 142 | PHE | Peptide |
| 20 | n | 145 | THR | Peptide |
| 20 | n | 146 | MET | Peptide |
| 20 | n | 284 | TYR | Sidechain |
| 20 | n | 303 | HIS | Sidechain |
| 20 | n | 326 | PHE | Sidechain |
| 20 | n | 378 | PHE | Peptide |
| 20 | n | 382 | ARG | Sidechain |
| 20 | n | 420 | PHE | Peptide |
| 20 | n | 466 | TYR | Sidechain |
| 20 | n | 526 | SER | Peptide |
| 20 | n | 551 | ASN | Peptide |
| 20 | n | 556 | HIS | Sidechain |
| 20 | n | 563 | PHE | Sidechain |
| 20 | n | 579 | ILE | Peptide |
| 20 | n | 592 | GLU | Peptide |
| 20 | n | 610 | LEU | Peptide |
| 20 | n | 621 | TYR | Peptide |
| 20 | n | 628 | HIS | Peptide |
| 20 | n | 66 | ARG | Sidechain |
| 20 | n | 692 | GLU | Peptide |
| 20 | n | 713 | ASP | Peptide |
| 20 | n | 738 | TYR | Sidechain |
| 20 | n | 751 | TYR | Sidechain |
| 20 | n | 77 | SER | Peptide |
| 20 | n | 781 | TYR | Sidechain |
| 20 | n | 839 | PHE | Sidechain |
| 20 | n | 881 | LYS | Peptide |
| 20 | n | 98 | LEU | Peptide |
| 20 | n | 984 | PHE | Sidechain |
| 21 | o | 39 | ARG | Sidechain |
| 21 | o | 65 | PHE | Sidechain |
| 21 | o | 80 | TYR | Sidechain |
| 21 | p | 35 | TYR | Sidechain |
| 21 | p | 53 | TYR | Sidechain |
| 21 | p | 56 | THR | Mainchain |
| 21 | p | 80 | TYR | Peptide |
| 21 | p | 86 | PHE | Sidechain |
| 21 | p | 89 | PHE | Sidechain |
| 21 | q | 56 | THR | Mainchain |
| 21 | q | 65 | PHE | Sidechain |
| 21 | q | 68 | TYR | Sidechain |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 21 | q | 71 | HIS | Sidechain |
| 21 | q | 79 | PHE | Sidechain |
| 21 | r | 65 | PHE | Sidechain |
| 21 | r | 75 | HIS | Sidechain |
| 21 | r | 78 | TYR | Sidechain |
| 21 | r | 89 | PHE | Sidechain |
| 21 | s | 53 | TYR | Sidechain |
| 21 | s | 56 | THR | Mainchain |
| 21 | s | 68 | TYR | Sidechain |
| 21 | s | 78 | TYR | Sidechain |
| 21 | s | 79 | PHE | Sidechain |
| 21 | t | 35 | TYR | Sidechain |
| 21 | t | 56 | THR | Mainchain |
| 21 | t | 68 | TYR | Sidechain |
| 21 | t | 76 | PHE | Sidechain |
| 21 | t | 80 | TYR | Sidechain |
| 21 | t | 86 | PHE | Sidechain |
| 12 | u | 112 | PHE | Sidechain |
| 12 | u | 132 | PHE | Sidechain |
| 12 | u | 266 | ARG | Sidechain |
| 12 | u | 344 | TYR | Sidechain |
| 12 | u | 374 | TYR | Sidechain |
| 12 | u | 422 | ARG | Sidechain |
| 12 | u | 428 | TYR | Sidechain |
| 12 | u | 44 | ARG | Sidechain |
| 12 | v | 132 | PHE | Sidechain |
| 12 | v | 154 | PHE | Sidechain |
| 12 | v | 195 | TYR | Sidechain |
| 12 | v | 209 | TYR | Sidechain |
| 12 | v | 247 | ARG | Sidechain |
| 12 | v | 25 | TYR | Sidechain |
| 12 | v | 285 | PHE | Sidechain |
| 12 | v | 290 | PHE | Sidechain |
| 12 | v | 328 | PHE | Sidechain |
| 12 | v | 353 | ARG | Sidechain |
| 12 | v | 374 | TYR | Sidechain |
| 12 | v | 394 | SER | Mainchain |
| 12 | v | 428 | TYR | Sidechain |
| 12 | v | 54 | TYR | Sidechain |
| 13 | x | 1117 | TYR | Sidechain |
| 13 | x | 1455 | ASN | Peptide |

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 0 | 8762 | 0 | 8808 | 270 | 0 |
| 1 | Y | 8770 | 0 | 8821 | 123 | 0 |
| 2 | 1 | 8919 | 0 | 8932 | 108 | 0 |
| 2 | Z | 8906 | 0 | 8917 | 109 | 0 |
| 3 | 5 | 181 | 0 | 38 | 0 | 0 |
| 3 | 6 | 181 | 0 | 38 | 7 | 0 |
| 4 | A | 1315 | 0 | 1274 | 9 | 0 |
| 4 | D | 1315 | 0 | 1275 | 16 | 0 |
| 4 | G | 1321 | 0 | 1280 | 6 | 0 |
| 4 | J | 1321 | 0 | 1280 | 22 | 0 |
| 4 | y | 946 | 0 | 404 | 19 | 0 |
| 4 | z | 962 | 0 | 410 | 24 | 0 |
| 5 | B | 1771 | 0 | 1832 | 11 | 0 |
| 5 | E | 1771 | 0 | 1832 | 70 | 0 |
| 5 | H | 1771 | 0 | 1832 | 39 | 0 |
| 5 | K | 1771 | 0 | 1832 | 11 | 0 |
| 6 | C | 1347 | 0 | 1376 | 10 | 0 |
| 6 | F | 1351 | 0 | 1379 | 12 | 0 |
| 6 | I | 1347 | 0 | 1376 | 8 | 0 |
| 6 | L | 1351 | 0 | 1379 | 8 | 0 |
| 7 | M | 11909 | 0 | 11617 | 105 | 0 |
| 7 | O | 11902 | 0 | 11608 | 120 | 0 |
| 8 | N | 10971 | 0 | 11316 | 148 | 0 |
| 8 | P | 10971 | 0 | 11315 | 215 | 0 |
| 9 | Q | 5184 | 0 | 4900 | 24 | 0 |
| 9 | R | 5287 | 0 | 4948 | 61 | 0 |
| 9 | S | 5197 | 0 | 4913 | 90 | 0 |
| 9 | T | 5287 | 0 | 4948 | 21 | 0 |
| 10 | U | 745 | 0 | 752 | 23 | 0 |
| 10 | W | 745 | 0 | 752 | 16 | 0 |
| 11 | V | 739 | 0 | 722 | 23 | 0 |
| 11 | X | 739 | 0 | 722 | 30 | 0 |
| 12 | u | 4214 | 0 | 3713 | 9 | 0 |
| 12 | v | 4063 | 0 | 3567 | 18 | 0 |
| 13 | w | 1088 | 0 | 656 | 1 | 0 |
| 13 | x | 1106 | 0 | 671 | 9 | 0 |
| 14 | a | 8279 | 0 | 8125 | 49 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 14 | h | 8279 | 0 | 8125 | 29 | 0 |
| 15 | b | 5424 | 0 | 5397 | 14 | 0 |
| 15 | i | 5327 | 0 | 5309 | 19 | 0 |
| 16 | c | 4520 | 0 | 4539 | 21 | 0 |
| 16 | j | 4520 | 0 | 4539 | 12 | 0 |
| 17 | d | 2160 | 0 | 2096 | 9 | 0 |
| 17 | k | 2160 | 0 | 2096 | 6 | 0 |
| 18 | e | 2407 | 0 | 2348 | 17 | 0 |
| 18 | l | 2438 | 0 | 2378 | 6 | 0 |
| 19 | f | 5261 | 0 | 5261 | 41 | 0 |
| 19 | m | 5261 | 0 | 5261 | 56 | 0 |
| 20 | g | 8627 | 0 | 8539 | 36 | 0 |
| 20 | n | 8627 | 0 | 8539 | 61 | 0 |
| 21 | o | 691 | 0 | 702 | 1 | 0 |
| 21 | p | 691 | 0 | 702 | 11 | 0 |
| 21 | q | 691 | 0 | 702 | 0 | 0 |
| 21 | r | 691 | 0 | 702 | 3 | 0 |
| 21 | s | 691 | 0 | 702 | 0 | 0 |
| 21 | t | 691 | 0 | 702 | 1 | 0 |
| All | All | 212962 | 0 | 208199 | 1948 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1948) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0:413:LEU:HD11 | 1:0:467:PHE:CD1 | 1.34 | 1.62 |
| 1:Y:412:ILE:CG2 | 1:Y:444:VAL:CG2 | 1.77 | 1.62 |
| 13:x:1300:ARG:CB | 21:p:51:VAL:HG21 | 1.28 | 1.59 |
| 8:N:322:HIS:CE1 | 8:N:359:LEU:HB3 | 1.34 | 1.58 |
| 1:Y:412:ILE:CG2 | 1:Y:444:VAL:HG21 | 1.20 | 1.58 |
| 1:0:401:ILE:CB | 1:0:462:LEU:HD23 | 1.19 | 1.57 |
| 2:1:1016:ASP:CA | 2:1:1040:LYS:HD2 | 1.13 | 1.56 |
| 1:0:129:SER:CB | 1:0:406:THR:H | 1.19 | 1.55 |
| 2:1:1016:ASP:HA | 2:1:1040:LYS:CD | 1.12 | 1.55 |
| 20:n:774:PHE:CZ | 20:n:777:ILE:HG21 | 1.38 | 1.54 |
| 1:0:413:LEU:HD21 | 1:0:467:PHE:CG | 1.42 | 1.53 |
| 4:y:595:ASP:CA | 4:z:598:LYS:CB | 1.85 | 1.53 |
| 1:0:401:ILE:HG13 | 1:0:462:LEU:CB | 1.13 | 1.53 |
| 9:R:746:PRO:HB3 | 9:R:753:ALA:N | 1.22 | 1.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0:131:VAL:CA | 1:0:511:LYS:HE3 | 1.38 | 1.52 |
| 4:y:595:ASP:HA | 4:z:598:LYS:CB | 1.09 | 1.50 |
| 10:U:304:LYS:CE | 11:V:271:ILE:HD11 | 1.42 | 1.50 |
| 7:O:1174:LYS:CB | 7:O:1319:LEU:HD23 | 1.39 | 1.49 |
| 1:0:401:ILE:HB | 1:0:462:LEU:CD2 | 1.40 | 1.47 |
| 10:U:304:LYS:HD3 | 11:V:271:ILE:CD1 | 1.44 | 1.46 |
| 1:0:413:LEU:CD1 | 1:0:467:PHE:CD1 | 1.98 | 1.46 |
| 8:N:379:ILE:CG1 | 8:N:403:ILE:HG21 | 1.47 | 1.45 |
| 1:0:129:SER:CA | 1:0:406:THR:H | 1.27 | 1.44 |
| 5:E:326:LYS:HD2 | 5:E:335:TRP:CE3 | 1.51 | 1.43 |
| 1:0:413:LEU:HD21 | 1:0:467:PHE:CD1 | 1.51 | 1.42 |
| 10:U:304:LYS:CD | 11:V:271:ILE:HD11 | 1.50 | 1.42 |
| 5:H:316:VAL:HG21 | 5:H:348:ILE:CB | 1.49 | 1.41 |
| 1:0:401:ILE:CG1 | 1:0:462:LEU:HB3 | 1.50 | 1.40 |
| 8:P:380:THR:HB | 8:P:400:PHE:CD1 | 1.57 | 1.40 |
| 19:f:27:ASN:HB2 | 19:f:435:PHE:CD2 | 1.54 | 1.40 |
| 1:0:413:LEU:HG | 1:0:467:PHE:CE1 | 1.54 | 1.39 |
| 7:O:1174:LYS:HB2 | 7:O:1319:LEU:CD2 | 1.52 | 1.38 |
| 2:1:127:ASP:OD1 | 2:1:457:SER:CB | 1.70 | 1.37 |
| 5:H:316:VAL:HG21 | 5:H:348:ILE:CG1 | 1.54 | 1.37 |
| 9:R:746:PRO:CG | 9:R:753:ALA:HA | 1.54 | 1.36 |
| 2:1:127:ASP:OD1 | 2:1:457:SER:HB2 | 1.19 | 1.36 |
| 9:S:268:ILE:CD1 | 9:S:514:LYS:HD2 | 1.55 | 1.36 |
| 1:Y:412:ILE:HG23 | 1:Y:444:VAL:CG2 | 1.37 | 1.36 |
| 1:0:131:VAL:N | 1:0:511:LYS:CE | 1.89 | 1.35 |
| 4:z:604:SER:O | 4:z:610:ALA:N | 1.57 | 1.34 |
| 1:0:413:LEU:CD2 | 1:0:467:PHE:CD1 | 2.10 | 1.33 |
| 1:0:413:LEU:CG | 1:0:467:PHE:CD1 | 2.11 | 1.32 |
| 1:0:413:LEU:CD1 | 1:0:467:PHE:HD1 | 1.33 | 1.32 |
| 1:0:129:SER:CA | 1:0:406:THR:N | 1.89 | 1.32 |
| 1:0:401:ILE:CG1 | 1:0:462:LEU:CB | 2.04 | 1.32 |
| 7:O:1174:LYS:O | 7:O:1319:LEU:HB2 | 1.27 | 1.31 |
| 1:0:130:GLY:C | 1:0:511:LYS:HZ1 | 1.37 | 1.31 |
| 1:0:129:SER:HA | 1:0:406:THR:N | 1.41 | 1.31 |
| 5:H:321:ALA:HB1 | 5:H:347:THR:O | 1.26 | 1.31 |
| 1:0:131:VAL:CA | 1:0:511:LYS:CE | 2.09 | 1.31 |
| 1:0:131:VAL:N | 1:0:511:LYS:HE3 | 0.98 | 1.30 |
| 20:n:774:PHE:CE1 | 20:n:777:ILE:HG21 | 1.66 | 1.30 |
| 1:0:130:GLY:O | 1:0:511:LYS:NZ | 1.67 | 1.28 |
| 8:P:777:ASP:O | 8:P:793:LEU:HG | 1.31 | 1.28 |
| 1:0:407:ALA:HB2 | 1:0:467:PHE:CZ | 1.65 | 1.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0:413:LEU:CG | 1:0:467:PHE:CE1 | 2.15 | 1.26 |
| 8:P:380:THR:OG1 | 8:P:400:PHE:HB2 | 1.19 | 1.26 |
| 1:0:129:SER:CB | 1:0:406:THR:N | 1.92 | 1.26 |
| 7:O:1174:LYS:CB | 7:O:1319:LEU:CD2 | 2.07 | 1.25 |
| 8:N:1384:ASP:OD1 | 8:N:1442:ILE:HD11 | 1.16 | 1.25 |
| 4:J:727:SER:O | 7:O:746:LYS:HG2 | 1.37 | 1.25 |
| 8:P:275:LEU:CD1 | 8:P:382:PHE:HE1 | 1.49 | 1.24 |
| 1:0:130:GLY:C | 1:0:511:LYS:NZ | 1.93 | 1.23 |
| 1:0:401:ILE:CG1 | 1:0:462:LEU:HD23 | 1.67 | 1.23 |
| 1:0:417:TYR:HB3 | 1:0:442:GLY:N | 1.53 | 1.23 |
| 3:6:36:UNK:CB | 7:M:1038:LEU:HD21 | 1.67 | 1.23 |
| 1:0:1277:SER:HB2 | 9:R:754:ARG:CG | 1.67 | 1.22 |
| 8:N:379:ILE:HG13 | 8:N:403:ILE:CD1 | 1.70 | 1.22 |
| 9:R:746:PRO:CB | 9:R:753:ALA:N | 2.01 | 1.22 |
| 2:1:1015:VAL:O | 2:1:1040:LYS:HD3 | 1.40 | 1.22 |
| 1:Y:403:GLY:HA3 | 1:Y:408:ARG:NE | 1.54 | 1.21 |
| 2:Z:1253:VAL:CG1 | 2:Z:1300:SER:OG | 1.87 | 1.21 |
| 2:Z:1253:VAL:HG12 | 2:Z:1300:SER:OG | 1.41 | 1.21 |
| 13:x:1296:THR:N | 21:p:47:LYS:NZ | 1.86 | 1.21 |
| 8:P:75:ILE:CD1 | 8:P:82:ASN:O | 1.88 | 1.21 |
| 1:0:409:ALA:C | 1:0:512:LYS:HG2 | 1.67 | 1.20 |
| 2:1:1175:ASN:HD21 | 9:S:754:ARG:CB | 1.52 | 1.20 |
| 1:0:401:ILE:CG1 | 1:0:462:LEU:CD2 | 2.17 | 1.20 |
| 1:0:1276:LEU:CB | 9:R:754:ARG:HE | 1.55 | 1.20 |
| 4:J:727:SER:C | 7:O:746:LYS:HZ3 | 1.47 | 1.19 |
| 11:X:297:ASP:HA | 11:X:302:ARG:O | 1.42 | 1.19 |
| 13:x:1300:ARG:CB | 21:p:51:VAL:CG2 | 2.20 | 1.18 |
| 1:0:409:ALA:O | 1:0:512:LYS:HG2 | 1.42 | 1.18 |
| 1:0:1277:SER:CB | 9:R:754:ARG:CG | 2.22 | 1.18 |
| 9:S:510:LEU:HB3 | 9:S:515:LEU:O | 1.43 | 1.18 |
| 9:R:746:PRO:HG3 | 9:R:753:ALA:CA | 1.71 | 1.17 |
| 1:0:129:SER:OG | 1:0:405:THR:HA | 1.42 | 1.17 |
| 20:n:774:PHE:CZ | 20:n:777:ILE:CG2 | 2.25 | 1.17 |
| 8:P:380:THR:CB | 8:P:400:PHE:CD1 | 2.28 | 1.17 |
| 8:P:1304:LYS:HE3 | 8:P:1304:LYS:HA | 1.24 | 1.17 |
| 1:Y:397:TYR:OH | 1:Y:461:ARG:HA | 1.44 | 1.17 |
| 1:0:398:ILE:HG21 | 1:0:446:LEU:HD22 | 1.24 | 1.16 |
| 8:N:380:THR:O | 8:N:414:ASN:ND2 | 1.75 | 1.16 |
| 1:0:131:VAL:HA | 1:0:511:LYS:CE | 1.72 | 1.16 |
| 8:N:322:HIS:CE1 | 8:N:359:LEU:CB | 2.27 | 1.16 |
| 8:P:72:ARG:O | 8:P:83:VAL:O | 1.63 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1:490:SER:O | 2:1:514:ARG:HB2 | 1.46 | 1.15 |
| 8:P:53:GLU:N | 8:P:133:ASP:OD2 | 1.76 | 1.15 |
| 5:E:378:HIS:O | 5:E:381:GLU:HG2 | 1.46 | 1.15 |
| 1:0:410:ALA:HB1 | 1:0:511:LYS:O | 1.48 | 1.14 |
| 5:E:317:ASN:O | 5:E:348:ILE:HD11 | 1.44 | 1.14 |
| 8:P:1227:VAL:HG13 | 8:P:1277:ILE:CD1 | 1.75 | 1.14 |
| 1:Y:412:ILE:HG21 | 1:Y:444:VAL:CG2 | 1.66 | 1.13 |
| 1:0:1276:LEU:HB3 | 9:R:754:ARG:HE | 1.01 | 1.13 |
| 1:Y:412:ILE:HG21 | 1:Y:444:VAL:CG1 | 1.77 | 1.13 |
| 8:N:69:ASN:HA | 8:N:72:ARG:NE | 1.64 | 1.12 |
| 8:P:1227:VAL:CG1 | 8:P:1277:ILE:HD13 | 1.79 | 1.12 |
| 2:1:1175:ASN:ND2 | 9:S:754:ARG:CB | 2.11 | 1.12 |
| 8:P:1227:VAL:HG11 | 8:P:1277:ILE:HG21 | 1.31 | 1.12 |
| 1:0:130:GLY:C | 1:0:511:LYS:CE | 2.20 | 1.12 |
| 1:0:131:VAL:HG13 | 1:0:511:LYS:CD | 1.77 | 1.12 |
| 1:Y:126:TYR:CE1 | 1:Y:405:THR:HB | 1.85 | 1.12 |
| 1:Y:791:MET:SD | 1:Y:923:ASP:OD2 | 2.06 | 1.12 |
| 8:N:379:ILE:CG1 | 8:N:403:ILE:CG2 | 2.28 | 1.11 |
| 10:U:304:LYS:CD | 11:V:271:ILE:CD1 | 2.15 | 1.11 |
| 1:0:467:PHE:HB2 | 1:0:511:LYS:HD2 | 1.26 | 1.11 |
| 2:1:513:LYS:HG2 | 2:1:539:TYR:OH | 1.50 | 1.11 |
| 8:N:69:ASN:HA | 8:N:72:ARG:HE | 1.05 | 1.11 |
| 9:S:268:ILE:HD11 | 9:S:514:LYS:CD | 1.80 | 1.11 |
| 1:0:1276:LEU:HB3 | 9:R:754:ARG:NE | 1.66 | 1.10 |
| 5:H:316:VAL:HG21 | 5:H:348:ILE:HB | 1.19 | 1.10 |
| 10:U:304:LYS:HE2 | 11:V:271:ILE:CD1 | 1.81 | 1.10 |
| 11:X:282:ASN:OD1 | 11:X:299:GLN:NE2 | 1.85 | 1.10 |
| 2:1:1178:ARG:HH22 | 9:S:754:ARG:C | 1.58 | 1.10 |
| 4:J:727:SER:O | 7:O:746:LYS:CG | 2.00 | 1.10 |
| 7:O:724:ASN:H | 7:O:1272:LEU:HD11 | 1.14 | 1.10 |
| 1:0:130:GLY:C | 1:0:511:LYS:HE3 | 1.75 | 1.10 |
| 11:X:282:ASN:CG | 11:X:299:GLN:HE21 | 1.60 | 1.10 |
| 2:Z:1253:VAL:CG1 | 2:Z:1300:SER:CB | 2.30 | 1.10 |
| 10:U:304:LYS:HE2 | 11:V:271:ILE:HD11 | 1.12 | 1.09 |
| 19:m:8:GLN:HG3 | 19:m:11:ARG:HH21 | 0.99 | 1.09 |
| 5:E:377:ASN:HB3 | 7:M:1041:PHE:CZ | 1.87 | 1.09 |
| 5:E:377:ASN:CB | 7:M:1041:PHE:HZ | 1.65 | 1.09 |
| 8:N:1384:ASP:OD1 | 8:N:1442:ILE:CD1 | 1.99 | 1.09 |
| 8:P:379:ILE:HG21 | 8:P:403:ILE:CG1 | 1.82 | 1.09 |
| 1:0:401:ILE:HG13 | 1:0:462:LEU:HB2 | 1.14 | 1.09 |
| 8:P:275:LEU:HD12 | 8:P:382:PHE:HE1 | 1.13 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:P:736:ILE:HD11 | 8:P:794:ILE:HG21 | 1.33 | 1.08 |
| 9:R:746:PRO:CG | 9:R:753:ALA:CA | 2.29 | 1.08 |
| 5:E:324:TYR:OH | 5:E:328:GLY:HA3 | 1.49 | 1.08 |
| 5:H:316:VAL:HG11 | 5:H:348:ILE:HD12 | 1.25 | 1.08 |
| 1:Y:412:ILE:CG2 | 1:Y:444:VAL:CB | 2.32 | 1.08 |
| 1:0:398:ILE:CG2 | 1:0:446:LEU:HD22 | 1.82 | 1.08 |
| 1:Y:412:ILE:HG21 | 1:Y:444:VAL:CB | 1.84 | 1.07 |
| 1:0:410:ALA:CB | 1:0:511:LYS:O | 2.02 | 1.07 |
| 5:H:316:VAL:HG21 | 5:H:348:ILE:HG13 | 1.36 | 1.07 |
| 19:m:8:GLN:HG3 | 19:m:11:ARG:NH2 | 1.67 | 1.07 |
| 8:P:275:LEU:CD1 | 8:P:382:PHE:CE1 | 2.37 | 1.07 |
| 14:a:715:THR:HG22 | 14:a:716:GLU:H | 0.90 | 1.07 |
| 8:N:70:LYS:HG3 | 8:N:72:ARG:NH2 | 1.70 | 1.07 |
| 4:y:605:THR:CB | 4:z:605:THR:HA | 1.85 | 1.06 |
| 5:E:326:LYS:HG2 | 5:E:327:PRO:HD2 | 1.33 | 1.06 |
| 8:N:379:ILE:CD1 | 8:N:403:ILE:HD13 | 1.85 | 1.06 |
| 1:0:129:SER:OG | 1:0:405:THR:CA | 2.02 | 1.06 |
| 5:H:316:VAL:CG2 | 5:H:348:ILE:HG13 | 1.85 | 1.06 |
| 1:0:1277:SER:CB | 9:R:754:ARG:HG3 | 1.83 | 1.05 |
| 8:P:75:ILE:HD11 | 8:P:82:ASN:O | 1.49 | 1.05 |
| 8:P:380:THR:OG1 | 8:P:400:PHE:CB | 2.03 | 1.05 |
| 5:H:316:VAL:CG2 | 5:H:348:ILE:CB | 2.34 | 1.05 |
| 4:z:688:HIS:CB | 21:p:37:LEU:HD21 | 1.86 | 1.05 |
| 5:H:316:VAL:CG2 | 5:H:348:ILE:HB | 1.86 | 1.05 |
| 1:0:131:VAL:HG13 | 1:0:511:LYS:HD3 | 1.07 | 1.05 |
| 8:P:400:PHE:HD2 | 8:P:596:LYS:CE | 1.69 | 1.05 |
| 8:P:778:VAL:CG2 | 8:P:795:ILE:HG13 | 1.87 | 1.05 |
| 1:0:417:TYR:OH | 1:0:517:LEU:HD23 | 1.54 | 1.04 |
| 5:E:381:GLU:HB3 | 7:M:1037:ASN:HB3 | 1.10 | 1.04 |
| 8:N:379:ILE:CG1 | 8:N:403:ILE:CD1 | 2.36 | 1.04 |
| 8:N:379:ILE:HG13 | 8:N:403:ILE:CB | 1.85 | 1.04 |
| 7:O:973:ASP:OD2 | 7:O:1039:ALA:HB2 | 1.54 | 1.04 |
| 2:1:1015:VAL:O | 2:1:1040:LYS:CD | 2.03 | 1.04 |
| 5:E:324:TYR:OH | 5:E:328:GLY:CA | 2.05 | 1.04 |
| 8:P:379:ILE:HG21 | 8:P:403:ILE:HG13 | 1.38 | 1.04 |
| 8:N:379:ILE:CD1 | 8:N:403:ILE:CD1 | 2.35 | 1.04 |
| 2:Z:1253:VAL:HG13 | 2:Z:1300:SER:CB | 1.86 | 1.04 |
| 1:0:398:ILE:O | 1:0:462:LEU:HD21 | 1.58 | 1.03 |
| 1:0:1277:SER:HB2 | 9:R:754:ARG:HG2 | 1.33 | 1.03 |
| 8:N:379:ILE:HG12 | 8:N:403:ILE:CG2 | 1.88 | 1.03 |
| 1:0:410:ALA:HA | 1:0:512:LYS:HA | 1.40 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:N:379:ILE:HG13 | 8:N:403:ILE:HG21 | 1.36 | 1.03 |
| 19:f:27:ASN:N | 19:f:394:ILE:HG21 | 1.72 | 1.03 |
| 1:Y:403:GLY:HA3 | 1:Y:408:ARG:HE | 1.09 | 1.03 |
| 7:O:1321:PRO:HG2 | 7:O:1324:ARG:HB2 | 1.41 | 1.02 |
| 1:Y:412:ILE:CG2 | 1:Y:444:VAL:CG1 | 2.36 | 1.02 |
| 5:E:467:LYS:HG3 | 7:M:1224:GLU:HB3 | 1.42 | 1.02 |
| 7:O:1174:LYS:HB3 | 7:O:1319:LEU:CD2 | 1.89 | 1.02 |
| 8:P:778:VAL:HG23 | 8:P:793:LEU:HD23 | 1.39 | 1.02 |
| 1:0:398:ILE:HG21 | 1:0:446:LEU:CD2 | 1.89 | 1.02 |
| 7:O:1321:PRO:HG2 | 7:O:1324:ARG:CB | 1.88 | 1.02 |
| 2:1:1175:ASN:ND2 | 9:S:754:ARG:HB2 | 1.72 | 1.02 |
| 19:m:453:GLU:HA | 19:m:483:VAL:HG21 | 1.40 | 1.02 |
| 4:J:727:SER:HB2 | 7:O:746:LYS:NZ | 1.74 | 1.01 |
| 7:O:1181:VAL:HG13 | 7:O:1318:LYS:HE2 | 1.40 | 1.01 |
| 2:1:1178:ARG:NH2 | 9:S:754:ARG:O | 1.92 | 1.01 |
| 5:H:316:VAL:CG2 | 5:H:348:ILE:CG1 | 2.38 | 1.01 |
| 8:N:1384:ASP:CG | 8:N:1442:ILE:HD11 | 1.85 | 1.01 |
| 1:0:417:TYR:HB3 | 1:0:442:GLY:CA | 1.91 | 1.01 |
| 8:P:75:ILE:HD12 | 8:P:82:ASN:O | 1.59 | 1.01 |
| 1:0:407:ALA:CB | 1:0:467:PHE:CZ | 2.43 | 1.01 |
| 2:1:123:TYR:CZ | 2:1:456:THR:HG21 | 1.96 | 1.00 |
| 8:P:1227:VAL:CG1 | 8:P:1277:ILE:CD1 | 2.38 | 1.00 |
| 9:S:268:ILE:CD1 | 9:S:514:LYS:CD | 2.36 | 1.00 |
| 8:P:1227:VAL:HG13 | 8:P:1277:ILE:HD12 | 1.38 | 1.00 |
| 4:z:607:LYS:O | 4:z:612:VAL:CB | 2.10 | 1.00 |
| 19:m:483:VAL:CG2 | 19:m:647:ALA:HB2 | 1.90 | 1.00 |
| 8:N:379:ILE:HG13 | 8:N:403:ILE:CG2 | 1.86 | 1.00 |
| 1:0:398:ILE:HG12 | 1:0:446:LEU:HD13 | 1.43 | 1.00 |
| 2:1:457:SER:C | 2:1:560:LEU:HD21 | 1.86 | 1.00 |
| 1:0:401:ILE:HG13 | 1:0:462:LEU:CG | 1.90 | 1.00 |
| 5:E:317:ASN:O | 5:E:348:ILE:CD1 | 2.10 | 1.00 |
| 8:P:359:LEU:HG | 8:P:399:VAL:HG13 | 1.42 | 1.00 |
| 7:O:1174:LYS:HB2 | 7:O:1319:LEU:HD23 | 1.03 | 1.00 |
| 8:N:379:ILE:HG12 | 8:N:403:ILE:HG21 | 1.03 | 0.99 |
| 19:m:454:ASP:N | 19:m:483:VAL:HG11 | 1.76 | 0.99 |
| 5:H:316:VAL:HG23 | 5:H:348:ILE:N | 1.76 | 0.99 |
| 8:P:359:LEU:HG | 8:P:399:VAL:CG1 | 1.92 | 0.99 |
| 1:Y:126:TYR:HE1 | 1:Y:405:THR:CB | 1.74 | 0.99 |
| 8:P:777:ASP:O | 8:P:793:LEU:CG | 2.11 | 0.99 |
| 9:R:746:PRO:HG3 | 9:R:753:ALA:HA | 0.99 | 0.99 |
| 1:0:413:LEU:CD2 | 1:0:467:PHE:CG | 2.39 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:1253:VAL:CG1 | 2:Z:1300:SER:HB3 | 1.93 | 0.98 |
| 19:f:27:ASN:CB | 19:f:435:PHE:CD2 | 2.46 | 0.98 |
| 2:1:1015:VAL:O | 2:1:1040:LYS:HG3 | 1.62 | 0.98 |
| 8:P:52:ILE:C | 8:P:133:ASP:OD2 | 2.05 | 0.98 |
| 4:J:727:SER:C | 7:O:746:LYS:NZ | 2.19 | 0.98 |
| 1:0:401:ILE:CB | 1:0:462:LEU:CD2 | 2.06 | 0.98 |
| 7:O:724:ASN:N | 7:O:1272:LEU:HD11 | 1.77 | 0.98 |
| 1:0:409:ALA:O | 1:0:512:LYS:CG | 2.12 | 0.98 |
| 1:0:413:LEU:HD13 | 1:0:444:VAL:CG2 | 1.94 | 0.98 |
| 10:U:304:LYS:HD3 | 11:V:271:ILE:HD12 | 1.43 | 0.98 |
| 5:E:326:LYS:CD | 5:E:335:TRP:CE3 | 2.46 | 0.97 |
| 14:a:715:THR:CG2 | 14:a:716:GLU:H | 1.75 | 0.97 |
| 2:1:1016:ASP:HA | 2:1:1040:LYS:CG | 1.93 | 0.97 |
| 7:M:1025:GLY:O | 7:M:1040:THR:HG21 | 1.64 | 0.97 |
| 1:0:131:VAL:CG1 | 1:0:511:LYS:CE | 2.41 | 0.97 |
| 8:P:719:ILE:HD11 | 8:P:793:LEU:O | 1.64 | 0.97 |
| 1:Y:403:GLY:CA | 1:Y:408:ARG:NE | 2.26 | 0.97 |
| 14:a:715:THR:HG22 | 14:a:716:GLU:N | 1.68 | 0.97 |
| 1:0:1277:SER:CB | 9:R:754:ARG:HB3 | 1.93 | 0.96 |
| 8:P:275:LEU:HD13 | 8:P:382:PHE:CE1 | 1.96 | 0.96 |
| 19:m:483:VAL:CG2 | 19:m:647:ALA:CB | 2.43 | 0.96 |
| 11:X:297:ASP:OD1 | 11:X:302:ARG:C | 2.07 | 0.96 |
| 5:H:321:ALA:CB | 5:H:347:THR:O | 2.13 | 0.96 |
| 7:O:1174:LYS:O | 7:O:1319:LEU:CB | 2.14 | 0.96 |
| 1:0:1276:LEU:HB2 | 9:R:754:ARG:HH21 | 1.31 | 0.96 |
| 1:0:129:SER:OG | 1:0:405:THR:C | 2.09 | 0.96 |
| 1:0:129:SER:OG | 1:0:406:THR:N | 1.99 | 0.96 |
| 1:0:401:ILE:HG13 | 1:0:462:LEU:HB3 | 1.01 | 0.95 |
| 8:P:400:PHE:CD2 | 8:P:596:LYS:CE | 2.47 | 0.95 |
| 1:0:131:VAL:CG1 | 1:0:511:LYS:HD3 | 1.97 | 0.95 |
| 5:E:381:GLU:HB3 | 7:M:1037:ASN:CB | 1.95 | 0.95 |
| 5:H:316:VAL:HG23 | 5:H:348:ILE:H | 1.28 | 0.95 |
| 1:0:467:PHE:CB | 1:0:511:LYS:HD2 | 1.96 | 0.95 |
| 2:1:1015:VAL:O | 2:1:1040:LYS:CG | 2.15 | 0.95 |
| 1:Y:126:TYR:HE1 | 1:Y:405:THR:HB | 1.21 | 0.95 |
| 2:Z:1253:VAL:HG13 | 2:Z:1300:SER:HB3 | 1.46 | 0.95 |
| 1:0:131:VAL:CG1 | 1:0:511:LYS:HE2 | 1.96 | 0.95 |
| 8:P:778:VAL:HG23 | 8:P:795:ILE:HG13 | 1.44 | 0.95 |
| 1:0:413:LEU:CD1 | 1:0:467:PHE:CE1 | 2.43 | 0.95 |
| 5:E:467:LYS:HD2 | 7:M:1224:GLU:OE1 | 1.66 | 0.95 |
| 1:0:131:VAL:HA | 1:0:511:LYS:HE2 | 1.46 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0:467:PHE:CD2 | 1:0:511:LYS:HD2 | 2.01 | 0.94 |
| 1:Y:412:ILE:CG2 | 1:Y:444:VAL:HG11 | 1.94 | 0.94 |
| 1:0:129:SER:HB3 | 1:0:406:THR:H | 1.31 | 0.94 |
| 1:0:398:ILE:HA | 1:0:462:LEU:CD2 | 1.98 | 0.94 |
| 5:E:326:LYS:HD2 | 5:E:335:TRP:CZ3 | 2.03 | 0.94 |
| 8:N:379:ILE:HD11 | 8:N:403:ILE:HD13 | 1.46 | 0.94 |
| 19:m:483:VAL:HG23 | 19:m:647:ALA:HB1 | 1.47 | 0.94 |
| 1:0:412:ILE:HG22 | 1:0:442:GLY:O | 1.68 | 0.94 |
| 1:0:375:SER:HB3 | 1:0:420:ILE:HD12 | 1.50 | 0.94 |
| 1:0:1277:SER:HB3 | 9:R:754:ARG:HG3 | 1.47 | 0.94 |
| 9:S:268:ILE:HD11 | 9:S:514:LYS:HD2 | 0.94 | 0.94 |
| 1:Y:412:ILE:CG2 | 1:Y:444:VAL:HG22 | 1.96 | 0.94 |
| 4:y:595:ASP:CB | 4:z:598:LYS:CB | 2.45 | 0.94 |
| 19:f:28:ASN:HD22 | 19:f:438:GLU:HG2 | 1.32 | 0.94 |
| 1:0:1277:SER:CB | 9:R:754:ARG:CB | 2.46 | 0.93 |
| 8:N:1305:ASN:CG | 8:N:1308:TYR:HB2 | 1.92 | 0.93 |
| 20:n:774:PHE:CE1 | 20:n:777:ILE:CG2 | 2.46 | 0.93 |
| 2:1:127:ASP:OD1 | 2:1:457:SER:HB3 | 1.65 | 0.93 |
| 13:x:1296:THR:H | 21:p:47:LYS:NZ | 1.54 | 0.93 |
| 1:0:1276:LEU:CB | 9:R:754:ARG:NE | 2.27 | 0.93 |
| 1:Y:403:GLY:CA | 1:Y:408:ARG:HE | 1.82 | 0.93 |
| 2:1:1178:ARG:NH2 | 9:S:754:ARG:C | 2.26 | 0.92 |
| 1:Y:397:TYR:OH | 1:Y:461:ARG:CA | 2.16 | 0.92 |
| 4:J:727:SER:HB2 | 7:O:746:LYS:HZ1 | 1.31 | 0.92 |
| 13:x:1296:THR:H | 21:p:47:LYS:HZ3 | 0.95 | 0.92 |
| 7:O:1174:LYS:HB3 | 7:O:1319:LEU:HD23 | 1.46 | 0.92 |
| 1:Y:403:GLY:HA2 | 1:Y:408:ARG:HG3 | 1.49 | 0.92 |
| 4:y:605:THR:CB | 4:z:605:THR:CA | 2.48 | 0.92 |
| 2:1:1016:ASP:CA | 2:1:1040:LYS:CD | 1.97 | 0.91 |
| 5:E:326:LYS:HD2 | 5:E:335:TRP:HE3 | 1.10 | 0.91 |
| 1:0:408:ARG:O | 1:0:512:LYS:HE2 | 1.71 | 0.91 |
| 9:S:514:LYS:CE | 9:S:514:LYS:HA | 2.00 | 0.91 |
| 13:x:1292:LYS:O | 21:p:47:LYS:NZ | 2.03 | 0.91 |
| 5:E:377:ASN:HB3 | 7:M:1041:PHE:HZ | 1.19 | 0.91 |
| 8:P:275:LEU:HD12 | 8:P:382:PHE:CE1 | 2.03 | 0.91 |
| 1:Y:412:ILE:HG22 | 1:Y:444:VAL:HG21 | 1.51 | 0.91 |
| 9:S:584:LYS:H | 11:X:302:ARG:HD2 | 1.33 | 0.91 |
| 1:0:131:VAL:HG12 | 1:0:511:LYS:HE2 | 1.49 | 0.91 |
| 13:x:1296:THR:N | 21:p:47:LYS:HZ3 | 1.34 | 0.91 |
| 1:0:1276:LEU:HB2 | 9:R:754:ARG:NH2 | 1.86 | 0.91 |
| 8:N:1303:LEU:HB3 | 8:N:1384:ASP:HB2 | 1.51 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1:1175:ASN:ND2 | 9:S:754:ARG:HB3 | 1.84 | 0.90 |
| 1:Y:126:TYR:HE1 | 1:Y:405:THR:CG2 | 1.84 | 0.90 |
| 8:P:1304:LYS:HA | 8:P:1304:LYS:CE | 1.99 | 0.90 |
| 19:m:452:LEU:O | 19:m:483:VAL:CG2 | 2.19 | 0.90 |
| 8:P:400:PHE:HD2 | 8:P:596:LYS:HE2 | 1.36 | 0.90 |
| 1:0:401:ILE:CD1 | 1:0:462:LEU:HB3 | 2.02 | 0.90 |
| 8:P:380:THR:HG1 | 8:P:400:PHE:HB2 | 1.32 | 0.90 |
| 2:Z:891:ARG:HG2 | 2:Z:891:ARG:HH11 | 1.36 | 0.90 |
| 19:m:28:ASN:HD22 | 19:m:438:GLU:HG2 | 1.37 | 0.90 |
| 19:f:29:GLU:HB2 | 19:f:33:ILE:HG21 | 1.53 | 0.90 |
| 9:S:584:LYS:HB2 | 11:X:302:ARG:HE | 1.37 | 0.89 |
| 1:0:1277:SER:HB3 | 9:R:754:ARG:CG | 2.00 | 0.89 |
| 1:0:1277:SER:HB3 | 9:R:754:ARG:HB3 | 1.55 | 0.89 |
| 2:1:1016:ASP:OD1 | 2:1:1040:LYS:HG2 | 1.73 | 0.89 |
| 1:0:129:SER:HA | 1:0:405:THR:C | 1.95 | 0.89 |
| 1:0:129:SER:HB3 | 1:0:406:THR:OG1 | 1.71 | 0.89 |
| 8:N:33:ASP:HB2 | 8:N:946:TRP:HB3 | 1.54 | 0.89 |
| 10:U:304:LYS:HD3 | 11:V:271:ILE:CG1 | 2.03 | 0.88 |
| 8:P:75:ILE:CG1 | 8:P:83:VAL:HA | 2.04 | 0.88 |
| 10:U:304:LYS:CE | 11:V:271:ILE:CD1 | 2.34 | 0.88 |
| 19:m:480:THR:CG2 | 20:n:979:SER:CB | 2.51 | 0.88 |
| 1:0:417:TYR:OH | 1:0:517:LEU:CD2 | 2.22 | 0.88 |
| 7:M:1234:GLY:HA2 | 7:M:1294:LYS:HD3 | 1.57 | 0.87 |
| 5:E:377:ASN:CB | 7:M:1041:PHE:CZ | 2.51 | 0.87 |
| 1:0:467:PHE:HB2 | 1:0:511:LYS:CD | 2.05 | 0.87 |
| 8:N:379:ILE:CG1 | 8:N:403:ILE:HD12 | 2.02 | 0.87 |
| 8:P:777:ASP:HB2 | 8:P:793:LEU:N | 1.89 | 0.86 |
| 1:Y:412:ILE:HG22 | 1:Y:444:VAL:HG11 | 1.55 | 0.86 |
| 9:S:584:LYS:H | 11:X:302:ARG:CD | 1.88 | 0.86 |
| 2:Z:745:ILE:O | 2:Z:815:PHE:CE1 | 2.28 | 0.86 |
| 8:N:379:ILE:HG13 | 8:N:403:ILE:HD12 | 1.54 | 0.86 |
| 2:1:1016:ASP:C | 2:1:1040:LYS:HD2 | 1.99 | 0.86 |
| 8:P:1053:LEU:HD23 | 8:P:1053:LEU:H | 1.41 | 0.85 |
| 4:y:595:ASP:C | 4:z:598:LYS:CB | 2.48 | 0.85 |
| 1:0:407:ALA:HB2 | 1:0:467:PHE:HZ | 1.38 | 0.85 |
| 1:0:1277:SER:HB3 | 9:R:754:ARG:CB | 2.06 | 0.85 |
| 1:0:401:ILE:HB | 1:0:462:LEU:CG | 2.06 | 0.85 |
| 9:S:268:ILE:HD13 | 9:S:514:LYS:HD2 | 1.59 | 0.85 |
| 8:N:1276:LYS:N | 8:N:1276:LYS:HD2 | 1.91 | 0.85 |
| 9:Q:232:PHE:HZ | 9:Q:513:LEU:HD22 | 1.42 | 0.85 |
| 8:P:380:THR:HB | 8:P:400:PHE:CE1 | 2.12 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:y:602:GLU:HA | 4:z:605:THR:CB | 2.07 | 0.84 |
| 19:m:483:VAL:HG22 | 19:m:647:ALA:HB2 | 1.58 | 0.84 |
| 1:0:417:TYR:HB3 | 1:0:442:GLY:H | 1.37 | 0.84 |
| 8:N:379:ILE:CG1 | 8:N:403:ILE:HD13 | 2.03 | 0.84 |
| 8:N:1057:LYS:NZ | 8:N:1057:LYS:HA | 1.92 | 0.84 |
| 19:m:483:VAL:HG23 | 19:m:647:ALA:CB | 2.06 | 0.84 |
| 1:0:412:ILE:O | 1:0:444:VAL:CG2 | 2.26 | 0.84 |
| 11:X:297:ASP:CA | 11:X:302:ARG:O | 2.25 | 0.84 |
| 5:E:326:LYS:HG2 | 5:E:327:PRO:CD | 2.06 | 0.84 |
| 7:O:1174:LYS:CA | 7:O:1319:LEU:HD23 | 2.07 | 0.84 |
| 9:R:746:PRO:HG2 | 9:R:753:ALA:HA | 1.59 | 0.84 |
| 8:P:736:ILE:HD11 | 8:P:794:ILE:CG2 | 2.06 | 0.84 |
| 1:0:467:PHE:HD2 | 1:0:511:LYS:HD2 | 1.42 | 0.83 |
| 2:Z:1254:GLY:C | 2:Z:1301:SER:CB | 2.52 | 0.83 |
| 1:0:401:ILE:CB | 1:0:462:LEU:CG | 2.56 | 0.83 |
| 4:z:688:HIS:CB | 21:p:37:LEU:CD2 | 2.56 | 0.83 |
| 7:M:1189:MET:HG2 | 8:N:166:ASN:HB3 | 1.61 | 0.83 |
| 5:E:467:LYS:CG | 7:M:1224:GLU:HB3 | 2.07 | 0.83 |
| 5:H:321:ALA:HA | 5:H:348:ILE:HG12 | 1.61 | 0.83 |
| 1:0:411:PRO:HB2 | 1:0:517:LEU:HD13 | 1.61 | 0.83 |
| 1:0:413:LEU:HD13 | 1:0:444:VAL:HG21 | 1.58 | 0.83 |
| 8:P:778:VAL:HG23 | 8:P:793:LEU:CD2 | 2.08 | 0.83 |
| 13:x:1296:THR:N | 21:p:47:LYS:HZ2 | 1.73 | 0.83 |
| 2:1:1175:ASN:HD21 | 9:S:754:ARG:CG | 1.92 | 0.83 |
| 8:N:322:HIS:ND1 | 8:N:359:LEU:HB3 | 1.93 | 0.82 |
| 1:Y:402:ILE:HD13 | 1:Y:413:LEU:HG | 1.58 | 0.82 |
| 1:Y:791:MET:HB2 | 1:Y:944:LEU:O | 1.79 | 0.82 |
| 19:m:480:THR:HG22 | 20:n:979:SER:CB | 2.09 | 0.82 |
| 1:0:412:ILE:O | 1:0:444:VAL:HG23 | 1.79 | 0.82 |
| 5:H:316:VAL:HG11 | 5:H:348:ILE:CD1 | 2.08 | 0.82 |
| 8:N:1384:ASP:CG | 8:N:1442:ILE:CD1 | 2.49 | 0.82 |
| 1:Y:412:ILE:HG21 | 1:Y:444:VAL:HG22 | 1.60 | 0.82 |
| 19:m:480:THR:HG21 | 20:n:979:SER:OG | 1.78 | 0.82 |
| 5:E:378:HIS:O | 5:E:381:GLU:CG | 2.27 | 0.82 |
| 8:N:379:ILE:HG13 | 8:N:403:ILE:CG1 | 2.09 | 0.82 |
| 1:0:467:PHE:HD2 | 1:0:511:LYS:CD | 1.92 | 0.82 |
| 8:N:322:HIS:HE1 | 8:N:359:LEU:HB3 | 1.01 | 0.82 |
| 1:0:398:ILE:C | 1:0:462:LEU:HD21 | 2.05 | 0.82 |
| 7:O:1174:LYS:CB | 7:O:1319:LEU:HD22 | 2.06 | 0.82 |
| 11:X:282:ASN:CG | 11:X:299:GLN:NE2 | 2.35 | 0.82 |
| 2:Z:1015:VAL:CG1 | 2:Z:1039:LEU:HD13 | 2.10 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:377:ASN:ND2 | 7:M:1041:PHE:CZ | 2.49 | 0.81 |
| 14:a:659:TYR:HE1 | 14:a:717:ASN:HD22 | 1.28 | 0.81 |
| 1:0:409:ALA:O | 1:0:512:LYS:CB | 2.27 | 0.81 |
| 2:1:123:TYR:OH | 2:1:456:THR:HG21 | 1.80 | 0.81 |
| 19:m:452:LEU:O | 19:m:483:VAL:HG21 | 1.80 | 0.81 |
| 3:6:36:UNK:CB | 7:M:1038:LEU:CD2 | 2.54 | 0.81 |
| 8:N:1056:LYS:H | 8:N:1056:LYS:HD2 | 1.46 | 0.81 |
| 1:0:375:SER:HB3 | 1:0:420:ILE:CD1 | 2.09 | 0.81 |
| 8:N:379:ILE:CD1 | 8:N:403:ILE:HD12 | 2.09 | 0.81 |
| 19:f:27:ASN:HB2 | 19:f:435:PHE:CE2 | 2.16 | 0.80 |
| 1:0:401:ILE:CG1 | 1:0:462:LEU:CG | 2.55 | 0.80 |
| 7:O:724:ASN:H | 7:O:1272:LEU:CD1 | 1.91 | 0.80 |
| 1:Y:397:TYR:OH | 1:Y:461:ARG:CB | 2.29 | 0.80 |
| 1:Y:397:TYR:CZ | 1:Y:461:ARG:HA | 2.16 | 0.80 |
| 8:N:379:ILE:HG13 | 8:N:403:ILE:HD13 | 1.63 | 0.80 |
| 7:O:979:LYS:HE2 | 7:O:1040:THR:OG1 | 1.81 | 0.80 |
| 1:0:413:LEU:HD13 | 1:0:444:VAL:HG22 | 1.61 | 0.80 |
| 16:c:783:ARG:O | 14:a:976:ALA:HB2 | 1.82 | 0.80 |
| 4:y:591:GLY:HA2 | 4:z:595:ASP:CB | 2.11 | 0.80 |
| 7:M:1025:GLY:O | 7:M:1040:THR:CG2 | 2.30 | 0.80 |
| 7:O:1253:ARG:HH21 | 7:O:1273:LYS:HG2 | 1.47 | 0.80 |
| 8:P:174:VAL:HG13 | 8:P:177:VAL:HB | 1.63 | 0.80 |
| 1:0:413:LEU:HD11 | 1:0:467:PHE:CE1 | 2.08 | 0.80 |
| 2:1:888:LEU:O | 2:1:888:LEU:HD23 | 1.80 | 0.79 |
| 8:P:53:GLU:CA | 8:P:133:ASP:OD2 | 2.30 | 0.79 |
| 8:P:380:THR:CB | 8:P:400:PHE:CG | 2.66 | 0.79 |
| 8:N:70:LYS:HG3 | 8:N:72:ARG:HH21 | 1.46 | 0.79 |
| 10:U:304:LYS:NZ | 11:V:360:TYR:HD2 | 1.79 | 0.79 |
| 1:Y:790:PHE:CE2 | 1:Y:909:PHE:HB3 | 2.17 | 0.79 |
| 4:z:604:SER:C | 4:z:610:ALA:N | 2.41 | 0.79 |
| 4:y:601:GLU:O | 4:z:605:THR:CB | 2.31 | 0.79 |
| 1:0:413:LEU:CD1 | 1:0:444:VAL:CG2 | 2.61 | 0.78 |
| 8:P:75:ILE:HD13 | 8:P:85:ASN:O | 1.82 | 0.78 |
| 2:1:123:TYR:CE1 | 2:1:456:THR:HG21 | 2.18 | 0.78 |
| 5:E:326:LYS:CD | 5:E:335:TRP:CZ3 | 2.67 | 0.78 |
| 7:O:724:ASN:N | 7:O:1272:LEU:CD1 | 2.46 | 0.78 |
| 8:P:174:VAL:HG12 | 8:P:178:GLN:H | 1.46 | 0.78 |
| 7:O:1321:PRO:HG2 | 7:O:1324:ARG:HB3 | 1.65 | 0.78 |
| 5:H:316:VAL:CG2 | 5:H:348:ILE:H | 1.97 | 0.78 |
| 1:0:398:ILE:HA | 1:0:462:LEU:HD21 | 1.66 | 0.77 |
| 8:P:1227:VAL:HG11 | 8:P:1277:ILE:CG2 | 2.14 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:1254:GLY:C | 2:Z:1301:SER:HB2 | 2.09 | 0.77 |
| 8:N:69:ASN:CA | 8:N:72:ARG:HE | 1.92 | 0.77 |
| 5:K:323:LEU:HD12 | 5:K:350:ILE:HD12 | 1.66 | 0.77 |
| 8:N:12:GLN:OE1 | 8:N:75:ILE:HD11 | 1.83 | 0.77 |
| 8:P:75:ILE:HG13 | 8:P:83:VAL:HA | 1.64 | 0.77 |
| 1:Y:789:VAL:HG21 | 1:Y:952:LEU:HD13 | 1.66 | 0.77 |
| 4:y:591:GLY:CA | 4:z:595:ASP:CB | 2.63 | 0.77 |
| 1:0:413:LEU:HG | 1:0:467:PHE:HE1 | 1.44 | 0.77 |
| 5:H:321:ALA:C | 5:H:323:LEU:H | 1.92 | 0.77 |
| 7:O:973:ASP:OD2 | 7:O:1039:ALA:CB | 2.31 | 0.77 |
| 1:0:401:ILE:HG12 | 1:0:462:LEU:CD2 | 2.13 | 0.77 |
| 7:M:1037:ASN:O | 7:M:1037:ASN:ND2 | 2.16 | 0.77 |
| 2:Z:1015:VAL:HG11 | 2:Z:1039:LEU:HD13 | 1.67 | 0.77 |
| 1:0:129:SER:HB3 | 1:0:406:THR:N | 1.93 | 0.77 |
| 9:S:514:LYS:HA | 9:S:514:LYS:HE3 | 1.65 | 0.77 |
| 14:a:659:TYR:HE1 | 14:a:717:ASN:ND2 | 1.83 | 0.76 |
| 1:0:413:LEU:CD1 | 1:0:444:VAL:HG21 | 2.15 | 0.76 |
| 8:P:477:LEU:HA | 8:P:553:ILE:HG23 | 1.66 | 0.76 |
| 9:R:746:PRO:CG | 9:R:753:ALA:N | 2.44 | 0.76 |
| 8:P:1053:LEU:CD2 | 8:P:1127:ASN:HB3 | 2.15 | 0.76 |
| 8:P:778:VAL:HG21 | 8:P:795:ILE:HG13 | 1.66 | 0.76 |
| 1:Y:402:ILE:HD12 | 1:Y:408:ARG:HA | 1.68 | 0.76 |
| 1:0:416:LYS:H | 1:0:416:LYS:HD2 | 1.50 | 0.76 |
| 2:1:127:ASP:CG | 2:1:457:SER:CB | 2.59 | 0.76 |
| 5:H:316:VAL:CG2 | 5:H:348:ILE:N | 2.48 | 0.76 |
| 8:P:160:LEU:HA | 8:P:165:ASN:ND2 | 2.00 | 0.76 |
| 1:0:401:ILE:HB | 1:0:462:LEU:HD23 | 0.77 | 0.76 |
| 8:N:354:GLU:HA | 8:N:359:LEU:HD11 | 1.67 | 0.76 |
| 2:Z:1015:VAL:HG11 | 2:Z:1039:LEU:CD1 | 2.16 | 0.76 |
| 2:1:1015:VAL:C | 2:1:1040:LYS:HD3 | 2.10 | 0.75 |
| 8:N:1384:ASP:CG | 8:N:1385:LEU:H | 1.93 | 0.75 |
| 7:O:1253:ARG:HH21 | 7:O:1273:LYS:CG | 1.98 | 0.75 |
| 19:f:27:ASN:HB2 | 19:f:435:PHE:HD2 | 1.42 | 0.75 |
| 2:1:860:LYS:HE3 | 2:1:891:ARG:HG3 | 1.68 | 0.75 |
| 7:O:1174:LYS:C | 7:O:1319:LEU:HD23 | 2.11 | 0.75 |
| 2:Z:1258:GLN:CD | 2:Z:1302:ALA:HB2 | 2.11 | 0.75 |
| 19:m:453:GLU:CA | 19:m:483:VAL:HG21 | 2.17 | 0.75 |
| 1:0:131:VAL:HG13 | 1:0:511:LYS:CE | 2.09 | 0.75 |
| 1:0:398:ILE:HG23 | 1:0:462:LEU:HD11 | 1.69 | 0.75 |
| 8:P:380:THR:HG21 | 8:P:400:PHE:CD2 | 2.21 | 0.75 |
| 8:P:1227:VAL:HG11 | 8:P:1277:ILE:HD13 | 1.65 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:N:18:VAL:HG22 | 8:N:34:ALA:HB1 | 1.67 | 0.75 |
| 8:N:1305:ASN:CB | 8:N:1308:TYR:HB2 | 2.15 | 0.75 |
| 7:O:1181:VAL:HG13 | 7:O:1318:LYS:CE | 2.15 | 0.75 |
| 7:O:1272:LEU:HD23 | 7:O:1272:LEU:N | 2.01 | 0.75 |
| 1:Y:130:GLY:HA2 | 1:Y:406:THR:CG2 | 2.17 | 0.75 |
| 3:6:36:UNK:CA | 7:M:1038:LEU:HD21 | 2.17 | 0.75 |
| 15:b:720:LEU:H | 15:b:720:LEU:HD12 | 1.52 | 0.75 |
| 19:m:8:GLN:CG | 19:m:11:ARG:HH21 | 1.90 | 0.74 |
| 7:M:1189:MET:CG | 8:N:166:ASN:HB3 | 2.17 | 0.74 |
| 1:0:401:ILE:CB | 1:0:462:LEU:HB3 | 2.16 | 0.74 |
| 8:P:22:MET:HE1 | 8:P:40:ILE:HG23 | 1.68 | 0.74 |
| 8:P:379:ILE:CG2 | 8:P:403:ILE:HG13 | 2.15 | 0.74 |
| 16:c:783:ARG:HH22 | 14:a:1017:TRP:HA | 1.52 | 0.74 |
| 1:0:413:LEU:HD21 | 1:0:467:PHE:CD2 | 2.21 | 0.74 |
| 19:m:452:LEU:O | 19:m:483:VAL:HG23 | 1.86 | 0.74 |
| 10:U:304:LYS:HZ1 | 11:V:360:TYR:HD2 | 1.28 | 0.74 |
| 19:f:364:GLU:OE1 | 19:f:375:ALA:HB1 | 1.88 | 0.74 |
| 5:H:318:GLU:HG2 | 5:H:346:GLN:HE21 | 1.52 | 0.73 |
| 19:f:374:GLU:OE2 | 19:f:414:THR:HG22 | 1.87 | 0.73 |
| 7:M:1234:GLY:HA2 | 7:M:1294:LYS:CD | 2.18 | 0.73 |
| 3:6:36:UNK:CB | 7:M:1038:LEU:HD11 | 2.19 | 0.73 |
| 1:0:411:PRO:HB2 | 1:0:517:LEU:CD1 | 2.18 | 0.73 |
| 4:J:727:SER:CB | 7:O:746:LYS:HZ3 | 2.01 | 0.73 |
| 9:S:747:PHE:HZ | 9:S:753:ALA:N | 1.86 | 0.73 |
| 1:0:398:ILE:CA | 1:0:462:LEU:HD21 | 2.19 | 0.73 |
| 8:N:379:ILE:HD12 | 8:N:403:ILE:CD1 | 2.19 | 0.73 |
| 8:P:719:ILE:HG13 | 8:P:794:ILE:HB | 1.67 | 0.73 |
| 9:T:263:MET:HE1 | 9:T:269:ASN:H | 1.53 | 0.73 |
| 1:0:401:ILE:CA | 1:0:462:LEU:HD23 | 2.13 | 0.73 |
| 1:0:1277:SER:HB2 | 9:R:754:ARG:CB | 2.15 | 0.73 |
| 9:R:617:LYS:H | 9:R:617:LYS:HD3 | 1.54 | 0.73 |
| 9:S:547:TYR:CD2 | 11:X:300:VAL:HA | 2.23 | 0.73 |
| 1:0:408:ARG:HH21 | 1:0:508:LYS:HE3 | 1.53 | 0.72 |
| 8:P:380:THR:HG21 | 8:P:400:PHE:CG | 2.23 | 0.72 |
| 1:0:408:ARG:NH2 | 1:0:508:LYS:HE3 | 2.04 | 0.72 |
| 9:T:432:ILE:HG22 | 9:T:473:ARG:HH21 | 1.55 | 0.72 |
| 1:0:401:ILE:HG13 | 1:0:462:LEU:CD2 | 2.02 | 0.72 |
| 2:1:1015:VAL:C | 2:1:1040:LYS:CD | 2.63 | 0.72 |
| 8:P:380:THR:OG1 | 8:P:400:PHE:CG | 2.42 | 0.72 |
| 8:P:778:VAL:HG21 | 8:P:795:ILE:CG1 | 2.19 | 0.72 |
| 1:Y:790:PHE:CZ | 1:Y:909:PHE:HB3 | 2.23 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 20:g:774:PHE:O | 20:g:778:ASN:ND2 | 2.22 | 0.72 |
| 4:y:591:GLY:O | 4:z:595:ASP:CB | 2.37 | 0.72 |
| 4:J:727:SER:C | 7:O:746:LYS:HG2 | 2.15 | 0.72 |
| 8:P:75:ILE:HG13 | 8:P:83:VAL:HG12 | 1.71 | 0.72 |
| 2:1:1016:ASP:CA | 2:1:1040:LYS:HD3 | 2.18 | 0.72 |
| 8:P:400:PHE:CD2 | 8:P:596:LYS:NZ | 2.58 | 0.71 |
| 1:Y:126:TYR:CE1 | 1:Y:405:THR:CG2 | 2.72 | 0.71 |
| 5:E:377:ASN:CG | 7:M:1041:PHE:CZ | 2.68 | 0.71 |
| 4:J:727:SER:HB2 | 7:O:746:LYS:HZ3 | 1.55 | 0.71 |
| 8:P:1227:VAL:CG2 | 8:P:1277:ILE:HD13 | 2.20 | 0.71 |
| 9:S:218:ILE:HD12 | 9:S:237:GLU:HB3 | 1.73 | 0.71 |
| 19:f:28:ASN:ND2 | 19:f:438:GLU:HG2 | 2.03 | 0.71 |
| 8:P:380:THR:HB | 8:P:400:PHE:HD1 | 1.51 | 0.71 |
| 1:0:407:ALA:HB2 | 1:0:467:PHE:CE2 | 2.24 | 0.71 |
| 4:y:605:THR:CB | 4:z:605:THR:O | 2.38 | 0.71 |
| 1:Y:403:GLY:HA2 | 1:Y:408:ARG:CG | 2.19 | 0.71 |
| 8:N:359:LEU:HD13 | 8:N:359:LEU:N | 2.04 | 0.70 |
| 10:U:304:LYS:HG2 | 11:V:271:ILE:HG13 | 1.73 | 0.70 |
| 1:0:417:TYR:CB | 1:0:442:GLY:CA | 2.69 | 0.70 |
| 1:0:410:ALA:HB2 | 1:0:511:LYS:O | 1.89 | 0.70 |
| 8:N:75:ILE:HG21 | 8:N:85:ASN:O | 1.91 | 0.70 |
| 7:O:1321:PRO:O | 7:O:1324:ARG:HB3 | 1.91 | 0.70 |
| 8:N:1056:LYS:HD2 | 8:N:1056:LYS:N | 2.07 | 0.70 |
| 9:Q:232:PHE:CZ | 9:Q:513:LEU:HD22 | 2.26 | 0.70 |
| 9:Q:672:GLN:HA | 9:R:373:ALA:HB2 | 1.73 | 0.70 |
| 1:0:131:VAL:CG1 | 1:0:511:LYS:CD | 2.57 | 0.70 |
| 2:1:1178:ARG:HH22 | 9:S:754:ARG:CA | 2.04 | 0.70 |
| 5:H:316:VAL:CG1 | 5:H:348:ILE:HD12 | 2.15 | 0.70 |
| 8:N:1384:ASP:OD1 | 8:N:1385:LEU:N | 2.23 | 0.70 |
| 7:O:1174:LYS:HB3 | 7:O:1319:LEU:HD22 | 1.68 | 0.70 |
| 9:S:584:LYS:HB2 | 11:X:302:ARG:NE | 2.05 | 0.70 |
| 5:K:322:ILE:HA | 5:K:335:TRP:HE1 | 1.56 | 0.70 |
| 8:P:362:LEU:HD13 | 8:P:379:ILE:HD11 | 1.73 | 0.70 |
| 8:P:1053:LEU:HD23 | 8:P:1127:ASN:HB3 | 1.74 | 0.70 |
| 1:0:395:PRO:HG3 | 1:0:419:LYS:HA | 1.74 | 0.70 |
| 8:N:379:ILE:HD12 | 8:N:403:ILE:HD12 | 1.71 | 0.70 |
| 1:Y:403:GLY:HA3 | 1:Y:408:ARG:CZ | 2.19 | 0.70 |
| 8:P:33:ASP:OD2 | 8:P:1010:GLU:HB2 | 1.91 | 0.70 |
| 4:J:727:SER:CB | 7:O:746:LYS:NZ | 2.51 | 0.70 |
| 19:m:27:ASN:HB2 | 19:m:398:ILE:HD11 | 1.74 | 0.69 |
| 12:v:396:CYS:SG | 12:v:401:ASP:HB2 | 2.32 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0:788:HIS:HB3 | 1:0:947:LEU:N | 2.07 | 0.69 |
| 1:0:1276:LEU:HB2 | 9:R:754:ARG:CZ | 2.22 | 0.69 |
| 2:1:888:LEU:HD23 | 2:1:888:LEU:C | 2.18 | 0.69 |
| 5:E:324:TYR:OH | 5:E:328:GLY:HA2 | 1.89 | 0.69 |
| 7:M:1034:LEU:C | 7:M:1034:LEU:HD23 | 2.17 | 0.69 |
| 1:0:397:TYR:O | 1:0:462:LEU:HD22 | 1.93 | 0.69 |
| 8:P:400:PHE:CD2 | 8:P:596:LYS:HE3 | 2.27 | 0.69 |
| 1:0:129:SER:CB | 1:0:405:THR:HA | 2.21 | 0.69 |
| 2:1:123:TYR:OH | 2:1:456:THR:CG2 | 2.40 | 0.69 |
| 10:W:305:TYR:H | 10:W:306:PRO:HD3 | 1.57 | 0.69 |
| 12:v:396:CYS:SG | 12:v:405:LEU:HD11 | 2.32 | 0.69 |
| 1:0:408:ARG:O | 1:0:512:LYS:CE | 2.40 | 0.69 |
| 2:Z:1015:VAL:HB | 2:Z:1039:LEU:HD13 | 1.75 | 0.69 |
| 1:0:413:LEU:HD21 | 1:0:467:PHE:CB | 2.19 | 0.69 |
| 8:P:359:LEU:HG | 8:P:399:VAL:HG11 | 1.73 | 0.69 |
| 8:P:1306:ASN:N | 8:P:1306:ASN:HD22 | 1.91 | 0.69 |
| 8:N:359:LEU:HD13 | 8:N:359:LEU:H | 1.56 | 0.69 |
| 2:Z:1258:GLN:HG2 | 2:Z:1301:SER:O | 1.91 | 0.69 |
| 8:P:327:PHE:CG | 8:P:382:PHE:HB3 | 2.27 | 0.68 |
| 8:P:778:VAL:CG2 | 8:P:793:LEU:HD23 | 2.22 | 0.68 |
| 4:y:595:ASP:O | 4:z:598:LYS:CB | 2.41 | 0.68 |
| 20:n:516:LEU:H | 20:n:516:LEU:HD12 | 1.57 | 0.68 |
| 20:n:774:PHE:CE2 | 20:n:777:ILE:CG2 | 2.76 | 0.68 |
| 1:0:413:LEU:HD12 | 1:0:444:VAL:HG11 | 1.75 | 0.68 |
| 7:O:724:ASN:CB | 7:O:1272:LEU:CD1 | 2.71 | 0.68 |
| 8:P:795:ILE:HB | 8:P:868:LEU:HB2 | 1.75 | 0.68 |
| 19:m:479:THR:OG1 | 20:n:978:GLY:O | 2.12 | 0.68 |
| 1:0:1276:LEU:HB2 | 9:R:754:ARG:NE | 2.08 | 0.68 |
| 8:P:778:VAL:CG2 | 8:P:795:ILE:CG1 | 2.69 | 0.68 |
| 20:n:700:GLU:O | 20:n:775:ILE:HG13 | 1.93 | 0.68 |
| 2:Z:1015:VAL:CB | 2:Z:1039:LEU:HD13 | 2.23 | 0.68 |
| 1:0:398:ILE:HG23 | 1:0:446:LEU:HD22 | 1.75 | 0.68 |
| 2:1:457:SER:C | 2:1:560:LEU:CD2 | 2.65 | 0.68 |
| 2:Z:891:ARG:HG2 | 2:Z:891:ARG:NH1 | 2.07 | 0.68 |
| 14:a:714:ILE:HD13 | 14:a:714:ILE:N | 2.09 | 0.68 |
| 1:Y:410:ALA:CB | 1:Y:511:LYS:O | 2.42 | 0.68 |
| 8:P:777:ASP:HB2 | 8:P:793:LEU:HB2 | 1.74 | 0.67 |
| 18:e:232:ALA:H | 18:e:312:TRP:HE1 | 1.43 | 0.67 |
| 2:1:513:LYS:HD3 | 2:1:539:TYR:HE2 | 1.58 | 0.67 |
| 5:E:467:LYS:HG3 | 7:M:1224:GLU:CB | 2.20 | 0.67 |
| 4:D:776:PHE:CD2 | 6:F:401:ILE:HG23 | 2.29 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:1257:GLY:O | 2:Z:1299:LYS:HD2 | 1.94 | 0.67 |
| 1:0:401:ILE:CG2 | 1:0:462:LEU:HB3 | 2.23 | 0.67 |
| 5:H:316:VAL:CB | 5:H:348:ILE:HG13 | 2.24 | 0.67 |
| 8:N:1058:GLU:O | 8:N:1061:THR:HG22 | 1.93 | 0.67 |
| 8:N:1303:LEU:HB3 | 8:N:1384:ASP:CB | 2.25 | 0.67 |
| 9:T:564:GLU:HA | 9:T:612:HIS:CE1 | 2.30 | 0.67 |
| 4:y:601:GLU:C | 4:z:605:THR:CB | 2.67 | 0.67 |
| 20:n:773:ASN:O | 20:n:773:ASN:ND2 | 2.27 | 0.67 |
| 14:a:266:ASP:H | 14:a:269:HIS:CE1 | 2.13 | 0.67 |
| 9:S:584:LYS:CB | 11:X:302:ARG:HE | 2.08 | 0.67 |
| 2:1:1015:VAL:C | 2:1:1040:LYS:HG3 | 2.19 | 0.67 |
| 8:P:1053:LEU:HD23 | 8:P:1053:LEU:N | 2.09 | 0.67 |
| 1:Y:398:ILE:HG23 | 1:Y:462:LEU:HD22 | 1.75 | 0.67 |
| 1:0:128:ASN:O | 1:0:405:THR:OG1 | 0.67 | 0.66 |
| 8:N:379:ILE:HG13 | 8:N:403:ILE:HB | 1.78 | 0.66 |
| 5:K:323:LEU:N | 5:K:323:LEU:HD23 | 2.11 | 0.66 |
| 8:P:445:LEU:HD23 | 8:P:446:ALA:H | 1.61 | 0.66 |
| 1:Y:412:ILE:HD13 | 1:Y:412:ILE:N | 2.10 | 0.66 |
| 1:0:717:TYR:HB2 | 1:0:885:ALA:HB3 | 1.77 | 0.66 |
| 1:Y:511:LYS:HE3 | 1:Y:512:LYS:HE3 | 1.77 | 0.66 |
| 1:0:417:TYR:CB | 1:0:442:GLY:N | 2.47 | 0.66 |
| 1:Y:412:ILE:HG22 | 1:Y:444:VAL:CB | 2.24 | 0.66 |
| 5:E:467:LYS:HD2 | 7:M:1224:GLU:CD | 2.19 | 0.66 |
| 6:I:356:GLN:HA | 6:L:292:HIS:CD2 | 2.31 | 0.66 |
| 7:O:1035:GLY:HA3 | 7:O:1041:PHE:CE1 | 2.31 | 0.66 |
| 1:0:129:SER:HB3 | 1:0:406:THR:CB | 2.25 | 0.66 |
| 9:R:266:LYS:HE2 | 9:R:266:LYS:HA | 1.77 | 0.66 |
| 8:N:354:GLU:CA | 8:N:359:LEU:HD11 | 2.26 | 0.65 |
| 1:0:398:ILE:HA | 1:0:462:LEU:HD22 | 1.76 | 0.65 |
| 1:0:413:LEU:CD2 | 1:0:467:PHE:CE1 | 2.66 | 0.65 |
| 4:J:755:LEU:HD23 | 4:J:755:LEU:H | 1.61 | 0.65 |
| 2:Z:888:LEU:C | 2:Z:888:LEU:HD23 | 2.21 | 0.65 |
| 2:1:1175:ASN:HD21 | 9:S:754:ARG:HB2 | 1.39 | 0.65 |
| 8:N:68:HIS:O | 8:N:72:ARG:NH2 | 2.30 | 0.65 |
| 2:1:1016:ASP:N | 2:1:1040:LYS:CD | 2.58 | 0.65 |
| 2:Z:745:ILE:HG22 | 2:Z:815:PHE:CD1 | 2.31 | 0.65 |
| 2:1:456:THR:O | 2:1:558:THR:HG21 | 1.96 | 0.65 |
| 10:U:304:LYS:CD | 11:V:271:ILE:CG1 | 2.67 | 0.65 |
| 1:0:413:LEU:HD11 | 1:0:467:PHE:HD1 | 0.60 | 0.65 |
| 8:P:1277:ILE:O | 8:P:1277:ILE:HG13 | 1.95 | 0.65 |
| 1:0:131:VAL:CB | 1:0:511:LYS:CE | 2.74 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:m:483:VAL:HG22 | 19:m:647:ALA:CB | 2.20 | 0.65 |
| 8:P:132:ASN:O | 8:P:135:PHE:N | 2.23 | 0.65 |
| 2:Z:344:GLN:HE22 | 2:Z:409:ILE:H | 1.42 | 0.65 |
| 2:1:513:LYS:CG | 2:1:539:TYR:OH | 2.38 | 0.65 |
| 2:1:1290:ASN:HD21 | 2:1:1328:ILE:HD12 | 1.61 | 0.64 |
| 8:P:719:ILE:HD11 | 8:P:793:LEU:C | 2.22 | 0.64 |
| 12:v:350:LEU:HD23 | 12:v:350:LEU:O | 1.97 | 0.64 |
| 19:m:480:THR:CG2 | 20:n:979:SER:HB2 | 2.26 | 0.64 |
| 8:N:1305:ASN:HB3 | 8:N:1308:TYR:HB2 | 1.77 | 0.64 |
| 8:P:1060:LEU:O | 8:P:1065:THR:HG21 | 1.97 | 0.64 |
| 8:P:1061:THR:CG2 | 8:P:1189:ASP:HB2 | 2.27 | 0.64 |
| 9:S:268:ILE:HG12 | 9:S:514:LYS:HG2 | 1.79 | 0.64 |
| 7:M:1236:ILE:HD12 | 7:M:1239:PHE:HA | 1.78 | 0.64 |
| 8:P:778:VAL:HA | 8:P:793:LEU:CD2 | 2.27 | 0.64 |
| 1:0:398:ILE:CG1 | 1:0:446:LEU:HD13 | 2.23 | 0.64 |
| 1:0:412:ILE:C | 1:0:444:VAL:CG2 | 2.70 | 0.64 |
| 1:0:398:ILE:CA | 1:0:462:LEU:CD2 | 2.72 | 0.64 |
| 1:0:467:PHE:CG | 1:0:511:LYS:HD2 | 2.32 | 0.64 |
| 8:P:795:ILE:HB | 8:P:868:LEU:CB | 2.28 | 0.64 |
| 19:m:480:THR:CG2 | 20:n:979:SER:OG | 2.46 | 0.64 |
| 8:N:1057:LYS:HD2 | 8:N:1057:LYS:N | 2.13 | 0.64 |
| 4:J:727:SER:CA | 7:O:746:LYS:HZ3 | 2.09 | 0.64 |
| 7:O:724:ASN:HB2 | 7:O:1272:LEU:HD12 | 1.80 | 0.64 |
| 12:u:396:CYS:SG | 12:u:404:PRO:HB2 | 2.38 | 0.64 |
| 1:0:131:VAL:H | 1:0:511:LYS:HE3 | 1.46 | 0.64 |
| 8:N:378:VAL:HG22 | 8:N:379:ILE:HD13 | 1.79 | 0.64 |
| 2:Z:1253:VAL:HG11 | 2:Z:1300:SER:HB3 | 1.75 | 0.64 |
| 16:c:781:TYR:HB2 | 14:a:1016:GLN:HE22 | 1.64 | 0.64 |
| 2:1:238:ASN:HD21 | 2:1:245:ASN:CG | 2.06 | 0.63 |
| 8:N:18:VAL:HG22 | 8:N:34:ALA:CB | 2.28 | 0.63 |
| 1:0:415:PRO:HD2 | 1:0:416:LYS:HZ2 | 1.63 | 0.63 |
| 8:N:354:GLU:CB | 8:N:359:LEU:HD11 | 2.28 | 0.63 |
| 9:S:747:PHE:CZ | 9:S:753:ALA:N | 2.66 | 0.63 |
| 2:Z:168:GLU:HA | 2:Z:575:ARG:HH22 | 1.63 | 0.63 |
| 19:m:458:ARG:HD2 | 19:m:478:ARG:O | 1.98 | 0.63 |
| 1:0:408:ARG:HH21 | 1:0:508:LYS:CE | 2.11 | 0.63 |
| 1:Y:403:GLY:CA | 1:Y:408:ARG:HG3 | 2.24 | 0.63 |
| 19:m:480:THR:HG22 | 20:n:979:SER:HB2 | 1.79 | 0.63 |
| 2:1:513:LYS:HG2 | 2:1:539:TYR:HH | 1.61 | 0.63 |
| 19:f:27:ASN:CB | 19:f:435:PHE:CE2 | 2.80 | 0.63 |
| 5:E:377:ASN:CG | 7:M:1041:PHE:HZ | 2.04 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:1254:GLY:CA | 2:Z:1301:SER:HB2 | 2.28 | 0.63 |
| 5:E:326:LYS:HG3 | 5:E:335:TRP:HZ3 | 1.62 | 0.63 |
| 8:N:379:ILE:CG2 | 8:N:400:PHE:CD1 | 2.82 | 0.63 |
| 8:N:380:THR:HG21 | 8:N:411:PHE:HB3 | 1.79 | 0.63 |
| 8:P:174:VAL:CG1 | 8:P:178:GLN:H | 2.12 | 0.63 |
| 8:P:719:ILE:HG13 | 8:P:794:ILE:CB | 2.29 | 0.63 |
| 1:0:411:PRO:HG3 | 1:0:514:SER:OG | 1.99 | 0.63 |
| 5:E:378:HIS:C | 5:E:381:GLU:HG2 | 2.24 | 0.62 |
| 1:0:412:ILE:O | 1:0:444:VAL:HG21 | 1.97 | 0.62 |
| 2:1:1171:ASP:HB3 | 9:S:754:ARG:HD2 | 1.81 | 0.62 |
| 8:N:1384:ASP:OD2 | 8:N:1442:ILE:CD1 | 2.46 | 0.62 |
| 8:P:777:ASP:C | 8:P:793:LEU:HG | 2.22 | 0.62 |
| 8:P:778:VAL:HG21 | 8:P:795:ILE:CD1 | 2.29 | 0.62 |
| 19:m:479:THR:HG21 | 20:n:1112:GLU:OE1 | 1.98 | 0.62 |
| 1:0:788:HIS:CD2 | 1:0:946:LYS:HG2 | 2.34 | 0.62 |
| 8:N:1354:GLU:OE1 | 8:N:1384:ASP:OD2 | 2.17 | 0.62 |
| 2:Z:745:ILE:HG22 | 2:Z:815:PHE:CE1 | 2.35 | 0.62 |
| 2:1:387:GLY:HA3 | 2:1:448:LEU:HD23 | 1.82 | 0.62 |
| 2:1:1016:ASP:C | 2:1:1040:LYS:CD | 2.67 | 0.62 |
| 8:P:778:VAL:HA | 8:P:793:LEU:HG | 1.80 | 0.62 |
| 9:R:274:GLY:HA2 | 9:R:484:LEU:HD22 | 1.80 | 0.62 |
| 2:Z:1253:VAL:HA | 2:Z:1299:LYS:O | 1.99 | 0.62 |
| 12:u:38:ILE:HG22 | 12:u:40:ASP:H | 1.64 | 0.62 |
| 14:a:715:THR:CG2 | 14:a:716:GLU:N | 2.44 | 0.62 |
| 1:0:398:ILE:O | 1:0:462:LEU:CD2 | 2.44 | 0.62 |
| 2:1:1175:ASN:HD22 | 9:S:754:ARG:HB2 | 1.61 | 0.62 |
| 8:N:1276:LYS:HA | 8:N:1276:LYS:HE3 | 1.79 | 0.62 |
| 4:G:791:ILE:HD12 | 4:G:792:GLN:H | 1.64 | 0.62 |
| 19:m:480:THR:HG22 | 20:n:979:SER:HB3 | 1.81 | 0.62 |
| 1:0:401:ILE:CG1 | 1:0:462:LEU:HD22 | 2.23 | 0.62 |
| 2:1:1338:LEU:HD23 | 2:1:1338:LEU:H | 1.65 | 0.61 |
| 1:0:416:LYS:H | 1:0:416:LYS:CD | 2.09 | 0.61 |
| 9:S:688:LEU:HD13 | 10:W:322:LEU:HD11 | 1.81 | 0.61 |
| 11:X:297:ASP:HA | 11:X:302:ARG:C | 2.25 | 0.61 |
| 1:0:400:ARG:HG2 | 1:0:400:ARG:HH11 | 1.64 | 0.61 |
| 1:0:410:ALA:HB2 | 1:0:511:LYS:C | 2.24 | 0.61 |
| 9:Q:232:PHE:CZ | 9:Q:513:LEU:CD2 | 2.83 | 0.61 |
| 8:N:1057:LYS:HA | 8:N:1057:LYS:HZ2 | 1.62 | 0.61 |
| 9:S:473:ARG:HA | 9:S:473:ARG:HE | 1.64 | 0.61 |
| 11:X:282:ASN:ND2 | 11:X:299:GLN:NE2 | 2.48 | 0.61 |
| 2:Z:960:GLN:HG2 | 2:Z:1039:LEU:HD11 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0:467:PHE:CD2 | 1:0:511:LYS:CD | 2.71 | 0.61 |
| 5:E:317:ASN:C | 5:E:348:ILE:HD11 | 2.25 | 0.61 |
| 20:g:774:PHE:CZ | 20:g:777:ILE:CG2 | 2.84 | 0.61 |
| 2:Z:1253:VAL:HG11 | 2:Z:1300:SER:CB | 2.28 | 0.61 |
| 5:E:318:GLU:HA | 5:E:348:ILE:HD11 | 1.83 | 0.61 |
| 5:H:318:GLU:HG2 | 5:H:346:GLN:HG2 | 1.83 | 0.61 |
| 8:P:1398:VAL:HG23 | 8:P:1399:ASN:H | 1.65 | 0.61 |
| 1:Y:397:TYR:CE2 | 1:Y:461:ARG:HA | 2.35 | 0.61 |
| 1:0:131:VAL:CB | 1:0:511:LYS:HE3 | 2.25 | 0.61 |
| 4:D:777:ASN:HD22 | 6:F:405:LEU:HD12 | 1.65 | 0.61 |
| 8:P:1276:LYS:N | 8:P:1321:LEU:CD1 | 2.63 | 0.61 |
| 2:Z:971:ALA:HB1 | 2:Z:1005:TYR:CZ | 2.35 | 0.61 |
| 1:0:467:PHE:HD2 | 1:0:511:LYS:NZ | 1.98 | 0.60 |
| 1:Y:126:TYR:CE1 | 1:Y:405:THR:CB | 2.59 | 0.60 |
| 2:Z:285:GLU:HB3 | 2:Z:306:LYS:HD3 | 1.83 | 0.60 |
| 2:Z:1210:ALA:HB2 | 2:Z:1218:ILE:HG13 | 1.84 | 0.60 |
| 16:j:257:MET:HE2 | 16:j:257:MET:HA | 1.84 | 0.60 |
| 8:N:379:ILE:HG21 | 8:N:400:PHE:CD1 | 2.37 | 0.60 |
| 8:P:1053:LEU:HD22 | 8:P:1127:ASN:HB3 | 1.83 | 0.60 |
| 9:R:746:PRO:HB3 | 9:R:753:ALA:CA | 2.25 | 0.60 |
| 19:f:27:ASN:N | 19:f:394:ILE:CG2 | 2.58 | 0.60 |
| 7:M:1226:VAL:O | 7:M:1226:VAL:HG12 | 2.00 | 0.60 |
| 8:P:1060:LEU:HD13 | 8:P:1060:LEU:N | 2.16 | 0.60 |
| 1:0:393:ILE:HG23 | 1:0:397:TYR:HD2 | 1.65 | 0.60 |
| 3:6:33:UNK:HA | 7:M:1038:LEU:HD13 | 1.83 | 0.60 |
| 1:Y:412:ILE:HG23 | 1:Y:444:VAL:HG21 | 0.61 | 0.60 |
| 12:v:301:ASN:HD22 | 12:v:302:ILE:H | 1.48 | 0.60 |
| 2:1:1175:ASN:HD21 | 9:S:754:ARG:CD | 2.14 | 0.60 |
| 1:Y:791:MET:C | 1:Y:791:MET:O | 2.45 | 0.60 |
| 5:E:322:ILE:HD12 | 5:E:322:ILE:H | 1.66 | 0.60 |
| 7:O:1188:THR:HG22 | 7:O:1189:MET:H | 1.66 | 0.60 |
| 9:R:746:PRO:HG3 | 9:R:753:ALA:N | 2.10 | 0.60 |
| 8:N:380:THR:O | 8:N:380:THR:HG23 | 2.01 | 0.59 |
| 9:T:608:GLN:H | 9:T:609:PRO:CD | 2.14 | 0.59 |
| 2:1:1015:VAL:C | 2:1:1040:LYS:CG | 2.75 | 0.59 |
| 8:P:75:ILE:CD1 | 8:P:83:VAL:HA | 2.32 | 0.59 |
| 8:P:736:ILE:CD1 | 8:P:794:ILE:HG21 | 2.20 | 0.59 |
| 8:N:379:ILE:CG1 | 8:N:403:ILE:CB | 2.70 | 0.59 |
| 8:N:1057:LYS:HA | 8:N:1057:LYS:HZ3 | 1.66 | 0.59 |
| 8:N:1277:ILE:HG13 | 8:N:1280:LEU:HG | 1.82 | 0.59 |
| 9:Q:269:ASN:HD21 | 9:Q:272:GLU:H | 1.51 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1:143:VAL:HG13 | 2:1:612:TYR:CE2 | 2.38 | 0.59 |
| 3:6:32:UNK:O | 7:M:1038:LEU:HD22 | 2.01 | 0.59 |
| 2:Z:1179:ASN:HD21 | 2:Z:1245:MET:HE1 | 1.67 | 0.59 |
| 1:0:413:LEU:CD1 | 1:0:444:VAL:CG1 | 2.80 | 0.59 |
| 8:P:736:ILE:CD1 | 8:P:794:ILE:CG2 | 2.80 | 0.59 |
| 1:Y:790:PHE:CZ | 1:Y:909:PHE:O | 2.56 | 0.59 |
| 1:0:375:SER:O | 1:0:420:ILE:HD11 | 2.03 | 0.59 |
| 7:M:461:LEU:HD23 | 7:M:461:LEU:H | 1.68 | 0.59 |
| 2:Z:745:ILE:HD11 | 2:Z:844:PHE:CE2 | 2.37 | 0.59 |
| 9:S:260:LEU:O | 9:S:513:LEU:HD11 | 2.02 | 0.59 |
| 9:S:268:ILE:HD13 | 9:S:514:LYS:CD | 2.20 | 0.59 |
| 1:Y:412:ILE:HG22 | 1:Y:444:VAL:CG1 | 2.18 | 0.59 |
| 14:h:991:LEU:HD23 | 14:h:991:LEU:H | 1.68 | 0.59 |
| 2:Z:1015:VAL:CG1 | 2:Z:1039:LEU:CD1 | 2.77 | 0.59 |
| 20:n:549:MET:HA | 20:n:552:THR:HG22 | 1.85 | 0.59 |
| 20:g:697:ASP:HB3 | 20:g:763:GLN:H | 1.67 | 0.59 |
| 7:M:951:ARG:HB3 | 7:M:1224:GLU:OE1 | 2.02 | 0.59 |
| 4:J:727:SER:O | 7:O:746:LYS:NZ | 2.30 | 0.59 |
| 8:P:380:THR:CG2 | 8:P:400:PHE:CG | 2.85 | 0.59 |
| 1:Y:410:ALA:HB2 | 1:Y:511:LYS:O | 2.02 | 0.59 |
| 20:n:699:MET:HE2 | 20:n:699:MET:HA | 1.85 | 0.59 |
| 8:N:322:HIS:HE1 | 8:N:359:LEU:CB | 1.92 | 0.58 |
| 1:Y:717:TYR:HB3 | 1:Y:885:ALA:HB2 | 1.85 | 0.58 |
| 8:P:719:ILE:CG1 | 8:P:794:ILE:HB | 2.33 | 0.58 |
| 1:Y:412:ILE:HG21 | 1:Y:444:VAL:HG13 | 1.76 | 0.58 |
| 1:Y:884:VAL:HG12 | 1:Y:884:VAL:O | 2.02 | 0.58 |
| 5:E:322:ILE:HD12 | 5:E:322:ILE:N | 2.17 | 0.58 |
| 1:Y:789:VAL:HG21 | 1:Y:952:LEU:CD1 | 2.33 | 0.58 |
| 14:h:109:THR:HG21 | 14:h:168:TYR:H | 1.68 | 0.58 |
| 19:m:453:GLU:C | 19:m:483:VAL:HG11 | 2.27 | 0.58 |
| 2:1:495:THR:HG23 | 2:1:535:GLU:N | 2.18 | 0.58 |
| 7:O:1321:PRO:HD2 | 7:O:1324:ARG:HD3 | 1.86 | 0.58 |
| 8:P:794:ILE:HG22 | 8:P:794:ILE:O | 2.03 | 0.58 |
| 2:Z:1109:LEU:HD12 | 2:Z:1156:LEU:HD23 | 1.85 | 0.58 |
| 19:f:27:ASN:C | 19:f:27:ASN:HD22 | 2.11 | 0.58 |
| 2:1:1178:ARG:HH22 | 9:S:754:ARG:CB | 2.17 | 0.58 |
| 1:0:131:VAL:CA | 1:0:511:LYS:HE2 | 2.09 | 0.58 |
| 6:I:350:PHE:CE1 | 6:I:354:LEU:HD11 | 2.39 | 0.58 |
| 8:P:380:THR:OG1 | 8:P:400:PHE:CD1 | 2.56 | 0.58 |
| 20:g:774:PHE:CZ | 20:g:777:ILE:HG21 | 2.39 | 0.58 |
| 1:0:401:ILE:HG21 | 1:0:462:LEU:HB3 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1:886:ASN:O | 2:1:890:GLU:HB3 | 2.03 | 0.58 |
| 8:P:777:ASP:O | 8:P:793:LEU:CB | 2.52 | 0.58 |
| 10:U:304:LYS:HD3 | 11:V:271:ILE:HG13 | 1.82 | 0.58 |
| 5:B:309:ARG:HH12 | 5:B:352:ILE:H | 1.51 | 0.58 |
| 6:I:370:ASP:OD1 | 6:I:370:ASP:N | 2.37 | 0.58 |
| 8:P:1247:PHE:CD2 | 8:P:1248:THR:HG23 | 2.38 | 0.58 |
| 1:Y:403:GLY:HA2 | 1:Y:408:ARG:CD | 2.34 | 0.57 |
| 2:Z:1254:GLY:C | 2:Z:1301:SER:HB3 | 2.29 | 0.57 |
| 8:N:1384:ASP:CG | 8:N:1385:LEU:N | 2.62 | 0.57 |
| 2:Z:745:ILE:HD11 | 2:Z:844:PHE:CZ | 2.39 | 0.57 |
| 1:0:467:PHE:HD2 | 1:0:511:LYS:HZ2 | 1.51 | 0.57 |
| 2:Z:745:ILE:O | 2:Z:745:ILE:HG22 | 2.02 | 0.57 |
| 5:E:381:GLU:CB | 7:M:1037:ASN:HB3 | 2.06 | 0.57 |
| 1:Y:130:GLY:CA | 1:Y:406:THR:HG21 | 2.34 | 0.57 |
| 1:0:394:GLU:O | 1:0:398:ILE:HD12 | 2.04 | 0.57 |
| 1:0:407:ALA:HB1 | 1:0:413:LEU:HG | 1.87 | 0.57 |
| 8:N:380:THR:HG22 | 8:N:411:PHE:CD2 | 2.39 | 0.57 |
| 8:P:1061:THR:HG22 | 8:P:1189:ASP:HB2 | 1.87 | 0.57 |
| 19:m:480:THR:HG21 | 20:n:979:SER:CB | 2.28 | 0.57 |
| 20:n:775:ILE:O | 20:n:775:ILE:HG12 | 2.04 | 0.57 |
| 8:N:70:LYS:CG | 8:N:72:ARG:NH2 | 2.59 | 0.57 |
| 8:N:733:ARG:HH12 | 8:N:796:SER:H | 1.51 | 0.57 |
| 7:O:561:CYS:HB3 | 7:O:612:LEU:HD11 | 1.84 | 0.57 |
| 7:M:602:ASN:CA | 7:M:606:VAL:HG23 | 2.35 | 0.57 |
| 1:Y:130:GLY:N | 1:Y:406:THR:HG21 | 2.19 | 0.57 |
| 10:U:304:LYS:CD | 11:V:271:ILE:HG13 | 2.34 | 0.57 |
| 14:a:206:LYS:O | 14:a:207:SER:HB2 | 2.04 | 0.57 |
| 1:0:417:TYR:CD2 | 1:0:442:GLY:HA2 | 2.40 | 0.57 |
| 8:N:1292:GLU:O | 8:N:1305:ASN:OD1 | 2.21 | 0.57 |
| 8:N:1316:LEU:HA | 8:N:1391:LEU:HD21 | 1.86 | 0.57 |
| 1:0:128:ASN:O | 1:0:405:THR:C | 2.38 | 0.56 |
| 1:0:467:PHE:CD2 | 1:0:511:LYS:NZ | 2.73 | 0.56 |
| 7:O:1026:PHE:CD1 | 7:O:1042:ILE:HA | 2.40 | 0.56 |
| 9:R:746:PRO:CB | 9:R:753:ALA:CA | 2.69 | 0.56 |
| 9:R:754:ARG:O | 9:R:758:GLN:HG2 | 2.05 | 0.56 |
| 2:Z:1286:HIS:CE1 | 2:Z:1324:ILE:HD12 | 2.40 | 0.56 |
| 1:0:401:ILE:HG12 | 1:0:462:LEU:HD22 | 1.84 | 0.56 |
| 4:D:722:LEU:HA | 4:D:726:VAL:HG23 | 1.87 | 0.56 |
| 8:P:1053:LEU:HD22 | 8:P:1127:ASN:CB | 2.34 | 0.56 |
| 1:Y:675:ALA:H | 1:Y:710:VAL:HG12 | 1.70 | 0.56 |
| 14:h:935:LEU:HD23 | 14:h:935:LEU:H | 1.69 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:m:454:ASP:N | 19:m:483:VAL:CG1 | 2.60 | 0.56 |
| 5:E:324:TYR:CZ | 5:E:328:GLY:CA | 2.88 | 0.56 |
| 8:P:1053:LEU:HD22 | 8:P:1127:ASN:H | 1.68 | 0.56 |
| 4:y:605:THR:CB | 4:z:605:THR:C | 2.78 | 0.56 |
| 6:L:302:ASP:HA | 6:L:305:ILE:HD12 | 1.87 | 0.56 |
| 9:S:510:LEU:HA | 9:S:513:LEU:HB2 | 1.85 | 0.56 |
| 14:h:1000:TYR:HA | 14:h:1004:ILE:HG22 | 1.88 | 0.56 |
| 19:m:578:ASP:OD2 | 19:m:639:THR:HG21 | 2.06 | 0.56 |
| 8:P:379:ILE:HG21 | 8:P:403:ILE:HG12 | 1.82 | 0.56 |
| 8:P:1469:LEU:HD11 | 8:P:1502:ILE:HG21 | 1.88 | 0.56 |
| 5:E:468:GLU:CB | 7:M:1224:GLU:HA | 2.36 | 0.56 |
| 8:P:379:ILE:HG21 | 8:P:403:ILE:CB | 2.33 | 0.56 |
| 1:Y:412:ILE:HD11 | 1:Y:513:SER:H | 1.70 | 0.56 |
| 2:Z:502:ILE:HG13 | 2:Z:572:PRO:HD3 | 1.88 | 0.56 |
| 19:m:142:SER:H | 19:m:203:SER:HA | 1.69 | 0.56 |
| 16:c:592:LEU:HD23 | 16:c:621:LEU:HD11 | 1.87 | 0.56 |
| 7:O:1035:GLY:HA3 | 7:O:1041:PHE:HE1 | 1.68 | 0.56 |
| 5:H:321:ALA:C | 5:H:323:LEU:N | 2.58 | 0.56 |
| 4:J:727:SER:O | 7:O:746:LYS:HG3 | 2.00 | 0.56 |
| 8:N:354:GLU:HA | 8:N:359:LEU:CD1 | 2.34 | 0.56 |
| 8:P:41:ARG:HG2 | 8:P:41:ARG:O | 2.06 | 0.56 |
| 8:P:723:LEU:CD2 | 8:P:794:ILE:HD11 | 2.36 | 0.56 |
| 5:E:324:TYR:HH | 5:E:328:GLY:HA3 | 1.64 | 0.56 |
| 8:P:1227:VAL:HG11 | 8:P:1277:ILE:CD1 | 2.29 | 0.56 |
| 9:S:682:GLU:OE2 | 10:W:322:LEU:CD2 | 2.53 | 0.56 |
| 2:Z:909:HIS:CE1 | 2:Z:926:ASN:HD22 | 2.23 | 0.56 |
| 12:v:395:LYS:HA | 12:v:395:LYS:HE2 | 1.88 | 0.56 |
| 9:S:547:TYR:HB2 | 11:X:299:GLN:C | 2.31 | 0.55 |
| 11:X:302:ARG:HH11 | 11:X:302:ARG:CG | 2.19 | 0.55 |
| 19:f:696:ASN:HB3 | 19:f:701:ILE:H | 1.71 | 0.55 |
| 2:1:1127:LEU:HD23 | 2:1:1127:LEU:H | 1.70 | 0.55 |
| 8:N:1423:ASN:HD21 | 8:N:1429:HIS:CG | 2.25 | 0.55 |
| 4:y:591:GLY:C | 4:z:595:ASP:CB | 2.79 | 0.55 |
| 5:E:387:GLN:HE21 | 5:E:388:GLN:HE22 | 1.54 | 0.55 |
| 7:M:323:LEU:HD23 | 7:M:323:LEU:C | 2.31 | 0.55 |
| 8:P:1276:LYS:N | 8:P:1321:LEU:CD2 | 2.69 | 0.55 |
| 1:Y:791:MET:H | 1:Y:831:LYS:HD3 | 1.70 | 0.55 |
| 12:v:83:PHE:CZ | 12:v:129:LYS:HB2 | 2.41 | 0.55 |
| 7:M:655:LYS:NZ | 7:M:659:ASN:HD21 | 2.03 | 0.55 |
| 7:O:724:ASN:CB | 7:O:1272:LEU:HD12 | 2.36 | 0.55 |
| 8:P:174:VAL:CG1 | 8:P:178:GLN:N | 2.69 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:P:778:VAL:HG21 | 8:P:795:ILE:HD12 | 1.88 | 0.55 |
| 11:X:297:ASP:N | 11:X:302:ARG:O | 2.39 | 0.55 |
| 2:1:932:ILE:HD13 | 9:T:609:PRO:HA | 1.88 | 0.55 |
| 5:H:316:VAL:HG21 | 5:H:348:ILE:CD1 | 2.32 | 0.55 |
| 6:L:307:SER:HA | 6:L:310:ARG:HE | 1.72 | 0.55 |
| 7:M:603:GLU:O | 7:M:607:ILE:N | 2.24 | 0.55 |
| 8:N:379:ILE:HG22 | 8:N:400:PHE:CD1 | 2.42 | 0.55 |
| 9:R:753:ALA:HB1 | 9:R:812:GLN:HG3 | 1.88 | 0.55 |
| 14:h:350:ASN:HA | 14:h:367:ASN:HA | 1.89 | 0.55 |
| 2:1:385:ARG:HH21 | 2:1:388:MET:HG3 | 1.71 | 0.55 |
| 8:N:380:THR:HB | 8:N:400:PHE:HE1 | 1.71 | 0.55 |
| 8:P:174:VAL:HG12 | 8:P:178:GLN:N | 2.19 | 0.55 |
| 1:0:1027:HIS:CE1 | 1:0:1057:VAL:HG11 | 2.42 | 0.55 |
| 8:P:75:ILE:HD11 | 8:P:83:VAL:HA | 1.88 | 0.55 |
| 10:W:305:TYR:H | 10:W:306:PRO:CD | 2.20 | 0.55 |
| 2:Z:807:ASP:OD2 | 2:Z:891:ARG:HB2 | 2.06 | 0.55 |
| 5:E:317:ASN:O | 5:E:348:ILE:HD12 | 2.04 | 0.55 |
| 8:N:41:ARG:C | 8:N:43:PHE:H | 2.15 | 0.55 |
| 16:c:221:LEU:HD22 | 16:c:231:TYR:CE1 | 2.41 | 0.55 |
| 4:D:758:LEU:O | 4:D:758:LEU:HD13 | 2.07 | 0.55 |
| 7:O:1043:SER:O | 7:O:1047:SER:OG | 2.24 | 0.55 |
| 7:O:1320:GLU:N | 7:O:1321:PRO:HD3 | 2.22 | 0.55 |
| 12:v:417:ILE:HD13 | 12:v:437:LEU:HD13 | 1.89 | 0.55 |
| 20:n:550:LEU:H | 20:n:550:LEU:HD23 | 1.72 | 0.55 |
| 11:X:302:ARG:HG2 | 11:X:302:ARG:NH1 | 2.22 | 0.54 |
| 1:0:240:LEU:HD21 | 1:0:282:ILE:HG21 | 1.89 | 0.54 |
| 1:0:413:LEU:HA | 1:0:444:VAL:HG21 | 1.88 | 0.54 |
| 14:a:719:PHE:CD2 | 14:a:746:CYS:SG | 3.01 | 0.54 |
| 1:0:409:ALA:CA | 1:0:512:LYS:HG2 | 2.36 | 0.54 |
| 5:H:318:GLU:CG | 5:H:346:GLN:HE21 | 2.17 | 0.54 |
| 9:Q:504:VAL:HG13 | 9:Q:538:LEU:CD2 | 2.37 | 0.54 |
| 9:S:482:LEU:HD13 | 9:S:491:ALA:HA | 1.89 | 0.54 |
| 15:i:584:GLN:HA | 15:i:637:ARG:HH22 | 1.72 | 0.54 |
| 8:N:322:HIS:CE1 | 8:N:359:LEU:CG | 2.91 | 0.54 |
| 2:1:1171:ASP:OD2 | 9:S:754:ARG:NH1 | 2.40 | 0.54 |
| 5:E:324:TYR:CD2 | 5:E:351:GLN:OE1 | 2.60 | 0.54 |
| 2:Z:745:ILE:O | 2:Z:815:PHE:CZ | 2.60 | 0.54 |
| 16:c:403:VAL:HG21 | 16:c:425:TYR:CD2 | 2.43 | 0.54 |
| 18:e:114:VAL:HG23 | 18:e:127:CYS:HB3 | 1.89 | 0.54 |
| 1:0:467:PHE:HD2 | 1:0:511:LYS:CE | 2.21 | 0.54 |
| 1:Y:126:TYR:HE1 | 1:Y:405:THR:HG22 | 1.70 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:v:307:ILE:HD12 | 12:v:390:ALA:HB1 | 1.89 | 0.54 |
| 19:m:8:GLN:HA | 19:m:8:GLN:NE2 | 2.22 | 0.54 |
| 1:0:401:ILE:HD12 | 1:0:462:LEU:HB3 | 1.87 | 0.54 |
| 7:O:297:ALA:H | 7:O:300:MET:HB2 | 1.72 | 0.54 |
| 8:P:34:ALA:HA | 8:P:40:ILE:HA | 1.89 | 0.54 |
| 14:a:719:PHE:HD2 | 14:a:746:CYS:SG | 2.29 | 0.54 |
| 1:0:128:ASN:O | 1:0:405:THR:CA | 1.81 | 0.54 |
| 10:U:304:LYS:CG | 11:V:271:ILE:HG13 | 2.36 | 0.54 |
| 4:y:605:THR:CB | 4:z:605:THR:CB | 2.86 | 0.54 |
| 7:O:1253:ARG:HH21 | 7:O:1273:LYS:CB | 2.21 | 0.53 |
| 1:0:401:ILE:CG1 | 1:0:462:LEU:HB2 | 2.04 | 0.53 |
| 1:0:790:PHE:O | 1:0:944:LEU:O | 2.26 | 0.53 |
| 7:O:707:LEU:CD2 | 7:O:776:VAL:HG22 | 2.38 | 0.53 |
| 7:O:724:ASN:HB2 | 7:O:1272:LEU:CD1 | 2.37 | 0.53 |
| 1:0:410:ALA:CA | 1:0:512:LYS:HA | 2.26 | 0.53 |
| 2:1:456:THR:O | 2:1:558:THR:CG2 | 2.57 | 0.53 |
| 8:N:322:HIS:ND1 | 8:N:359:LEU:CB | 2.62 | 0.53 |
| 8:P:1469:LEU:HD11 | 8:P:1502:ILE:CG2 | 2.38 | 0.53 |
| 1:Y:111:LEU:HD11 | 1:Y:771:TYR:CE1 | 2.43 | 0.53 |
| 20:n:917:LEU:H | 20:n:917:LEU:HD12 | 1.73 | 0.53 |
| 5:E:377:ASN:ND2 | 7:M:1041:PHE:CE1 | 2.76 | 0.53 |
| 8:N:69:ASN:C | 8:N:72:ARG:HH21 | 2.16 | 0.53 |
| 9:S:510:LEU:CB | 9:S:515:LEU:O | 2.36 | 0.53 |
| 9:S:515:LEU:CD2 | 9:S:563:ASN:ND2 | 2.71 | 0.53 |
| 15:i:406:LEU:N | 15:i:407:PRO:HD2 | 2.24 | 0.53 |
| 14:a:935:LEU:HD23 | 14:a:935:LEU:H | 1.72 | 0.53 |
| 8:N:380:THR:CG2 | 8:N:411:PHE:HD2 | 2.21 | 0.53 |
| 8:P:1461:ILE:HG21 | 8:P:1509:GLN:HE22 | 1.73 | 0.53 |
| 9:S:688:LEU:CD1 | 10:W:322:LEU:HD11 | 2.39 | 0.53 |
| 2:Z:1253:VAL:HG13 | 2:Z:1299:LYS:O | 2.08 | 0.53 |
| 1:0:416:LYS:HD2 | 1:0:416:LYS:N | 2.23 | 0.53 |
| 5:E:326:LYS:CD | 5:E:335:TRP:HE3 | 2.01 | 0.53 |
| 5:E:377:ASN:CG | 7:M:1041:PHE:CE1 | 2.86 | 0.53 |
| 7:O:1325:SER:HA | 7:O:1328:ILE:HD12 | 1.91 | 0.53 |
| 8:P:188:ILE:HG21 | 8:P:218:ASN:HD22 | 1.73 | 0.53 |
| 4:y:602:GLU:CA | 4:z:605:THR:CB | 2.85 | 0.53 |
| 4:A:689:SER:HB2 | 6:C:326:LEU:HD21 | 1.90 | 0.53 |
| 8:N:13:LEU:HD11 | 8:N:34:ALA:HB2 | 1.91 | 0.53 |
| 8:P:1227:VAL:CG1 | 8:P:1277:ILE:HD12 | 2.21 | 0.53 |
| 10:W:283:ILE:HG23 | 10:W:284:LYS:N | 2.24 | 0.53 |
| 8:N:379:ILE:HG21 | 8:N:400:PHE:HD1 | 1.72 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:Q:232:PHE:HZ | 9:Q:513:LEU:CD2 | 2.14 | 0.53 |
| 1:0:398:ILE:HA | 1:0:462:LEU:CD1 | 2.39 | 0.53 |
| 7:M:661:VAL:HG11 | 7:M:715:ASN:HB3 | 1.90 | 0.53 |
| 8:P:22:MET:HE1 | 8:P:40:ILE:CG2 | 2.39 | 0.53 |
| 9:S:268:ILE:HD11 | 9:S:514:LYS:CG | 2.37 | 0.53 |
| 1:Y:403:GLY:HA2 | 1:Y:408:ARG:NE | 2.22 | 0.53 |
| 1:0:417:TYR:HB3 | 1:0:442:GLY:HA3 | 1.89 | 0.53 |
| 15:i:375:LEU:HD22 | 15:i:398:ILE:HG21 | 1.90 | 0.53 |
| 20:n:974:ARG:HH22 | 20:n:1044:ARG:HA | 1.74 | 0.53 |
| 1:0:130:GLY:HA2 | 1:0:511:LYS:CG | 2.39 | 0.52 |
| 2:Z:1257:GLY:C | 2:Z:1299:LYS:HD2 | 2.33 | 0.52 |
| 8:P:380:THR:CG2 | 8:P:400:PHE:CD1 | 2.91 | 0.52 |
| 2:Z:927:HIS:CG | 2:Z:928:LEU:H | 2.26 | 0.52 |
| 1:0:398:ILE:HG12 | 1:0:446:LEU:CD1 | 2.30 | 0.52 |
| 8:N:72:ARG:O | 8:N:83:VAL:HB | 2.08 | 0.52 |
| 1:0:788:HIS:HB3 | 1:0:947:LEU:H | 1.72 | 0.52 |
| 7:M:336:LYS:HE3 | 7:M:336:LYS:H | 1.74 | 0.52 |
| 8:N:1278:ILE:HG22 | 8:N:1282:ASN:ND2 | 2.25 | 0.52 |
| 8:P:1160:ILE:H | 8:P:1160:ILE:HD12 | 1.73 | 0.52 |
| 9:Q:546:ARG:HG3 | 9:Q:546:ARG:HH11 | 1.74 | 0.52 |
| 14:h:737:ILE:HD12 | 14:h:739:PHE:CD2 | 2.45 | 0.52 |
| 1:0:398:ILE:HG21 | 1:0:446:LEU:HD21 | 1.87 | 0.52 |
| 1:0:408:ARG:C | 1:0:512:LYS:HE2 | 2.33 | 0.52 |
| 1:0:717:TYR:HB2 | 1:0:885:ALA:CB | 2.38 | 0.52 |
| 1:Y:126:TYR:CZ | 1:Y:405:THR:HB | 2.40 | 0.52 |
| 1:Y:412:ILE:HG23 | 1:Y:444:VAL:HG22 | 1.63 | 0.52 |
| 2:Z:854:THR:HB | 2:Z:856:ASN:HD21 | 1.73 | 0.52 |
| 4:z:604:SER:CB | 4:z:610:ALA:HB2 | 2.39 | 0.52 |
| 14:a:220:TYR:HB3 | 14:a:222:SER:H | 1.73 | 0.52 |
| 7:O:674:PHE:CZ | 7:O:678:LEU:HD11 | 2.44 | 0.52 |
| 8:P:778:VAL:HA | 8:P:793:LEU:CG | 2.40 | 0.52 |
| 2:Z:232:ILE:HD13 | 2:Z:288:TYR:CE2 | 2.44 | 0.52 |
| 1:0:401:ILE:HG21 | 1:0:462:LEU:CB | 2.39 | 0.52 |
| 5:H:316:VAL:HB | 5:H:348:ILE:HG13 | 1.91 | 0.52 |
| 7:M:602:ASN:HA | 7:M:606:VAL:CG2 | 2.40 | 0.52 |
| 15:i:78:ASN:HD21 | 15:i:95:ILE:HG13 | 1.74 | 0.52 |
| 10:U:304:LYS:HB3 | 11:V:270:ALA:CA | 2.39 | 0.52 |
| 16:c:147:SER:H | 17:d:11:LEU:HD13 | 1.75 | 0.52 |
| 1:0:395:PRO:HA | 1:0:398:ILE:HD12 | 1.92 | 0.52 |
| 4:A:697:LEU:HD22 | 6:C:333:ILE:HG23 | 1.91 | 0.52 |
| 5:K:506:ILE:HG13 | 5:K:507:ASN:H | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:130:GLY:CA | 1:Y:406:THR:CG2 | 2.87 | 0.52 |
| 9:S:547:TYR:CG | 11:X:300:VAL:HA | 2.45 | 0.52 |
| 20:n:228:ILE:HD12 | 20:n:295:TRP:CZ3 | 2.44 | 0.52 |
| 20:g:775:ILE:HA | 20:g:778:ASN:HD22 | 1.74 | 0.52 |
| 9:R:573:HIS:CD2 | 9:R:623:ILE:HD11 | 2.45 | 0.51 |
| 14:a:806:SER:O | 14:a:807:ILE:HD13 | 2.10 | 0.51 |
| 8:N:70:LYS:HG3 | 8:N:72:ARG:HH22 | 1.63 | 0.51 |
| 9:Q:504:VAL:HG13 | 9:Q:538:LEU:HD23 | 1.93 | 0.51 |
| 19:f:29:GLU:CB | 19:f:33:ILE:HG21 | 2.35 | 0.51 |
| 20:g:852:ILE:H | 20:g:854:HIS:CE1 | 2.28 | 0.51 |
| 1:0:413:LEU:HD12 | 1:0:444:VAL:CG1 | 2.40 | 0.51 |
| 12:u:209:TYR:H | 12:u:210:PRO:HD2 | 1.76 | 0.51 |
| 12:u:366:LEU:H | 12:u:369:GLN:HE21 | 1.59 | 0.51 |
| 19:f:433:ALA:HA | 19:f:436:LEU:HD13 | 1.90 | 0.51 |
| 5:E:380:LEU:HB3 | 7:M:1036:PRO:HA | 1.93 | 0.51 |
| 7:M:602:ASN:HA | 7:M:606:VAL:HG21 | 1.93 | 0.51 |
| 8:P:400:PHE:CE2 | 8:P:596:LYS:HE3 | 2.45 | 0.51 |
| 2:Z:872:ASN:HA | 2:Z:909:HIS:CE1 | 2.46 | 0.51 |
| 7:O:336:LYS:HE3 | 7:O:336:LYS:H | 1.75 | 0.51 |
| 8:P:51:LEU:O | 8:P:133:ASP:HB2 | 2.10 | 0.51 |
| 8:P:1052:LYS:HD2 | 8:P:1056:LYS:HA | 1.93 | 0.51 |
| 1:Y:717:TYR:C | 1:Y:885:ALA:CB | 2.84 | 0.51 |
| 2:Z:1255:SER:N | 2:Z:1301:SER:CB | 2.74 | 0.51 |
| 14:h:206:LYS:O | 14:h:207:SER:HB2 | 2.11 | 0.51 |
| 6:L:345:LEU:HD23 | 6:L:345:LEU:H | 1.75 | 0.51 |
| 7:O:1164:PHE:CE1 | 7:O:1168:ILE:HD11 | 2.45 | 0.51 |
| 7:O:1253:ARG:NH2 | 7:O:1273:LYS:HG2 | 2.22 | 0.51 |
| 9:R:599:ARG:H | 9:R:599:ARG:NE | 2.09 | 0.51 |
| 10:W:283:ILE:CG2 | 10:W:284:LYS:N | 2.72 | 0.51 |
| 2:Z:1112:ALA:HB1 | 2:Z:1156:LEU:CD1 | 2.41 | 0.51 |
| 4:D:711:LEU:HB2 | 5:E:411:ARG:HE | 1.75 | 0.51 |
| 7:M:159:LYS:HA | 7:M:159:LYS:HE2 | 1.92 | 0.51 |
| 7:M:1492:LEU:HD13 | 7:M:1546:ILE:HD12 | 1.93 | 0.51 |
| 9:S:584:LYS:CA | 11:X:302:ARG:HE | 2.24 | 0.51 |
| 20:n:605:ARG:HH21 | 20:n:628:HIS:HB2 | 1.76 | 0.51 |
| 20:g:212:LEU:HD21 | 20:g:272:ASN:HB2 | 1.92 | 0.51 |
| 5:H:318:GLU:HG2 | 5:H:346:GLN:NE2 | 2.21 | 0.51 |
| 19:m:313:LEU:HD22 | 19:m:313:LEU:N | 2.26 | 0.51 |
| 20:n:853:LYS:HG2 | 20:n:861:ILE:HG22 | 1.92 | 0.51 |
| 20:n:1015:LEU:HG | 20:n:1015:LEU:O | 2.10 | 0.51 |
| 19:f:126:LEU:HD21 | 19:f:190:ALA:HA | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0:412:ILE:HD13 | 1:0:514:SER:HB3 | 1.93 | 0.51 |
| 1:0:584:GLY:HA3 | 1:0:673:TYR:CD1 | 2.46 | 0.51 |
| 8:P:719:ILE:HG13 | 8:P:794:ILE:CG1 | 2.41 | 0.51 |
| 14:h:999:CYS:O | 14:h:1003:VAL:HG12 | 2.11 | 0.51 |
| 20:n:86:LEU:H | 20:n:456:ILE:HG23 | 1.76 | 0.51 |
| 1:0:1415:ILE:HD12 | 1:0:1419:ALA:HB2 | 1.94 | 0.50 |
| 5:K:323:LEU:HD12 | 5:K:350:ILE:CD1 | 2.39 | 0.50 |
| 8:P:141:LEU:HD23 | 8:P:141:LEU:H | 1.76 | 0.50 |
| 18:e:221:ALA:HB1 | 18:e:226:ARG:HH22 | 1.76 | 0.50 |
| 1:0:409:ALA:O | 1:0:512:LYS:HB3 | 2.09 | 0.50 |
| 4:D:725:VAL:O | 4:D:725:VAL:HG12 | 2.09 | 0.50 |
| 5:E:381:GLU:HG3 | 5:E:382:LYS:N | 2.26 | 0.50 |
| 7:M:702:LYS:HG3 | 7:M:703:TYR:H | 1.76 | 0.50 |
| 7:M:1027:GLN:HB2 | 7:M:1036:PRO:HG3 | 1.93 | 0.50 |
| 8:N:1278:ILE:C | 8:N:1280:LEU:H | 2.19 | 0.50 |
| 7:O:1026:PHE:HD1 | 7:O:1042:ILE:HA | 1.76 | 0.50 |
| 17:k:58:ARG:HG3 | 17:k:259:ARG:HH12 | 1.76 | 0.50 |
| 20:n:256:ILE:HD13 | 20:n:256:ILE:H | 1.76 | 0.50 |
| 1:0:398:ILE:C | 1:0:462:LEU:CD2 | 2.83 | 0.50 |
| 8:P:1227:VAL:HG22 | 8:P:1277:ILE:HD13 | 1.93 | 0.50 |
| 8:P:1276:LYS:N | 8:P:1321:LEU:HD11 | 2.26 | 0.50 |
| 1:Y:126:TYR:CE1 | 1:Y:405:THR:HG22 | 2.45 | 0.50 |
| 2:Z:872:ASN:HA | 2:Z:909:HIS:HE1 | 1.75 | 0.50 |
| 19:m:628:PHE:CE2 | 19:m:664:LEU:HA | 2.45 | 0.50 |
| 5:E:467:LYS:CD | 7:M:1224:GLU:HB3 | 2.41 | 0.50 |
| 8:N:380:THR:HG22 | 8:N:411:PHE:HD2 | 1.77 | 0.50 |
| 7:O:6:ILE:HB | 7:O:7:PRO:HD3 | 1.94 | 0.50 |
| 5:B:328:GLY:H | 5:B:351:GLN:HE21 | 1.60 | 0.50 |
| 5:E:326:LYS:HG3 | 5:E:335:TRP:CZ3 | 2.45 | 0.50 |
| 8:P:132:ASN:O | 8:P:135:PHE:HB3 | 2.12 | 0.50 |
| 8:P:885:VAL:HG21 | 8:P:922:PHE:H | 1.76 | 0.50 |
| 2:Z:1253:VAL:HG13 | 2:Z:1300:SER:OG | 1.87 | 0.50 |
| 1:0:281:ARG:HH12 | 1:0:385:LYS:HD2 | 1.75 | 0.50 |
| 4:D:702:ARG:HA | 4:D:702:ARG:HE | 1.76 | 0.50 |
| 4:D:755:LEU:HD23 | 4:D:755:LEU:H | 1.77 | 0.50 |
| 5:H:316:VAL:CG2 | 5:H:348:ILE:CA | 2.89 | 0.50 |
| 9:S:515:LEU:HD21 | 9:S:563:ASN:ND2 | 2.26 | 0.50 |
| 1:0:202:GLN:HG2 | 1:0:254:LEU:H | 1.77 | 0.50 |
| 1:0:788:HIS:CD2 | 1:0:946:LYS:HA | 2.46 | 0.50 |
| 2:1:1266:SER:HA | 2:1:1270:ILE:HD12 | 1.93 | 0.50 |
| 4:D:722:LEU:HA | 4:D:726:VAL:CG2 | 2.42 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:767:VAL:HG11 | 5:E:399:LEU:HD13 | 1.93 | 0.50 |
| 2:Z:1253:VAL:HG13 | 2:Z:1299:LYS:C | 2.37 | 0.50 |
| 17:d:84:GLU:HG3 | 17:d:89:TRP:CD2 | 2.46 | 0.50 |
| 20:g:785:HIS:HA | 20:g:788:TRP:HB3 | 1.92 | 0.50 |
| 4:J:755:LEU:H | 4:J:755:LEU:CD2 | 2.25 | 0.50 |
| 7:M:1034:LEU:HD23 | 7:M:1034:LEU:O | 2.12 | 0.50 |
| 2:1:123:TYR:CE1 | 2:1:456:THR:CG2 | 2.93 | 0.49 |
| 8:N:1423:ASN:HD21 | 8:N:1429:HIS:CD2 | 2.29 | 0.49 |
| 16:c:781:TYR:HB2 | 14:a:1016:GLN:NE2 | 2.26 | 0.49 |
| 5:E:443:LEU:HD21 | 6:F:377:ILE:HG23 | 1.94 | 0.49 |
| 9:R:736:LEU:HA | 9:R:739:MET:HE3 | 1.92 | 0.49 |
| 10:U:304:LYS:HB3 | 11:V:270:ALA:N | 2.27 | 0.49 |
| 20:n:334:TRP:HE1 | 20:n:351:ILE:HB | 1.76 | 0.49 |
| 20:n:751:TYR:CZ | 20:n:782:ASP:HA | 2.47 | 0.49 |
| 1:0:412:ILE:C | 1:0:444:VAL:HG23 | 2.36 | 0.49 |
| 7:O:1290:ILE:O | 7:O:1294:LYS:HG2 | 2.12 | 0.49 |
| 1:Y:124:ARG:HH22 | 1:Y:404:THR:HG21 | 1.78 | 0.49 |
| 19:m:446:SER:O | 19:m:478:ARG:NH2 | 2.46 | 0.49 |
| 8:N:75:ILE:O | 8:N:75:ILE:HG22 | 2.12 | 0.49 |
| 8:P:362:LEU:HB3 | 8:P:379:ILE:HD11 | 1.93 | 0.49 |
| 1:Y:977:LYS:HA | 1:Y:977:LYS:HE2 | 1.94 | 0.49 |
| 19:m:355:LEU:HD22 | 19:m:355:LEU:H | 1.78 | 0.49 |
| 7:M:1064:THR:HG23 | 7:M:1115:GLN:H | 1.76 | 0.49 |
| 1:Y:130:GLY:HA2 | 1:Y:406:THR:HG22 | 1.94 | 0.49 |
| 21:o:14:SER:HB2 | 21:o:16:ILE:HG22 | 1.95 | 0.49 |
| 14:a:10:ASN:HD21 | 14:a:418:GLN:HB3 | 1.77 | 0.49 |
| 7:M:1424:GLU:HA | 7:M:1427:LEU:HD12 | 1.95 | 0.49 |
| 7:O:1042:ILE:HG13 | 7:O:1042:ILE:O | 2.11 | 0.49 |
| 7:O:1115:GLN:HB3 | 7:O:1193:ARG:HE | 1.76 | 0.49 |
| 1:0:409:ALA:O | 1:0:512:LYS:CA | 2.61 | 0.49 |
| 5:H:321:ALA:O | 5:H:323:LEU:N | 2.46 | 0.49 |
| 7:O:473:SER:C | 7:O:474:LEU:HD12 | 2.38 | 0.49 |
| 1:Y:130:GLY:HA2 | 1:Y:406:THR:HG21 | 1.94 | 0.49 |
| 1:Y:397:TYR:OH | 1:Y:461:ARG:HG2 | 2.12 | 0.49 |
| 7:M:1027:GLN:OE1 | 7:M:1036:PRO:HG3 | 2.12 | 0.49 |
| 8:P:1040:VAL:HG12 | 8:P:1043:LEU:HD12 | 1.94 | 0.49 |
| 9:S:260:LEU:HB3 | 9:S:513:LEU:HD12 | 1.95 | 0.49 |
| 9:S:548:SER:HB3 | 11:X:299:GLN:HA | 1.93 | 0.49 |
| 1:Y:403:GLY:CA | 1:Y:408:ARG:CD | 2.90 | 0.49 |
| 20:n:162:GLY:H | 20:n:176:GLU:HA | 1.77 | 0.49 |
| 7:M:1235:ASN:O | 7:M:1290:ILE:HG12 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:562:LEU:HG | 7:O:612:LEU:HD13 | 1.95 | 0.49 |
| 1:Y:1348:ARG:HH12 | 1:Y:1367:LEU:HD22 | 1.77 | 0.49 |
| 2:Z:991:ALA:HA | 2:Z:995:LYS:HE3 | 1.94 | 0.49 |
| 19:f:271:ILE:HG12 | 19:f:292:GLN:HE21 | 1.78 | 0.49 |
| 2:1:457:SER:C | 2:1:558:THR:CB | 2.85 | 0.49 |
| 5:E:318:GLU:HG2 | 5:E:348:ILE:HG12 | 1.93 | 0.49 |
| 5:E:415:LEU:HD13 | 6:F:350:PHE:CE1 | 2.48 | 0.49 |
| 10:W:305:TYR:N | 10:W:306:PRO:CD | 2.76 | 0.49 |
| 2:Z:1258:GLN:NE2 | 2:Z:1302:ALA:HB2 | 2.27 | 0.49 |
| 7:M:873:ASN:HD21 | 7:M:1241:LYS:HG3 | 1.77 | 0.48 |
| 16:j:581:LEU:HD12 | 16:j:664:GLU:OE1 | 2.12 | 0.48 |
| 3:6:36:UNK:CB | 7:M:1038:LEU:CD1 | 2.91 | 0.48 |
| 5:E:355:PHE:CB | 6:F:287:GLN:HE22 | 2.26 | 0.48 |
| 7:O:1250:LYS:HZ2 | 7:O:1250:LYS:HB3 | 1.78 | 0.48 |
| 20:n:987:LEU:HD22 | 20:n:1005:LEU:HD21 | 1.95 | 0.48 |
| 15:b:250:ASN:HA | 15:b:253:VAL:HG12 | 1.95 | 0.48 |
| 1:0:919:VAL:HG23 | 1:0:920:GLU:H | 1.78 | 0.48 |
| 2:1:960:GLN:H | 2:1:961:PRO:CD | 2.27 | 0.48 |
| 7:O:1181:VAL:CG1 | 7:O:1318:LYS:HE2 | 2.27 | 0.48 |
| 8:P:923:LEU:HD23 | 8:P:923:LEU:H | 1.78 | 0.48 |
| 9:T:345:LEU:HD13 | 9:T:348:GLU:OE2 | 2.12 | 0.48 |
| 15:b:720:LEU:H | 15:b:720:LEU:CD1 | 2.23 | 0.48 |
| 20:g:317:LEU:HA | 20:g:320:LEU:HD12 | 1.95 | 0.48 |
| 7:O:172:ASN:H | 7:O:172:ASN:HD22 | 1.61 | 0.48 |
| 7:O:707:LEU:HD21 | 7:O:776:VAL:HG22 | 1.95 | 0.48 |
| 9:S:348:GLU:HA | 9:S:351:GLN:HE21 | 1.77 | 0.48 |
| 9:S:514:LYS:HE3 | 9:S:514:LYS:CA | 2.42 | 0.48 |
| 9:T:621:HIS:CE1 | 9:T:648:GLU:HG3 | 2.49 | 0.48 |
| 2:Z:822:PHE:CZ | 2:Z:870:VAL:HG11 | 2.49 | 0.48 |
| 14:a:1017:TRP:HE1 | 14:a:1020:ASN:HB2 | 1.77 | 0.48 |
| 1:0:416:LYS:CD | 1:0:416:LYS:N | 2.76 | 0.48 |
| 7:O:1274:ASP:O | 7:O:1278:GLU:HG3 | 2.13 | 0.48 |
| 8:P:359:LEU:CG | 8:P:399:VAL:HG13 | 2.29 | 0.48 |
| 9:S:515:LEU:HD21 | 9:S:563:ASN:HD21 | 1.79 | 0.48 |
| 1:Y:397:TYR:OH | 1:Y:461:ARG:CG | 2.61 | 0.48 |
| 1:Y:402:ILE:HB | 1:Y:407:ALA:HB3 | 1.95 | 0.48 |
| 2:Z:882:ASP:O | 2:Z:886:ASN:HB2 | 2.13 | 0.48 |
| 12:v:638:ILE:CB | 15:i:372:ALA:HB1 | 2.43 | 0.48 |
| 8:N:82:ASN:HD22 | 8:N:84:ASP:H | 1.61 | 0.48 |
| 9:R:628:ALA:HB1 | 9:R:644:TYR:CD1 | 2.49 | 0.48 |
| 2:Z:1015:VAL:HG11 | 2:Z:1039:LEU:HD11 | 1.92 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:c:455:GLN:OE1 | 16:c:455:GLN:HA | 2.13 | 0.48 |
| 5:E:377:ASN:O | 7:M:1037:ASN:HB2 | 2.13 | 0.48 |
| 8:N:1056:LYS:N | 8:N:1056:LYS:CD | 2.73 | 0.48 |
| 9:Q:533:ARG:HB2 | 9:Q:571:LEU:HD22 | 1.95 | 0.48 |
| 9:S:268:ILE:HD11 | 9:S:514:LYS:N | 2.29 | 0.48 |
| 1:Y:1413:VAL:HA | 1:Y:1416:PHE:CD2 | 2.49 | 0.48 |
| 16:j:336:ALA:HB2 | 16:j:361:LEU:HB3 | 1.96 | 0.48 |
| 7:M:1272:LEU:HB2 | 7:M:1273:LYS:H | 1.48 | 0.48 |
| 8:N:898:VAL:HG22 | 8:N:898:VAL:O | 2.13 | 0.48 |
| 7:O:152:HIS:CD2 | 7:O:229:PHE:CE1 | 3.02 | 0.48 |
| 1:Y:403:GLY:CA | 1:Y:408:ARG:CG | 2.89 | 0.48 |
| 1:Y:790:PHE:HD1 | 1:Y:831:LYS:HE3 | 1.79 | 0.48 |
| 7:M:740:LEU:HD13 | 7:M:749:ILE:CG2 | 2.43 | 0.48 |
| 14:a:878:HIS:CD2 | 14:a:878:HIS:H | 2.32 | 0.48 |
| 5:B:419:LEU:HD11 | 6:C:354:LEU:HD11 | 1.95 | 0.48 |
| 15:b:693:GLU:HA | 15:b:696:GLU:HG3 | 1.96 | 0.48 |
| 1:0:131:VAL:CB | 1:0:511:LYS:HE2 | 2.43 | 0.47 |
| 1:0:412:ILE:C | 1:0:444:VAL:HG21 | 2.39 | 0.47 |
| 2:1:888:LEU:C | 2:1:888:LEU:CD2 | 2.86 | 0.47 |
| 7:O:1395:PRO:HA | 7:O:1440:ILE:HD12 | 1.96 | 0.47 |
| 2:Z:457:SER:CA | 2:Z:513:LYS:HG2 | 2.44 | 0.47 |
| 1:0:1113:ILE:O | 1:0:1113:ILE:HG22 | 2.14 | 0.47 |
| 5:E:514:THR:HA | 5:E:517:GLN:HE21 | 1.79 | 0.47 |
| 8:P:719:ILE:CD1 | 8:P:794:ILE:HB | 2.44 | 0.47 |
| 1:Y:402:ILE:HG21 | 1:Y:413:LEU:CG | 2.44 | 0.47 |
| 14:h:229:PHE:CZ | 14:h:230:HIS:NE2 | 2.82 | 0.47 |
| 16:j:579:ARG:HH12 | 17:k:86:ASN:HA | 1.80 | 0.47 |
| 2:1:710:TYR:CE2 | 2:1:714:LEU:HD22 | 2.49 | 0.47 |
| 2:1:1292:ILE:HG22 | 2:1:1296:PHE:CZ | 2.49 | 0.47 |
| 5:K:322:ILE:HA | 5:K:335:TRP:NE1 | 2.26 | 0.47 |
| 7:M:773:LYS:HG3 | 7:M:777:GLN:HE21 | 1.79 | 0.47 |
| 8:N:13:LEU:CD1 | 8:N:34:ALA:HB2 | 2.44 | 0.47 |
| 8:N:33:ASP:CB | 8:N:946:TRP:HB3 | 2.36 | 0.47 |
| 7:O:152:HIS:CG | 7:O:229:PHE:CE1 | 3.03 | 0.47 |
| 15:i:90:LEU:HD21 | 18:l:12:VAL:HG11 | 1.96 | 0.47 |
| 18:e:117:ALA:HB2 | 18:e:173:TRP:CD2 | 2.48 | 0.47 |
| 2:1:457:SER:C | 2:1:558:THR:HB | 2.39 | 0.47 |
| 2:1:1008:ILE:O | 2:1:1012:VAL:HG23 | 2.15 | 0.47 |
| 7:O:1465:GLN:HE21 | 7:O:1469:ARG:HG3 | 1.80 | 0.47 |
| 8:P:1276:LYS:N | 8:P:1321:LEU:HD13 | 2.29 | 0.47 |
| 9:S:688:LEU:CD1 | 10:W:322:LEU:CD1 | 2.93 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:788:HIS:CE1 | 1:Y:947:LEU:H | 2.32 | 0.47 |
| 2:Z:138:PHE:CE2 | 2:Z:559:ALA:HB2 | 2.48 | 0.47 |
| 20:g:504:PHE:HA | 20:g:507:ILE:HG22 | 1.96 | 0.47 |
| 20:g:690:ARG:HA | 20:g:690:ARG:HE | 1.79 | 0.47 |
| 7:O:145:LEU:HG | 7:O:219:HIS:CG | 2.50 | 0.47 |
| 7:O:858:GLY:H | 7:O:861:GLN:HG2 | 1.80 | 0.47 |
| 8:P:1200:GLU:O | 8:P:1200:GLU:HG3 | 2.13 | 0.47 |
| 9:S:215:TYR:CE2 | 9:S:505:HIS:CE1 | 3.02 | 0.47 |
| 9:S:585:GLU:HG2 | 11:X:302:ARG:HG3 | 1.96 | 0.47 |
| 9:S:754:ARG:HE | 9:S:758:GLN:NE2 | 2.11 | 0.47 |
| 1:Y:397:TYR:OH | 1:Y:461:ARG:HB3 | 2.11 | 0.47 |
| 1:Y:1466:ILE:HG23 | 1:Y:1468:TYR:H | 1.78 | 0.47 |
| 2:Z:285:GLU:HB3 | 2:Z:306:LYS:CD | 2.43 | 0.47 |
| 2:Z:409:ILE:HG23 | 2:Z:424:VAL:HG22 | 1.96 | 0.47 |
| 1:0:402:ILE:HD12 | 1:0:467:PHE:CE1 | 2.50 | 0.47 |
| 2:1:123:TYR:HE1 | 2:1:456:THR:CB | 2.28 | 0.47 |
| 7:M:623:VAL:HG11 | 7:M:627:VAL:HG21 | 1.97 | 0.47 |
| 8:N:459:ASP:HA | 8:N:463:PHE:CE2 | 2.50 | 0.47 |
| 7:O:1347:ILE:H | 7:O:1347:ILE:HD13 | 1.79 | 0.47 |
| 8:P:387:LEU:HD21 | 8:P:444:ASN:HB2 | 1.95 | 0.47 |
| 8:P:723:LEU:HD23 | 8:P:794:ILE:HD11 | 1.95 | 0.47 |
| 9:R:608:GLN:HB3 | 9:R:609:PRO:HD3 | 1.96 | 0.47 |
| 9:S:577:ARG:HE | 9:S:623:ILE:HG23 | 1.80 | 0.47 |
| 9:T:443:ILE:H | 9:T:443:ILE:HD12 | 1.78 | 0.47 |
| 13:x:1300:ARG:CB | 21:p:51:VAL:HG11 | 2.45 | 0.47 |
| 17:d:106:GLN:HG3 | 17:d:152:SER:HA | 1.97 | 0.47 |
| 20:g:680:GLY:H | 20:g:683:GLU:HB2 | 1.79 | 0.47 |
| 14:a:959:GLU:HG3 | 14:a:961:PHE:H | 1.80 | 0.47 |
| 5:E:401:ALA:HB2 | 6:F:336:PHE:CD1 | 2.50 | 0.47 |
| 4:J:665:TRP:CH2 | 6:L:301:HIS:CE1 | 3.03 | 0.47 |
| 8:N:1278:ILE:C | 8:N:1280:LEU:N | 2.73 | 0.47 |
| 9:S:758:GLN:HE22 | 9:S:819:MET:HE1 | 1.79 | 0.47 |
| 2:Z:1254:GLY:N | 2:Z:1299:LYS:O | 2.47 | 0.47 |
| 14:a:873:LEU:HB3 | 14:a:908:LEU:HD21 | 1.97 | 0.47 |
| 1:0:408:ARG:C | 1:0:512:LYS:NZ | 2.69 | 0.47 |
| 8:N:1081:ILE:HA | 8:N:1084:LEU:HD12 | 1.97 | 0.47 |
| 9:S:584:LYS:H | 11:X:302:ARG:NE | 2.13 | 0.47 |
| 1:Y:270:VAL:HG11 | 1:Y:273:ILE:HG23 | 1.97 | 0.47 |
| 14:h:922:LEU:HD21 | 14:h:934:GLU:OE2 | 2.14 | 0.47 |
| 8:P:15:PHE:CD2 | 8:P:72:ARG:HD3 | 2.50 | 0.47 |
| 14:h:210:ARG:HG2 | 14:h:210:ARG:HH11 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 19:m:387:ARG:HH22 | 19:m:419:LEU:HB3 | 1.80 | 0.47 |
| 20:n:451:ASN:HD21 | 20:n:510:ASN:C | 2.22 | 0.47 |
| 1:0:213:LYS:HG2 | 1:0:272:ASP:HA | 1.96 | 0.46 |
| 5:H:320:GLU:O | 5:H:323:LEU:HD12 | 2.14 | 0.46 |
| 8:N:380:THR:CG2 | 8:N:411:PHE:CD2 | 2.97 | 0.46 |
| 8:P:166:ASN:HA | 8:P:174:VAL:N | 2.30 | 0.46 |
| 2:Z:139:GLN:HB3 | 2:Z:613:CYS:HB3 | 1.97 | 0.46 |
| 16:c:400:GLU:HG3 | 16:c:425:TYR:CE1 | 2.50 | 0.46 |
| 18:e:107:SER:HA | 18:e:135:ARG:HE | 1.80 | 0.46 |
| 2:1:123:TYR:CE1 | 2:1:456:THR:CB | 2.98 | 0.46 |
| 2:1:514:ARG:HD3 | 2:1:514:ARG:HA | 1.48 | 0.46 |
| 9:Q:209:ARG:HD3 | 11:V:351:THR:H | 1.80 | 0.46 |
| 9:T:414:LEU:HD22 | 9:T:437:TRP:CZ3 | 2.50 | 0.46 |
| 1:Y:853:PHE:HB3 | 1:Y:897:ILE:HG23 | 1.97 | 0.46 |
| 19:f:27:ASN:C | 19:f:27:ASN:ND2 | 2.73 | 0.46 |
| 1:0:417:TYR:HA | 1:0:441:VAL:HB | 1.98 | 0.46 |
| 1:0:1387:ILE:CG1 | 1:0:1426:MET:HE1 | 2.45 | 0.46 |
| 5:B:459:LEU:HD21 | 6:C:394:ILE:HG23 | 1.96 | 0.46 |
| 8:P:357:ASP:OD1 | 8:P:357:ASP:N | 2.49 | 0.46 |
| 9:R:599:ARG:H | 9:R:599:ARG:HE | 1.64 | 0.46 |
| 9:T:595:ARG:HH12 | 9:T:691:ARG:HG3 | 1.80 | 0.46 |
| 11:V:378:ARG:HA | 11:V:378:ARG:HE | 1.81 | 0.46 |
| 1:Y:790:PHE:HA | 1:Y:831:LYS:HD3 | 1.96 | 0.46 |
| 7:M:121:VAL:HG11 | 7:M:196:ILE:HA | 1.97 | 0.46 |
| 7:O:1321:PRO:CG | 7:O:1324:ARG:HB3 | 2.43 | 0.46 |
| 8:P:40:ILE:HB | 8:P:41:ARG:H | 1.46 | 0.46 |
| 8:P:400:PHE:CD2 | 8:P:596:LYS:HE2 | 2.28 | 0.46 |
| 9:R:599:ARG:HE | 2:Z:880:SER:HB2 | 1.79 | 0.46 |
| 2:Z:436:GLY:HA3 | 2:Z:443:ILE:HD11 | 1.97 | 0.46 |
| 15:b:672:TYR:HA | 15:b:731:LEU:HD21 | 1.96 | 0.46 |
| 1:0:401:ILE:CB | 1:0:462:LEU:CB | 2.75 | 0.46 |
| 7:M:602:ASN:N | 7:M:606:VAL:HG23 | 2.30 | 0.46 |
| 8:N:322:HIS:ND1 | 8:N:359:LEU:HA | 2.31 | 0.46 |
| 8:P:994:ILE:HD12 | 8:P:995:LEU:H | 1.81 | 0.46 |
| 9:R:541:TYR:CE1 | 9:R:556:TYR:CD2 | 3.03 | 0.46 |
| 18:l:244:LYS:HB2 | 18:l:297:LEU:HD11 | 1.97 | 0.46 |
| 20:n:228:ILE:HD12 | 20:n:295:TRP:HZ3 | 1.81 | 0.46 |
| 20:g:824:ASN:CG | 20:g:872:ILE:HG23 | 2.41 | 0.46 |
| 6:I:451:MET:HE1 | 9:S:65:ASP:O | 2.15 | 0.46 |
| 8:P:1595:LYS:HD3 | 8:P:1595:LYS:H | 1.80 | 0.46 |
| 9:R:439:HIS:CD2 | 9:R:465:ILE:HB | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:1156:LEU:HD13 | 2:Z:1156:LEU:HA | 1.78 | 0.46 |
| 14:h:342:LEU:HD13 | 14:h:379:ILE:CD1 | 2.45 | 0.46 |
| 20:g:947:ILE:HG22 | 20:g:948:GLN:HE21 | 1.80 | 0.46 |
| 4:A:702:ARG:NE | 4:A:702:ARG:HA | 2.30 | 0.46 |
| 7:M:788:LEU:HD21 | 7:M:874:LYS:HB2 | 1.98 | 0.46 |
| 7:M:1037:ASN:HD22 | 7:M:1037:ASN:C | 2.09 | 0.46 |
| 7:O:1188:THR:HG22 | 7:O:1189:MET:N | 2.31 | 0.46 |
| 8:P:878:PHE:CG | 8:P:879:ILE:N | 2.82 | 0.46 |
| 9:S:260:LEU:HB3 | 9:S:513:LEU:CD1 | 2.45 | 0.46 |
| 9:S:439:HIS:CD2 | 9:S:465:ILE:HG21 | 2.51 | 0.46 |
| 2:Z:887:VAL:O | 2:Z:887:VAL:HG12 | 2.16 | 0.46 |
| 14:h:674:LEU:HD21 | 14:h:728:ILE:HG21 | 1.98 | 0.46 |
| 19:m:8:GLN:HB3 | 19:m:11:ARG:NE | 2.30 | 0.46 |
| 15:b:682:LEU:HD13 | 14:a:1031:ARG:CZ | 2.46 | 0.46 |
| 14:a:811:LEU:HG | 14:a:815:PHE:CE2 | 2.51 | 0.46 |
| 1:0:130:GLY:HA2 | 1:0:511:LYS:HG2 | 1.96 | 0.46 |
| 2:1:960:GLN:H | 2:1:961:PRO:HD2 | 1.81 | 0.46 |
| 8:N:189:LEU:HD21 | 8:N:840:LEU:HD12 | 1.97 | 0.46 |
| 7:O:183:ARG:HD2 | 7:O:360:LEU:HD12 | 1.98 | 0.46 |
| 8:P:719:ILE:CD1 | 8:P:793:LEU:O | 2.51 | 0.46 |
| 15:i:461:MET:SD | 18:l:335:TYR:HB2 | 2.55 | 0.46 |
| 7:M:940:ASN:HA | 7:M:943:ARG:HE | 1.81 | 0.46 |
| 7:M:1189:MET:HG3 | 8:N:166:ASN:HB3 | 1.96 | 0.46 |
| 7:O:1336:ILE:HG23 | 7:O:1384:LEU:HD22 | 1.96 | 0.46 |
| 8:P:160:LEU:HD22 | 8:P:165:ASN:HD21 | 1.81 | 0.46 |
| 8:P:476:ASP:O | 8:P:553:ILE:CG2 | 2.64 | 0.46 |
| 9:Q:820:ILE:HG22 | 9:Q:820:ILE:O | 2.16 | 0.46 |
| 9:S:268:ILE:HD11 | 9:S:514:LYS:CA | 2.45 | 0.46 |
| 2:1:1274:LYS:HB3 | 9:S:819:MET:HB2 | 1.97 | 0.46 |
| 7:M:467:LEU:HD12 | 7:M:603:GLU:HB3 | 1.98 | 0.46 |
| 8:N:380:THR:CG2 | 8:N:411:PHE:HB3 | 2.44 | 0.46 |
| 8:P:380:THR:HG23 | 8:P:396:THR:CG2 | 2.46 | 0.46 |
| 8:P:719:ILE:CG1 | 8:P:794:ILE:CG1 | 2.94 | 0.46 |
| 9:Q:282:PHE:HA | 9:Q:285:TYR:HB3 | 1.98 | 0.46 |
| 11:X:282:ASN:OD1 | 11:X:299:GLN:CG | 2.64 | 0.46 |
| 1:Y:402:ILE:HG21 | 1:Y:413:LEU:HD11 | 1.98 | 0.46 |
| 19:m:29:GLU:OE2 | 19:m:29:GLU:HA | 2.14 | 0.46 |
| 14:a:2:ALA:HA | 14:a:379:ILE:HA | 1.99 | 0.46 |
| 1:0:402:ILE:CD1 | 1:0:467:PHE:HE1 | 2.28 | 0.45 |
| 2:1:249:THR:OG1 | 2:1:251:LEU:HD12 | 2.15 | 0.45 |
| 2:1:612:TYR:HB3 | 2:1:614:TYR:CE2 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:P:1304:LYS:HE3 | 8:P:1304:LYS:CA | 2.18 | 0.45 |
| 9:S:584:LYS:N | 11:X:302:ARG:HD2 | 2.15 | 0.45 |
| 16:j:303:VAL:HG11 | 19:m:242:LEU:HD21 | 1.98 | 0.45 |
| 21:r:60:ILE:HD13 | 21:r:87:LEU:HD23 | 1.98 | 0.45 |
| 19:f:126:LEU:CD2 | 19:f:190:ALA:HA | 2.45 | 0.45 |
| 14:a:959:GLU:OE1 | 14:a:959:GLU:HA | 2.16 | 0.45 |
| 2:1:266:TYR:CE1 | 2:1:268:ARG:HB2 | 2.51 | 0.45 |
| 7:M:916:ILE:HD12 | 7:M:948:LEU:HD11 | 1.98 | 0.45 |
| 7:M:1223:LEU:HD23 | 7:M:1223:LEU:HA | 1.89 | 0.45 |
| 8:P:42:GLN:HE21 | 8:P:42:GLN:HB3 | 1.54 | 0.45 |
| 8:P:400:PHE:CE2 | 8:P:596:LYS:CE | 2.98 | 0.45 |
| 9:R:807:LYS:HA | 9:R:810:ALA:HB3 | 1.98 | 0.45 |
| 9:S:417:ARG:HH21 | 9:S:423:LYS:HE3 | 1.81 | 0.45 |
| 14:h:1027:LEU:HD22 | 14:h:1030:LEU:HD12 | 1.97 | 0.45 |
| 15:i:78:ASN:HD21 | 15:i:95:ILE:CG1 | 2.29 | 0.45 |
| 20:n:400:PHE:CD2 | 20:n:459:GLY:HA2 | 2.51 | 0.45 |
| 20:g:707:PRO:HB2 | 20:g:709:PHE:CE2 | 2.51 | 0.45 |
| 14:a:68:ILE:HG12 | 14:a:138:LEU:HD13 | 1.98 | 0.45 |
| 2:1:274:PHE:CD2 | 2:1:284:TRP:HB2 | 2.51 | 0.45 |
| 4:D:665:TRP:CD2 | 6:F:305:ILE:HD11 | 2.51 | 0.45 |
| 8:N:464:ALA:HA | 8:N:562:TRP:CZ3 | 2.52 | 0.45 |
| 8:N:522:LYS:H | 8:N:522:LYS:HD3 | 1.81 | 0.45 |
| 7:O:428:GLN:O | 7:O:432:LEU:HG | 2.16 | 0.45 |
| 8:P:1211:ILE:HG23 | 8:P:1226:PHE:CE2 | 2.51 | 0.45 |
| 9:R:776:ILE:HG12 | 9:R:824:MET:HE3 | 1.97 | 0.45 |
| 11:X:302:ARG:HH11 | 11:X:302:ARG:HG2 | 1.80 | 0.45 |
| 12:u:351:ILE:HG23 | 13:w:1453:PHE:CE2 | 2.52 | 0.45 |
| 1:0:281:ARG:HH12 | 1:0:385:LYS:CD | 2.29 | 0.45 |
| 5:E:468:GLU:HB3 | 7:M:1224:GLU:HA | 1.97 | 0.45 |
| 5:H:309:ARG:HB3 | 5:H:330:VAL:HG23 | 1.98 | 0.45 |
| 6:I:356:GLN:HE21 | 6:L:292:HIS:HD2 | 1.65 | 0.45 |
| 2:Z:233:LEU:HD22 | 2:Z:248:ASN:HA | 1.98 | 0.45 |
| 19:f:211:ILE:HG22 | 19:f:267:LEU:HD13 | 1.99 | 0.45 |
| 4:A:711:LEU:HD13 | 5:B:411:ARG:HB2 | 1.97 | 0.45 |
| 7:M:1439:GLU:HA | 7:M:1442:TRP:CZ2 | 2.52 | 0.45 |
| 9:S:764:ASP:H | 9:S:767:ILE:HG13 | 1.81 | 0.45 |
| 16:j:142:ARG:HE | 17:k:57:TRP:CG | 2.34 | 0.45 |
| 1:0:790:PHE:O | 1:0:944:LEU:C | 2.58 | 0.45 |
| 5:B:415:LEU:O | 5:B:419:LEU:HD12 | 2.16 | 0.45 |
| 7:O:620:THR:HG21 | 7:O:660:LEU:HD21 | 1.98 | 0.45 |
| 7:O:1499:LEU:HD23 | 7:O:1499:LEU:H | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:P:275:LEU:HD23 | 8:P:276:ASN:H | 1.81 | 0.45 |
| 10:U:304:LYS:CE | 11:V:271:ILE:CG1 | 2.95 | 0.45 |
| 1:Y:394:GLU:H | 1:Y:394:GLU:HG3 | 1.62 | 0.45 |
| 1:Y:887:GLN:HA | 1:Y:887:GLN:NE2 | 2.30 | 0.45 |
| 12:v:197:LEU:HD11 | 12:v:299:ALA:HB3 | 1.99 | 0.45 |
| 20:g:647:LYS:NZ | 20:g:651:ASN:HD21 | 2.15 | 0.45 |
| 14:a:719:PHE:CD2 | 14:a:746:CYS:CB | 3.00 | 0.45 |
| 14:a:719:PHE:CE1 | 14:a:721:MET:HE3 | 2.52 | 0.45 |
| 7:M:324:ILE:CG2 | 7:M:355:LEU:H | 2.30 | 0.45 |
| 16:c:183:PHE:HD1 | 16:c:183:PHE:H | 1.65 | 0.45 |
| 14:a:399:THR:HA | 14:a:669:ARG:CD | 2.47 | 0.45 |
| 1:0:412:ILE:CG2 | 1:0:442:GLY:O | 2.54 | 0.45 |
| 6:C:292:HIS:HA | 6:C:295:LYS:HZ2 | 1.82 | 0.45 |
| 5:H:320:GLU:O | 5:H:348:ILE:HG12 | 2.16 | 0.45 |
| 2:Z:1298:ASP:C | 2:Z:1300:SER:N | 2.75 | 0.45 |
| 12:v:387:MET:HA | 12:v:390:ALA:HB3 | 1.98 | 0.45 |
| 14:h:666:ASN:HD22 | 14:h:742:GLU:HB3 | 1.81 | 0.45 |
| 20:g:690:ARG:HA | 20:g:690:ARG:NE | 2.32 | 0.45 |
| 2:1:998:TYR:HA | 2:1:1001:ARG:HB2 | 1.99 | 0.45 |
| 4:A:700:ILE:HG22 | 4:D:642:THR:HG21 | 1.99 | 0.45 |
| 5:H:315:LYS:HA | 5:H:347:THR:HA | 1.98 | 0.45 |
| 8:N:81:ILE:HD13 | 8:N:87:PRO:HD2 | 1.98 | 0.45 |
| 7:O:561:CYS:CB | 7:O:612:LEU:HD11 | 2.47 | 0.45 |
| 7:O:1501:SER:H | 7:O:1517:ALA:HB2 | 1.82 | 0.45 |
| 8:P:360:GLN:NE2 | 8:P:655:VAL:HG21 | 2.32 | 0.45 |
| 8:P:477:LEU:O | 8:P:553:ILE:HG23 | 2.16 | 0.45 |
| 9:R:274:GLY:CA | 9:R:484:LEU:HD22 | 2.47 | 0.45 |
| 20:n:450:ARG:HB2 | 20:n:453:ILE:HD11 | 1.97 | 0.45 |
| 1:0:692:SER:HA | 1:0:696:ARG:HD3 | 1.99 | 0.45 |
| 2:1:860:LYS:CE | 2:1:891:ARG:HG3 | 2.43 | 0.45 |
| 6:I:355:GLN:O | 6:L:292:HIS:CE1 | 2.70 | 0.45 |
| 9:S:554:VAL:O | 9:S:558:VAL:HG23 | 2.16 | 0.45 |
| 9:S:682:GLU:OE2 | 10:W:322:LEU:HD23 | 2.16 | 0.45 |
| 1:Y:174:GLY:O | 1:Y:183:TRP:CE3 | 2.70 | 0.45 |
| 2:Z:807:ASP:CB | 2:Z:887:VAL:HG13 | 2.47 | 0.45 |
| 19:f:50:ALA:HB1 | 19:f:69:GLU:HB2 | 1.98 | 0.45 |
| 20:g:510:ASN:HB2 | 20:g:511:PRO:HD3 | 1.98 | 0.45 |
| 20:g:1095:ILE:HA | 20:g:1098:THR:HG22 | 1.99 | 0.45 |
| 14:a:228:LEU:HD12 | 14:a:233:TYR:O | 2.16 | 0.45 |
| 2:1:1210:ALA:O | 2:1:1214:ASP:HA | 2.17 | 0.44 |
| 8:N:1305:ASN:OD1 | 8:N:1308:TYR:HB2 | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:Q:277:TYR:C | 9:Q:277:TYR:CD1 | 2.95 | 0.44 |
| 1:Y:276:HIS:CE1 | 1:Y:278:ARG:HB2 | 2.51 | 0.44 |
| 2:Z:1258:GLN:NE2 | 2:Z:1299:LYS:HB2 | 2.31 | 0.44 |
| 19:m:248:TYR:CD2 | 19:m:317:LEU:HD23 | 2.52 | 0.44 |
| 15:b:732:ARG:HE | 17:d:90:SER:HB3 | 1.82 | 0.44 |
| 16:c:637:LEU:HD12 | 16:c:640:GLY:HA3 | 1.98 | 0.44 |
| 20:g:95:GLY:HA3 | 20:g:461:ASP:HA | 1.98 | 0.44 |
| 4:A:676:ILE:HD12 | 5:B:376:LEU:HA | 1.99 | 0.44 |
| 7:O:1454:VAL:HG22 | 7:O:1520:ALA:HB3 | 1.99 | 0.44 |
| 8:P:161:ALA:H | 8:P:165:ASN:HD22 | 1.65 | 0.44 |
| 8:P:1524:TYR:CD2 | 8:P:1525:PHE:CE1 | 3.05 | 0.44 |
| 2:Z:491:THR:O | 2:Z:514:ARG:HB2 | 2.18 | 0.44 |
| 20:n:940:ASP:H | 20:n:941:ILE:HG12 | 1.81 | 0.44 |
| 1:0:399:SER:HA | 1:0:402:ILE:HG12 | 2.00 | 0.44 |
| 2:1:548:LEU:C | 2:1:548:LEU:HD12 | 2.43 | 0.44 |
| 6:C:337:LYS:O | 6:C:340:ILE:HG22 | 2.18 | 0.44 |
| 7:M:1221:LEU:HD23 | 7:M:1221:LEU:C | 2.41 | 0.44 |
| 7:O:1482:THR:HB | 7:O:1486:LEU:HD23 | 1.99 | 0.44 |
| 8:P:777:ASP:CB | 8:P:793:LEU:HB2 | 2.45 | 0.44 |
| 18:e:337:ASN:O | 18:e:338:GLU:HB3 | 2.16 | 0.44 |
| 19:f:242:LEU:HB2 | 19:f:312:GLU:HA | 1.99 | 0.44 |
| 14:a:720:PHE:HD1 | 14:a:720:PHE:HA | 1.68 | 0.44 |
| 2:1:491:THR:HB | 2:1:513:LYS:HB2 | 2.00 | 0.44 |
| 5:E:356:GLU:H | 5:E:356:GLU:CD | 2.26 | 0.44 |
| 5:E:466:LEU:HD11 | 6:F:398:VAL:HG13 | 1.99 | 0.44 |
| 5:H:513:LEU:HD12 | 5:H:514:THR:HG23 | 2.00 | 0.44 |
| 7:M:336:LYS:H | 7:M:336:LYS:CE | 2.30 | 0.44 |
| 7:M:419:THR:HG23 | 7:M:771:ARG:H | 1.82 | 0.44 |
| 7:M:602:ASN:CA | 7:M:606:VAL:CG2 | 2.96 | 0.44 |
| 7:M:1464:ILE:HB | 7:M:1532:ARG:HG2 | 2.00 | 0.44 |
| 9:S:637:ILE:O | 9:S:637:ILE:HG22 | 2.17 | 0.44 |
| 10:U:279:ASP:OD1 | 10:U:307:ILE:HG13 | 2.17 | 0.44 |
| 15:i:508:LEU:HB3 | 18:l:119:ALA:H | 1.83 | 0.44 |
| 18:l:242:ILE:O | 18:l:297:LEU:HD12 | 2.17 | 0.44 |
| 20:n:110:ILE:H | 20:n:110:ILE:HD12 | 1.83 | 0.44 |
| 5:E:322:ILE:H | 5:E:322:ILE:CD1 | 2.21 | 0.44 |
| 8:P:795:ILE:HB | 8:P:868:LEU:HB3 | 2.00 | 0.44 |
| 8:P:885:VAL:CG2 | 8:P:922:PHE:H | 2.29 | 0.44 |
| 8:P:1227:VAL:CB | 8:P:1277:ILE:HD13 | 2.45 | 0.44 |
| 9:S:688:LEU:HD13 | 10:W:322:LEU:CD1 | 2.47 | 0.44 |
| 1:Y:202:GLN:HG2 | 1:Y:254:LEU:H | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Z:1316:VAL:HB | 2:Z:1321:LEU:HD11 | 1.99 | 0.44 |
| 12:u:422:ARG:HE | 12:u:439:LEU:CD1 | 2.30 | 0.44 |
| 14:a:719:PHE:CD2 | 14:a:746:CYS:HB2 | 2.53 | 0.44 |
| 1:0:688:LYS:HG3 | 1:0:690:ASN:H | 1.83 | 0.44 |
| 2:1:1041:LYS:HA | 2:1:1041:LYS:HD3 | 1.57 | 0.44 |
| 4:A:769:ILE:HD11 | 6:C:394:ILE:HG23 | 2.00 | 0.44 |
| 4:G:670:VAL:HG11 | 5:H:315:LYS:HD2 | 1.99 | 0.44 |
| 8:N:1056:LYS:H | 8:N:1056:LYS:CD | 2.08 | 0.44 |
| 8:P:174:VAL:CG1 | 8:P:177:VAL:HB | 2.40 | 0.44 |
| 1:Y:411:PRO:HG2 | 1:Y:512:LYS:C | 2.41 | 0.44 |
| 12:u:302:ILE:O | 12:u:302:ILE:HG13 | 2.18 | 0.44 |
| 12:v:114:TYR:CE1 | 12:v:144:VAL:HG11 | 2.52 | 0.44 |
| 20:n:998:ASN:HD22 | 20:n:1101:ARG:HG3 | 1.82 | 0.44 |
| 1:0:1379:GLN:HB2 | 1:0:1421:VAL:HG11 | 2.00 | 0.44 |
| 5:B:401:ALA:HB1 | 6:C:336:PHE:CZ | 2.52 | 0.44 |
| 8:N:379:ILE:HG22 | 8:N:400:PHE:CE1 | 2.52 | 0.44 |
| 8:P:75:ILE:CD1 | 8:P:85:ASN:O | 2.60 | 0.44 |
| 8:P:260:ARG:HD2 | 8:P:260:ARG:HA | 1.92 | 0.44 |
| 8:P:333:ARG:HH12 | 8:P:347:THR:CG2 | 2.31 | 0.44 |
| 2:Z:1039:LEU:HB3 | 2:Z:1040:LYS:H | 1.45 | 0.44 |
| 14:a:84:LEU:HD11 | 14:a:481:HIS:CE1 | 2.52 | 0.44 |
| 1:0:409:ALA:CB | 1:0:512:LYS:HG2 | 2.47 | 0.44 |
| 2:1:513:LYS:HD3 | 2:1:539:TYR:CE2 | 2.44 | 0.44 |
| 9:S:253:LEU:O | 9:S:257:TRP:CD1 | 2.71 | 0.44 |
| 2:Z:1130:ARG:HD2 | 2:Z:1199:VAL:HG12 | 2.00 | 0.44 |
| 20:n:230:PHE:CD1 | 20:n:297:LEU:HD21 | 2.53 | 0.44 |
| 20:n:1095:ILE:HA | 20:n:1098:THR:HG22 | 2.00 | 0.44 |
| 1:0:417:TYR:O | 1:0:440:THR:HB | 2.18 | 0.44 |
| 7:O:724:ASN:HB3 | 7:O:1272:LEU:CD1 | 2.47 | 0.44 |
| 9:R:638:TYR:CG | 9:R:639:ASP:N | 2.85 | 0.44 |
| 19:m:511:ILE:HG23 | 19:m:549:PHE:CD1 | 2.52 | 0.44 |
| 16:c:276:ILE:HD12 | 16:c:280:ILE:HD11 | 2.00 | 0.44 |
| 18:e:191:ALA:HB3 | 18:e:211:HIS:CE1 | 2.53 | 0.44 |
| 5:E:352:ILE:HG23 | 5:E:358:LEU:HD11 | 2.00 | 0.43 |
| 7:M:1034:LEU:C | 7:M:1034:LEU:CD2 | 2.88 | 0.43 |
| 8:N:733:ARG:HH12 | 8:N:796:SER:N | 2.15 | 0.43 |
| 8:P:53:GLU:HA | 8:P:133:ASP:OD2 | 2.17 | 0.43 |
| 8:P:75:ILE:HD11 | 8:P:82:ASN:C | 2.36 | 0.43 |
| 9:S:268:ILE:HD11 | 9:S:514:LYS:CB | 2.47 | 0.43 |
| 9:S:514:LYS:HA | 9:S:514:LYS:NZ | 2.33 | 0.43 |
| 9:T:232:PHE:CD1 | 9:T:232:PHE:N | 2.86 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:e:334:THR:HG22 | 18:e:336:SER:H | 1.83 | 0.43 |
| 19:f:105:PHE:HB2 | 19:f:302:LEU:HD21 | 2.00 | 0.43 |
| 20:g:1099:TYR:CD1 | 20:g:1104:ILE:HD11 | 2.53 | 0.43 |
| 1:0:401:ILE:HG12 | 1:0:462:LEU:HD23 | 1.74 | 0.43 |
| 5:E:326:LYS:CG | 5:E:335:TRP:CZ3 | 3.00 | 0.43 |
| 8:P:462:SER:O | 8:P:463:PHE:CD1 | 2.70 | 0.43 |
| 8:P:777:ASP:O | 8:P:793:LEU:HB2 | 2.18 | 0.43 |
| 8:P:1078:ILE:HG23 | 8:P:1119:ASN:HD22 | 1.83 | 0.43 |
| 9:R:408:ARG:C | 9:R:408:ARG:HD3 | 2.43 | 0.43 |
| 1:Y:789:VAL:O | 1:Y:789:VAL:HG12 | 2.17 | 0.43 |
| 2:Z:642:SER:CB | 2:Z:714:LEU:HD23 | 2.48 | 0.43 |
| 2:Z:1048:MET:HA | 2:Z:1048:MET:HE2 | 1.99 | 0.43 |
| 17:k:238:ASN:HD22 | 17:k:241:GLY:H | 1.64 | 0.43 |
| 5:E:519:GLY:O | 5:E:523:LEU:HB2 | 2.19 | 0.43 |
| 5:K:323:LEU:N | 5:K:323:LEU:CD2 | 2.80 | 0.43 |
| 7:M:778:LEU:HB3 | 7:M:779:PRO:HD3 | 1.99 | 0.43 |
| 8:N:943:VAL:HG12 | 8:N:945:ASP:H | 1.83 | 0.43 |
| 7:O:298:ASP:O | 7:O:299:THR:HB | 2.18 | 0.43 |
| 9:Q:755:LYS:HA | 9:Q:758:GLN:HE22 | 1.83 | 0.43 |
| 9:R:542:THR:HG22 | 9:R:556:TYR:HB3 | 2.00 | 0.43 |
| 1:Y:148:PHE:CZ | 1:Y:652:TYR:HA | 2.54 | 0.43 |
| 1:Y:1313:VAL:H | 1:Y:1314:PRO:CD | 2.32 | 0.43 |
| 2:Z:811:LEU:HD13 | 2:Z:867:LEU:HD23 | 2.00 | 0.43 |
| 20:n:577:TYR:O | 20:n:578:LYS:CB | 2.66 | 0.43 |
| 18:e:191:ALA:HB3 | 18:e:211:HIS:HE1 | 1.83 | 0.43 |
| 19:f:578:ASP:HA | 19:f:581:LEU:HG | 1.99 | 0.43 |
| 1:0:158:ASP:O | 1:0:162:HIS:CG | 2.71 | 0.43 |
| 1:0:408:ARG:O | 1:0:512:LYS:CG | 2.67 | 0.43 |
| 7:M:1027:GLN:H | 7:M:1036:PRO:HD3 | 1.83 | 0.43 |
| 9:R:590:LEU:HD12 | 9:R:591:GLY:H | 1.83 | 0.43 |
| 1:Y:1009:HIS:HA | 1:Y:1012:ARG:HE | 1.83 | 0.43 |
| 2:Z:384:ILE:HG12 | 2:Z:434:PHE:CZ | 2.53 | 0.43 |
| 2:Z:927:HIS:CG | 2:Z:928:LEU:N | 2.86 | 0.43 |
| 12:v:278:LEU:HD23 | 12:v:337:TRP:HA | 2.01 | 0.43 |
| 19:m:33:ILE:HD12 | 19:m:34:ASP:H | 1.84 | 0.43 |
| 19:f:7:TYR:O | 19:f:7:TYR:CG | 2.70 | 0.43 |
| 1:0:395:PRO:HG2 | 1:0:419:LYS:HG3 | 2.00 | 0.43 |
| 2:1:117:TYR:CD1 | 2:1:120:GLY:O | 2.72 | 0.43 |
| 5:B:296:LYS:HD2 | 6:C:279:GLN:HE22 | 1.83 | 0.43 |
| 4:J:727:SER:O | 7:O:746:LYS:CE | 2.66 | 0.43 |
| 4:J:800:HIS:CD2 | 5:K:516:GLN:HG3 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:N:1249:GLN:CD | 8:N:1249:GLN:H | 2.26 | 0.43 |
| 7:O:174:LEU:HD22 | 7:O:174:LEU:H | 1.83 | 0.43 |
| 7:O:1318:LYS:HB2 | 7:O:1321:PRO:HG3 | 1.99 | 0.43 |
| 8:P:1053:LEU:HD22 | 8:P:1127:ASN:N | 2.34 | 0.43 |
| 9:S:682:GLU:OE2 | 10:W:322:LEU:HD21 | 2.18 | 0.43 |
| 9:S:754:ARG:CG | 9:S:754:ARG:HH11 | 2.30 | 0.43 |
| 11:X:357:LYS:O | 11:X:357:LYS:HG3 | 2.18 | 0.43 |
| 1:Y:434:LEU:HD13 | 1:Y:447:TYR:HB3 | 2.00 | 0.43 |
| 1:Y:1084:VAL:HG23 | 1:Y:1085:ALA:N | 2.34 | 0.43 |
| 2:Z:807:ASP:CG | 2:Z:887:VAL:HG13 | 2.43 | 0.43 |
| 15:b:69:PHE:CE1 | 18:e:328:VAL:HG11 | 2.53 | 0.43 |
| 1:0:129:SER:HG | 1:0:406:THR:N | 2.13 | 0.43 |
| 7:M:1250:LYS:HB2 | 7:M:1275:ALA:HB1 | 2.00 | 0.43 |
| 8:N:1412:LEU:HD13 | 8:N:1418:LEU:HD11 | 2.00 | 0.43 |
| 7:O:861:GLN:OE1 | 7:O:861:GLN:HA | 2.18 | 0.43 |
| 7:O:868:ALA:HA | 7:O:871:ILE:HD12 | 2.01 | 0.43 |
| 8:P:379:ILE:CG2 | 8:P:403:ILE:HB | 2.48 | 0.43 |
| 9:Q:314:LYS:HG3 | 9:Q:316:ALA:H | 1.84 | 0.43 |
| 9:Q:514:LYS:HA | 9:Q:514:LYS:HD2 | 1.41 | 0.43 |
| 9:R:417:ARG:H | 9:R:420:LEU:HD21 | 1.83 | 0.43 |
| 9:S:747:PHE:CZ | 9:S:753:ALA:HA | 2.54 | 0.43 |
| 1:Y:410:ALA:HB3 | 1:Y:413:LEU:HD23 | 2.01 | 0.43 |
| 1:Y:832:VAL:HG11 | 1:Y:910:LEU:HD11 | 2.00 | 0.43 |
| 1:Y:1002:LEU:HD13 | 1:Y:1005:ARG:HB2 | 2.00 | 0.43 |
| 2:Z:120:GLY:HA3 | 2:Z:453:PHE:H | 1.82 | 0.43 |
| 12:u:209:TYR:CE2 | 12:u:335:MET:HG3 | 2.54 | 0.43 |
| 15:i:122:ARG:HD3 | 15:i:493:ALA:H | 1.83 | 0.43 |
| 20:n:699:MET:HA | 20:n:699:MET:CE | 2.48 | 0.43 |
| 15:b:486:ILE:HD12 | 15:b:503:VAL:HG21 | 2.00 | 0.43 |
| 1:0:108:ILE:HD13 | 1:0:777:ILE:HG21 | 2.00 | 0.43 |
| 4:D:658:TYR:CD2 | 6:F:294:LEU:HD11 | 2.53 | 0.43 |
| 5:E:298:SER:H | 6:F:280:LEU:HD21 | 1.84 | 0.43 |
| 7:M:482:PHE:CZ | 7:M:514:CYS:SG | 3.11 | 0.43 |
| 8:N:1278:ILE:HG22 | 8:N:1282:ASN:CG | 2.44 | 0.43 |
| 9:R:514:LYS:HD3 | 9:R:515:LEU:H | 1.84 | 0.43 |
| 11:X:352:GLY:HA3 | 11:X:355:TRP:HB3 | 2.01 | 0.43 |
| 2:Z:514:ARG:HG3 | 2:Z:514:ARG:HH11 | 1.84 | 0.43 |
| 1:0:375:SER:CB | 1:0:420:ILE:CD1 | 2.89 | 0.43 |
| 1:0:395:PRO:HB3 | 1:0:418:LEU:HB3 | 2.01 | 0.43 |
| 1:0:787:ARG:HG2 | 1:0:833:SER:O | 2.18 | 0.43 |
| 2:1:264:ILE:HG21 | 2:1:347:VAL:H | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:1:491:THR:O | 2:1:513:LYS:HB3 | 2.19 | 0.43 |
| 2:1:891:ARG:HA | 2:1:891:ARG:HD3 | 1.43 | 0.43 |
| 2:1:1178:ARG:H | 2:1:1178:ARG:HD3 | 1.83 | 0.43 |
| 7:O:1043:SER:HB3 | 7:O:1047:SER:N | 2.34 | 0.43 |
| 9:Q:209:ARG:CD | 11:V:351:THR:H | 2.31 | 0.43 |
| 9:R:820:ILE:O | 9:R:820:ILE:HG22 | 2.19 | 0.43 |
| 9:S:755:LYS:HD2 | 9:S:755:LYS:HA | 1.45 | 0.43 |
| 10:W:255:ILE:H | 10:W:255:ILE:HD12 | 1.84 | 0.43 |
| 2:Z:1298:ASP:C | 2:Z:1300:SER:H | 2.25 | 0.43 |
| 15:i:306:TRP:CZ3 | 15:i:310:VAL:HG21 | 2.53 | 0.43 |
| 19:m:480:THR:CG2 | 20:n:979:SER:HB3 | 2.42 | 0.43 |
| 16:c:647:GLN:CD | 16:c:647:GLN:H | 2.27 | 0.43 |
| 2:1:351:ARG:HH22 | 2:1:446:LEU:HD13 | 1.84 | 0.43 |
| 5:B:380:LEU:O | 5:B:384:THR:HG23 | 2.19 | 0.43 |
| 7:M:1032:ILE:HD12 | 7:M:1033:SER:H | 1.83 | 0.43 |
| 7:O:1339:ILE:HG23 | 7:O:1384:LEU:HD13 | 2.01 | 0.43 |
| 10:W:305:TYR:N | 10:W:306:PRO:HD3 | 2.30 | 0.43 |
| 1:Y:243:PHE:CE2 | 1:Y:258:ASN:HA | 2.54 | 0.43 |
| 12:u:577:LEU:CB | 4:y:687:GLU:HA | 2.48 | 0.43 |
| 14:h:983:GLN:NE2 | 14:h:1003:VAL:HG11 | 2.34 | 0.43 |
| 19:f:665:MET:HE1 | 19:f:714:TYR:HB2 | 2.00 | 0.43 |
| 20:g:819:GLN:HB3 | 20:g:824:ASN:HB3 | 2.01 | 0.43 |
| 1:0:111:LEU:HD23 | 1:0:774:ALA:HB1 | 2.01 | 0.43 |
| 8:P:75:ILE:HG13 | 8:P:83:VAL:CG1 | 2.45 | 0.43 |
| 8:P:379:ILE:CG2 | 8:P:403:ILE:CB | 2.97 | 0.43 |
| 8:P:1303:LEU:N | 8:P:1353:SER:HB3 | 2.33 | 0.43 |
| 19:m:27:ASN:CB | 19:m:398:ILE:HD11 | 2.46 | 0.43 |
| 19:f:96:LEU:HG | 19:f:97:HIS:CD2 | 2.54 | 0.43 |
| 2:1:491:THR:C | 2:1:513:LYS:HA | 2.44 | 0.42 |
| 8:N:1167:LEU:HD12 | 8:N:1183:PHE:HB2 | 2.01 | 0.42 |
| 7:O:1036:PRO:HD2 | 7:O:1038:LEU:HD12 | 2.01 | 0.42 |
| 7:O:1178:LEU:HD21 | 7:O:1319:LEU:HB3 | 2.01 | 0.42 |
| 14:h:359:THR:HA | 14:h:455:THR:HG21 | 2.01 | 0.42 |
| 14:h:497:MET:SD | 14:h:511:ARG:HA | 2.57 | 0.42 |
| 15:i:75:SER:HB3 | 15:i:95:ILE:HD12 | 2.01 | 0.42 |
| 19:m:558:ILE:HG22 | 19:m:558:ILE:O | 2.19 | 0.42 |
| 21:r:53:TYR:HB2 | 21:r:57:TRP:HE1 | 1.84 | 0.42 |
| 19:f:576:ASN:HD22 | 19:f:576:ASN:HA | 1.54 | 0.42 |
| 1:0:408:ARG:C | 1:0:512:LYS:CE | 2.92 | 0.42 |
| 8:N:195:LEU:HD13 | 8:N:269:THR:HG22 | 2.01 | 0.42 |
| 8:N:322:HIS:ND1 | 8:N:359:LEU:CA | 2.82 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:723:GLU:HB3 | 7:O:1272:LEU:HD21 | 2.01 | 0.42 |
| 8:P:1276:LYS:N | 8:P:1321:LEU:HD21 | 2.33 | 0.42 |
| 16:j:572:ILE:HD12 | 16:j:572:ILE:HA | 1.92 | 0.42 |
| 19:m:480:THR:OG1 | 20:n:1108:ALA:HB1 | 2.18 | 0.42 |
| 20:n:447:VAL:HG23 | 20:n:566:ASN:HB2 | 2.01 | 0.42 |
| 2:1:141:GLN:HB3 | 2:1:615:ARG:HH21 | 1.84 | 0.42 |
| 7:M:1226:VAL:HG23 | 7:M:1236:ILE:HG12 | 2.01 | 0.42 |
| 8:N:1277:ILE:HD11 | 8:N:1280:LEU:CD1 | 2.49 | 0.42 |
| 8:P:387:LEU:HD11 | 8:P:444:ASN:HB2 | 2.00 | 0.42 |
| 9:Q:428:VAL:HG12 | 9:Q:428:VAL:O | 2.19 | 0.42 |
| 10:W:255:ILE:HD13 | 10:W:314:VAL:HG22 | 2.01 | 0.42 |
| 2:Z:1040:LYS:HD3 | 2:Z:1040:LYS:HA | 1.65 | 0.42 |
| 12:v:130:VAL:HG13 | 12:v:144:VAL:HG22 | 2.01 | 0.42 |
| 14:h:245:ILE:HD13 | 14:h:311:LEU:HB2 | 2.01 | 0.42 |
| 16:j:592:LEU:HD23 | 16:j:621:LEU:HD21 | 2.01 | 0.42 |
| 20:n:258:SER:H | 20:n:289:LYS:HG3 | 1.83 | 0.42 |
| 18:e:16:VAL:HG12 | 18:e:63:TRP:CD1 | 2.54 | 0.42 |
| 1:0:400:ARG:HH11 | 1:0:400:ARG:CG | 2.32 | 0.42 |
| 6:I:331:LYS:HD3 | 6:I:331:LYS:HA | 1.94 | 0.42 |
| 4:J:755:LEU:HD22 | 5:K:443:LEU:HD13 | 2.01 | 0.42 |
| 7:M:1318:LYS:H | 7:M:1318:LYS:HG3 | 1.63 | 0.42 |
| 8:P:260:ARG:HH11 | 8:P:263:SER:HB2 | 1.84 | 0.42 |
| 8:P:359:LEU:HD12 | 8:P:359:LEU:HA | 1.85 | 0.42 |
| 9:S:71:TYR:O | 9:S:84:ASP:HA | 2.19 | 0.42 |
| 2:Z:745:ILE:CD1 | 2:Z:844:PHE:CZ | 3.03 | 0.42 |
| 20:g:649:PHE:HA | 20:g:652:HIS:HB2 | 2.02 | 0.42 |
| 14:a:896:LEU:O | 14:a:897:SER:HB3 | 2.18 | 0.42 |
| 2:1:885:VAL:HG21 | 2:1:901:ILE:HB | 2.02 | 0.42 |
| 5:K:311:PHE:CE1 | 5:K:351:GLN:HB3 | 2.54 | 0.42 |
| 8:P:1061:THR:HG21 | 8:P:1189:ASP:HB2 | 2.00 | 0.42 |
| 8:P:1399:ASN:HA | 8:P:1400:PRO:HD3 | 1.86 | 0.42 |
| 9:Q:761:SER:HB2 | 2:Z:1315:GLY:HA2 | 2.01 | 0.42 |
| 9:S:321:LYS:H | 9:S:325:LEU:HD23 | 1.84 | 0.42 |
| 9:T:487:LEU:HD23 | 9:T:487:LEU:HA | 1.91 | 0.42 |
| 1:0:421:VAL:CG2 | 1:0:441:VAL:HG22 | 2.50 | 0.42 |
| 1:0:1275:ILE:HG22 | 1:0:1275:ILE:O | 2.20 | 0.42 |
| 2:1:889:LYS:O | 2:1:889:LYS:HG3 | 2.19 | 0.42 |
| 2:1:1374:PRO:HB2 | 2:1:1375:ASN:HD22 | 1.84 | 0.42 |
| 7:M:907:HIS:CD2 | 7:M:907:HIS:C | 2.98 | 0.42 |
| 8:N:380:THR:HB | 8:N:400:PHE:CE1 | 2.51 | 0.42 |
| 8:N:589:GLU:CD | 8:N:589:GLU:H | 2.27 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:O:875:VAL:HG11 | 7:O:912:PHE:CE1 | 2.55 | 0.42 |
| 7:O:1339:ILE:HD12 | 7:O:1353:LEU:HB3 | 2.01 | 0.42 |
| 9:Q:322:ILE:CG2 | 9:Q:427:ALA:HA | 2.49 | 0.42 |
| 9:S:600:ILE:HG23 | 9:S:601:PRO:HD2 | 2.01 | 0.42 |
| 10:W:255:ILE:HD12 | 10:W:255:ILE:N | 2.35 | 0.42 |
| 2:Z:111:LEU:HD23 | 2:Z:111:LEU:HA | 1.87 | 0.42 |
| 14:h:916:ARG:O | 14:h:917:ASP:HB3 | 2.20 | 0.42 |
| 15:i:571:TYR:HA | 15:i:574:LEU:HD12 | 2.00 | 0.42 |
| 17:k:80:LEU:HA | 17:k:80:LEU:HD23 | 1.88 | 0.42 |
| 18:l:230:LEU:N | 18:l:230:LEU:HD12 | 2.34 | 0.42 |
| 20:n:891:ILE:HA | 20:n:926:VAL:HG11 | 2.02 | 0.42 |
| 1:0:413:LEU:HD11 | 1:0:444:VAL:HG13 | 2.01 | 0.42 |
| 7:M:1460:LEU:HD23 | 7:M:1460:LEU:H | 1.84 | 0.42 |
| 8:N:754:TYR:HA | 8:N:756:TRP:CE2 | 2.55 | 0.42 |
| 8:P:793:LEU:HB3 | 8:P:794:ILE:H | 1.56 | 0.42 |
| 8:P:1060:LEU:HD13 | 8:P:1060:LEU:H | 1.81 | 0.42 |
| 1:Y:402:ILE:CB | 1:Y:407:ALA:HB3 | 2.50 | 0.42 |
| 1:Y:413:LEU:HA | 1:Y:413:LEU:HD13 | 1.73 | 0.42 |
| 1:Y:1109:PHE:HA | 1:Y:1146:TYR:CE1 | 2.55 | 0.42 |
| 14:h:224:ILE:HG22 | 14:h:276:VAL:HA | 2.01 | 0.42 |
| 14:h:399:THR:HA | 14:h:669:ARG:HG2 | 2.01 | 0.42 |
| 15:i:183:ASN:HD21 | 15:i:214:ARG:HB2 | 1.85 | 0.42 |
| 16:j:299:LEU:HD22 | 16:j:387:LEU:HD21 | 2.01 | 0.42 |
| 20:n:571:VAL:HG13 | 20:n:576:ASN:HB2 | 2.02 | 0.42 |
| 15:b:69:PHE:CZ | 18:e:328:VAL:HG11 | 2.55 | 0.42 |
| 18:e:32:HIS:O | 18:e:58:ILE:HD13 | 2.20 | 0.42 |
| 18:e:111:LEU:HA | 18:e:129:GLY:HA3 | 2.01 | 0.42 |
| 20:g:506:LYS:HE2 | 20:g:570:PHE:CD2 | 2.55 | 0.42 |
| 20:g:852:ILE:H | 20:g:854:HIS:HE1 | 1.68 | 0.42 |
| 14:a:399:THR:HA | 14:a:669:ARG:HD3 | 2.01 | 0.42 |
| 7:O:1397:SER:HB2 | 7:O:1401:LEU:HB2 | 2.02 | 0.42 |
| 9:T:758:GLN:HE22 | 1:Y:1271:ILE:HG22 | 1.85 | 0.42 |
| 2:Z:759:ILE:HD12 | 2:Z:805:ILE:HG13 | 2.02 | 0.42 |
| 2:Z:948:ARG:HH21 | 2:Z:951:VAL:HG21 | 1.84 | 0.42 |
| 2:Z:1170:GLN:HE22 | 2:Z:1199:VAL:HA | 1.85 | 0.42 |
| 12:v:168:LYS:H | 12:v:168:LYS:HD2 | 1.85 | 0.42 |
| 19:f:678:LEU:HG | 19:f:679:LYS:H | 1.84 | 0.42 |
| 20:g:275:ILE:HA | 20:g:280:THR:HG22 | 2.02 | 0.42 |
| 20:g:774:PHE:CE1 | 20:g:777:ILE:HG21 | 2.55 | 0.42 |
| 14:a:800:GLU:HG2 | 14:a:800:GLU:O | 2.20 | 0.42 |
| 1:0:1446:LYS:HA | 1:0:1446:LYS:HE3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:E:304:THR:C | 5:E:306:THR:H | 2.28 | 0.42 |
| 5:H:316:VAL:HG22 | 5:H:348:ILE:HB | 1.91 | 0.42 |
| 4:J:754:ASN:HB2 | 7:O:892:LYS:HE3 | 2.01 | 0.42 |
| 8:N:33:ASP:HB2 | 8:N:946:TRP:CB | 2.37 | 0.42 |
| 7:O:323:LEU:HD21 | 7:O:345:ARG:HA | 2.00 | 0.42 |
| 1:Y:437:VAL:HG21 | 1:Y:531:PHE:CD1 | 2.55 | 0.42 |
| 2:Z:1084:LEU:HD23 | 2:Z:1084:LEU:C | 2.45 | 0.42 |
| 15:i:306:TRP:CH2 | 15:i:310:VAL:HG21 | 2.55 | 0.42 |
| 16:j:569:GLU:HG3 | 16:j:609:LYS:HB2 | 2.02 | 0.42 |
| 15:b:162:VAL:O | 15:b:162:VAL:HG22 | 2.20 | 0.42 |
| 20:g:1005:LEU:C | 20:g:1008:MET:HE2 | 2.45 | 0.42 |
| 14:a:223:VAL:HG22 | 14:a:236:VAL:HB | 2.02 | 0.42 |
| 1:0:407:ALA:HB1 | 1:0:413:LEU:CG | 2.48 | 0.42 |
| 4:G:791:ILE:HD12 | 4:G:792:GLN:N | 2.33 | 0.42 |
| 8:N:1436:GLU:H | 8:N:1439:LEU:HB3 | 1.85 | 0.42 |
| 8:P:275:LEU:HD13 | 8:P:382:PHE:CD1 | 2.49 | 0.42 |
| 8:P:835:LEU:HA | 8:P:838:LYS:H | 1.84 | 0.42 |
| 9:R:226:ARG:HD3 | 9:R:562:LEU:HB2 | 2.01 | 0.42 |
| 12:v:396:CYS:SG | 12:v:401:ASP:CB | 3.05 | 0.42 |
| 15:i:271:LEU:HB2 | 15:i:272:PRO:HD3 | 2.02 | 0.42 |
| 20:n:1148:ILE:HD12 | 20:n:1149:ASN:H | 1.85 | 0.42 |
| 19:f:387:ARG:HD2 | 19:f:416:TYR:CZ | 2.55 | 0.42 |
| 19:f:506:ILE:HB | 19:f:509:HIS:ND1 | 2.35 | 0.42 |
| 14:a:389:LEU:O | 14:a:393:HIS:HB2 | 2.19 | 0.42 |
| 5:E:359:ASN:HA | 6:F:294:LEU:HD12 | 2.02 | 0.41 |
| 5:E:529:LYS:HE3 | 9:R:78:LEU:H | 1.84 | 0.41 |
| 8:N:69:ASN:HA | 8:N:72:ARG:CZ | 2.42 | 0.41 |
| 8:N:1412:LEU:HD13 | 8:N:1418:LEU:CD1 | 2.50 | 0.41 |
| 7:O:145:LEU:HG | 7:O:219:HIS:CD2 | 2.55 | 0.41 |
| 1:Y:1154:ASP:HB3 | 1:Y:1156:LEU:H | 1.85 | 0.41 |
| 20:g:774:PHE:CZ | 20:g:777:ILE:HG22 | 2.54 | 0.41 |
| 1:0:120:VAL:HG22 | 1:0:121:LEU:H | 1.85 | 0.41 |
| 2:1:158:GLU:HG3 | 2:1:161:SER:H | 1.85 | 0.41 |
| 4:D:665:TRP:CE3 | 6:F:305:ILE:HD11 | 2.55 | 0.41 |
| 7:M:761:LEU:HD22 | 7:M:843:VAL:HG21 | 2.01 | 0.41 |
| 7:O:916:ILE:HG13 | 7:O:917:PHE:H | 1.85 | 0.41 |
| 8:P:1061:THR:O | 8:P:1061:THR:OG1 | 2.30 | 0.41 |
| 9:R:612:HIS:CD2 | 2:Z:969:ARG:HG2 | 2.55 | 0.41 |
| 9:R:755:LYS:HA | 9:R:755:LYS:HD2 | 1.63 | 0.41 |
| 9:T:437:TRP:CZ2 | 9:T:441:MET:HG3 | 2.55 | 0.41 |
| 1:Y:790:PHE:CD1 | 1:Y:831:LYS:HE3 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:1313:VAL:H | 1:Y:1314:PRO:HD2 | 1.84 | 0.41 |
| 2:Z:866:ILE:O | 2:Z:870:VAL:HG13 | 2.20 | 0.41 |
| 14:h:305:VAL:H | 14:h:305:VAL:HG23 | 1.58 | 0.41 |
| 16:c:148:TYR:CE2 | 17:d:258:TRP:CZ3 | 3.08 | 0.41 |
| 14:a:161:ARG:HA | 14:a:161:ARG:HE | 1.84 | 0.41 |
| 1:0:139:LYS:HA | 1:0:599:LEU:HD22 | 2.02 | 0.41 |
| 1:0:241:PHE:HB3 | 1:0:243:PHE:CE2 | 2.56 | 0.41 |
| 7:M:1158:THR:HG23 | 7:M:1309:LEU:HD22 | 2.02 | 0.41 |
| 8:N:499:LEU:HD23 | 8:N:524:THR:OG1 | 2.20 | 0.41 |
| 8:N:1277:ILE:HD11 | 8:N:1280:LEU:HD11 | 2.02 | 0.41 |
| 8:N:1303:LEU:O | 8:N:1384:ASP:HA | 2.20 | 0.41 |
| 7:O:1035:GLY:O | 7:O:1041:PHE:CZ | 2.73 | 0.41 |
| 21:r:59:VAL:HG12 | 21:r:61:VAL:HG23 | 2.01 | 0.41 |
| 14:a:714:ILE:N | 14:a:714:ILE:CD1 | 2.78 | 0.41 |
| 1:0:130:GLY:HA2 | 1:0:511:LYS:HG3 | 2.02 | 0.41 |
| 1:0:402:ILE:HD13 | 1:0:467:PHE:HE1 | 1.85 | 0.41 |
| 1:0:406:THR:HG23 | 1:0:408:ARG:NE | 2.36 | 0.41 |
| 1:0:407:ALA:HB1 | 1:0:467:PHE:CZ | 2.46 | 0.41 |
| 2:1:766:PHE:CD2 | 2:1:773:PHE:CE2 | 3.08 | 0.41 |
| 4:D:684:VAL:HG13 | 4:D:688:HIS:CE1 | 2.55 | 0.41 |
| 5:H:356:GLU:HA | 6:I:290:ILE:HG21 | 2.01 | 0.41 |
| 7:M:152:HIS:CE1 | 7:M:223:LEU:HD11 | 2.55 | 0.41 |
| 7:M:740:LEU:HD13 | 7:M:749:ILE:HG22 | 2.02 | 0.41 |
| 8:P:396:THR:HB | 8:P:444:ASN:HD22 | 1.85 | 0.41 |
| 8:P:551:ASN:HB3 | 8:P:552:LEU:H | 1.47 | 0.41 |
| 9:Q:546:ARG:HG3 | 9:Q:546:ARG:NH1 | 2.36 | 0.41 |
| 10:U:304:LYS:HE2 | 11:V:271:ILE:CG1 | 2.46 | 0.41 |
| 1:Y:145:PHE:CE1 | 1:Y:673:TYR:CE1 | 3.09 | 0.41 |
| 2:Z:205:LYS:HZ1 | 2:Z:223:ILE:HG13 | 1.85 | 0.41 |
| 2:Z:1112:ALA:HB1 | 2:Z:1156:LEU:HD11 | 2.00 | 0.41 |
| 14:h:255:GLN:HB3 | 14:h:257:TYR:CE2 | 2.56 | 0.41 |
| 16:j:560:LEU:HD22 | 16:j:595:LEU:HD22 | 2.02 | 0.41 |
| 17:k:267:ASN:HD22 | 17:k:267:ASN:HA | 1.74 | 0.41 |
| 19:m:174:LYS:O | 19:m:178:HIS:CD2 | 2.73 | 0.41 |
| 20:n:163:GLY:O | 20:n:164:LEU:HB2 | 2.20 | 0.41 |
| 16:c:769:PRO:HG3 | 14:a:1011:ASP:HB3 | 2.02 | 0.41 |
| 18:e:61:ILE:HD12 | 18:e:61:ILE:HA | 2.00 | 0.41 |
| 1:0:140:ASN:HA | 1:0:146:THR:HG23 | 2.02 | 0.41 |
| 7:M:664:LEU:HD12 | 7:M:664:LEU:HA | 1.91 | 0.41 |
| 7:M:798:ASN:HD22 | 7:M:1221:LEU:HA | 1.85 | 0.41 |
| 7:M:815:PHE:HB3 | 7:M:818:TYR:HB3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:N:101:PHE:HB3 | 8:N:102:PHE:H | 1.71 | 0.41 |
| 8:N:1210:LEU:HD13 | 8:N:1210:LEU:HA | 1.86 | 0.41 |
| 7:O:184:ASP:HA | 7:O:187:LEU:HD12 | 2.03 | 0.41 |
| 7:O:432:LEU:HD22 | 7:O:488:PHE:CD1 | 2.55 | 0.41 |
| 8:P:445:LEU:HD23 | 8:P:446:ALA:N | 2.32 | 0.41 |
| 8:P:466:THR:HG22 | 8:P:467:LYS:H | 1.85 | 0.41 |
| 8:P:1303:LEU:HB3 | 8:P:1304:LYS:H | 1.62 | 0.41 |
| 9:Q:557:LEU:HD12 | 9:Q:579:LEU:HD22 | 2.02 | 0.41 |
| 10:U:279:ASP:O | 10:U:307:ILE:HD11 | 2.20 | 0.41 |
| 1:Y:511:LYS:HG3 | 1:Y:512:LYS:HG3 | 2.03 | 0.41 |
| 17:d:219:ARG:H | 17:d:239:GLU:HB2 | 1.85 | 0.41 |
| 19:f:668:HIS:CD2 | 19:f:714:TYR:CD1 | 3.08 | 0.41 |
| 1:0:393:ILE:HG23 | 1:0:397:TYR:CD2 | 2.52 | 0.41 |
| 1:0:408:ARG:NH2 | 1:0:508:LYS:CE | 2.75 | 0.41 |
| 1:0:409:ALA:O | 1:0:512:LYS:HA | 2.20 | 0.41 |
| 2:1:457:SER:C | 2:1:558:THR:OG1 | 2.64 | 0.41 |
| 4:D:719:GLU:OE1 | 7:M:688:SER:HB2 | 2.19 | 0.41 |
| 4:G:640:LEU:HD23 | 4:G:640:LEU:HA | 1.88 | 0.41 |
| 4:G:777:ASN:H | 9:S:45:SER:CB | 2.32 | 0.41 |
| 8:N:18:VAL:CG2 | 8:N:34:ALA:HB1 | 2.45 | 0.41 |
| 7:O:1417:LEU:HD12 | 7:O:1418:SER:H | 1.85 | 0.41 |
| 9:R:811:ARG:HH11 | 9:R:815:ILE:HD11 | 1.85 | 0.41 |
| 9:T:754:ARG:O | 9:T:757:ALA:HB3 | 2.21 | 0.41 |
| 1:Y:790:PHE:CZ | 1:Y:913:LEU:HD23 | 2.55 | 0.41 |
| 2:Z:807:ASP:HB3 | 2:Z:887:VAL:CG1 | 2.51 | 0.41 |
| 15:i:504:ILE:O | 15:i:504:ILE:HG22 | 2.20 | 0.41 |
| 19:m:237:ILE:HD12 | 19:m:240:HIS:HA | 2.01 | 0.41 |
| 20:n:685:GLY:HA3 | 20:n:759:TRP:CE3 | 2.56 | 0.41 |
| 20:n:772:ASP:HB3 | 20:n:773:ASN:H | 1.45 | 0.41 |
| 20:g:705:LYS:HG3 | 20:g:706:LEU:HD23 | 2.01 | 0.41 |
| 1:0:1143:GLN:HG3 | 1:0:1177:ILE:HD11 | 2.02 | 0.41 |
| 2:1:1049:ASN:HB2 | 9:T:514:LYS:CG | 2.51 | 0.41 |
| 7:M:948:LEU:CD2 | 7:M:951:ARG:HH21 | 2.33 | 0.41 |
| 8:N:190:GLN:HE22 | 8:N:837:ASP:HA | 1.86 | 0.41 |
| 8:N:1083:ALA:HA | 8:N:1086:ILE:HD12 | 2.01 | 0.41 |
| 8:N:1620:THR:HG23 | 9:Q:99:ASN:HA | 2.02 | 0.41 |
| 7:O:1318:LYS:HB3 | 7:O:1319:LEU:H | 1.56 | 0.41 |
| 8:P:1278:ILE:H | 8:P:1278:ILE:HG12 | 1.58 | 0.41 |
| 9:T:512:SER:HA | 9:T:562:LEU:HD11 | 2.03 | 0.41 |
| 11:X:299:GLN:HG2 | 11:X:300:VAL:HG12 | 2.03 | 0.41 |
| 1:Y:121:LEU:H | 1:Y:121:LEU:HD12 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:791:MET:N | 1:Y:831:LYS:HD3 | 2.34 | 0.41 |
| 12:v:128:LYS:O | 12:v:129:LYS:HB3 | 2.21 | 0.41 |
| 12:v:155:ASP:H | 12:v:161:GLU:HG3 | 1.85 | 0.41 |
| 16:j:451:TRP:HA | 16:j:473:ALA:HB1 | 2.03 | 0.41 |
| 19:m:70:LEU:HD22 | 19:m:344:ARG:HE | 1.86 | 0.41 |
| 16:c:650:HIS:H | 17:d:130:PHE:HB2 | 1.86 | 0.41 |
| 19:f:72:ALA:HA | 19:f:75:TRP:CE3 | 2.56 | 0.41 |
| 19:f:694:VAL:O | 19:f:694:VAL:HG12 | 2.21 | 0.41 |
| 20:g:774:PHE:O | 20:g:774:PHE:CD2 | 2.73 | 0.41 |
| 14:a:396:ASP:HA | 14:a:399:THR:HG23 | 2.03 | 0.41 |
| 14:a:807:ILE:O | 14:a:807:ILE:HG22 | 2.20 | 0.41 |
| 6:C:336:PHE:O | 6:C:336:PHE:CG | 2.74 | 0.41 |
| 5:E:435:LYS:HE3 | 5:E:436:MET:HE2 | 2.03 | 0.41 |
| 4:J:797:LEU:HD13 | 6:L:443:VAL:HG22 | 2.03 | 0.41 |
| 7:M:940:ASN:HB3 | 7:M:943:ARG:HH21 | 1.86 | 0.41 |
| 10:U:335:MET:HE2 | 10:U:335:MET:HB2 | 1.93 | 0.41 |
| 1:Y:176:PHE:CZ | 1:Y:232:LEU:HD11 | 2.56 | 0.41 |
| 1:Y:278:ARG:HH21 | 1:Y:366:GLY:HA2 | 1.84 | 0.41 |
| 1:Y:1198:ASN:H | 1:Y:1201:TRP:HD1 | 1.69 | 0.41 |
| 2:Z:1157:SER:HA | 2:Z:1160:ILE:HD11 | 2.02 | 0.41 |
| 19:m:77:LEU:HD23 | 19:m:77:LEU:HA | 1.92 | 0.41 |
| 17:d:79:VAL:HG11 | 17:d:116:LEU:HD21 | 2.02 | 0.41 |
| 20:g:884:HIS:CE1 | 20:g:909:ASP:HB2 | 2.56 | 0.41 |
| 20:g:1005:LEU:O | 20:g:1008:MET:HE2 | 2.21 | 0.41 |
| 2:1:348:ASP:HB3 | 2:1:353:VAL:H | 1.85 | 0.41 |
| 2:1:1317:SER:CB | 9:S:823:ARG:HH22 | 2.33 | 0.41 |
| 4:A:665:TRP:HE1 | 5:B:369:VAL:HG11 | 1.85 | 0.41 |
| 7:M:781:LEU:CD2 | 7:M:868:ALA:HB2 | 2.50 | 0.41 |
| 7:M:966:LEU:HD23 | 7:M:966:LEU:HA | 1.90 | 0.41 |
| 8:N:467:LYS:HE2 | 8:N:586:LEU:H | 1.86 | 0.41 |
| 8:N:1489:PRO:CG | 8:N:1620:THR:HG21 | 2.51 | 0.41 |
| 7:O:497:CYS:HA | 7:O:500:TRP:CH2 | 2.55 | 0.41 |
| 8:P:1223:ASN:O | 8:P:1261:ILE:HG23 | 2.20 | 0.41 |
| 9:S:436:LEU:HA | 9:S:439:HIS:CE1 | 2.56 | 0.41 |
| 9:T:593:ILE:HD13 | 9:T:593:ILE:HA | 1.97 | 0.41 |
| 1:Y:412:ILE:HG22 | 1:Y:444:VAL:CG2 | 2.14 | 0.41 |
| 1:Y:1088:PHE:CE1 | 1:Y:1185:TYR:CE1 | 3.08 | 0.41 |
| 2:Z:194:ILE:HD13 | 2:Z:194:ILE:N | 2.35 | 0.41 |
| 2:Z:720:PHE:HD1 | 2:Z:723:ILE:HD11 | 1.86 | 0.41 |
| 2:Z:966:PHE:HA | 2:Z:969:ARG:HH21 | 1.85 | 0.41 |
| 14:h:200:ASN:HD21 | 14:h:252:THR:HG22 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 15:b:511:TYR:CE2 | 15:b:538:ILE:HG22 | 2.56 | 0.41 |
| 17:d:17:LEU:N | 17:d:17:LEU:HD12 | 2.36 | 0.41 |
| 18:e:183:LEU:N | 18:e:183:LEU:HD23 | 2.36 | 0.41 |
| 18:e:192:ILE:HG22 | 18:e:207:LYS:HG2 | 2.03 | 0.41 |
| 20:g:948:GLN:HE22 | 20:g:951:LEU:HD22 | 1.86 | 0.41 |
| 14:a:382:VAL:HG12 | 14:a:498:HIS:HB2 | 2.03 | 0.41 |
| 4:A:726:VAL:HG13 | 4:A:726:VAL:O | 2.20 | 0.41 |
| 5:E:384:THR:HG21 | 7:M:1036:PRO:HB3 | 2.03 | 0.41 |
| 8:P:34:ALA:HB3 | 8:P:43:PHE:HD2 | 1.85 | 0.41 |
| 8:P:587:GLN:HG3 | 8:P:588:HIS:H | 1.86 | 0.41 |
| 8:P:661:MET:HA | 8:P:664:LEU:HG | 2.03 | 0.41 |
| 8:P:772:THR:HG22 | 8:P:775:PHE:CZ | 2.55 | 0.41 |
| 9:T:238:PHE:HA | 9:T:241:ILE:HG13 | 2.01 | 0.41 |
| 9:T:613:VAL:CG2 | 9:T:616:GLU:HA | 2.51 | 0.41 |
| 20:n:892:LEU:HD23 | 20:n:892:LEU:HA | 1.91 | 0.41 |
| 16:c:566:ASP:HB3 | 16:c:567:LEU:HD22 | 2.03 | 0.41 |
| 19:f:665:MET:HE1 | 19:f:714:TYR:CA | 2.51 | 0.41 |
| 1:0:400:ARG:HG2 | 1:0:400:ARG:NH1 | 2.34 | 0.40 |
| 2:1:203:LYS:HG2 | 2:1:263:ILE:H | 1.85 | 0.40 |
| 5:K:406:VAL:HA | 5:K:409:GLU:HG2 | 2.02 | 0.40 |
| 8:P:1053:LEU:H | 8:P:1053:LEU:CD2 | 2.09 | 0.40 |
| 1:Y:779:ARG:HG2 | 1:Y:782:ARG:HH21 | 1.87 | 0.40 |
| 14:h:323:LEU:HB2 | 14:h:326:SER:HA | 2.02 | 0.40 |
| 14:h:579:ILE:HD12 | 14:h:579:ILE:H | 1.85 | 0.40 |
| 19:m:478:ARG:HE | 19:m:536:ARG:NH2 | 2.19 | 0.40 |
| 20:n:741:GLY:HA2 | 20:n:796:ASN:HD21 | 1.85 | 0.40 |
| 15:b:271:LEU:HD22 | 15:b:271:LEU:H | 1.86 | 0.40 |
| 20:g:578:LYS:HA | 20:g:578:LYS:HD3 | 1.90 | 0.40 |
| 2:1:1317:SER:HB2 | 9:S:823:ARG:HH22 | 1.86 | 0.40 |
| 8:N:1515:LEU:HB3 | 8:N:1516:PRO:HD3 | 2.02 | 0.40 |
| 8:P:777:ASP:HB2 | 8:P:793:LEU:CB | 2.46 | 0.40 |
| 8:P:1276:LYS:N | 8:P:1321:LEU:HD22 | 2.36 | 0.40 |
| 9:R:579:LEU:O | 9:R:583:THR:HG23 | 2.21 | 0.40 |
| 9:S:590:LEU:HB2 | 9:S:646:LEU:HD11 | 2.03 | 0.40 |
| 2:Z:867:LEU:CD1 | 2:Z:888:LEU:HB2 | 2.51 | 0.40 |
| 20:n:539:PHE:CZ | 20:n:588:ILE:HA | 2.57 | 0.40 |
| 21:t:59:VAL:HG12 | 21:t:61:VAL:HG23 | 2.03 | 0.40 |
| 16:c:321:LEU:HD12 | 16:c:321:LEU:HA | 1.99 | 0.40 |
| 16:c:638:ILE:HD11 | 16:c:766:LYS:H | 1.84 | 0.40 |
| 19:f:665:MET:HE1 | 19:f:714:TYR:HA | 2.02 | 0.40 |
| 14:a:177:PHE:CD2 | 14:a:223:VAL:HG21 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:0:412:ILE:CD1 | 1:0:514:SER:HB3 | 2.51 | 0.40 |
| 1:0:413:LEU:CD1 | 1:0:444:VAL:HG22 | 2.36 | 0.40 |
| 4:G:684:VAL:HG13 | 5:H:382:LYS:HZ1 | 1.87 | 0.40 |
| 7:M:1036:PRO:HB2 | 7:M:1037:ASN:H | 1.63 | 0.40 |
| 8:P:972:LEU:HD22 | 8:P:1022:TYR:CD2 | 2.56 | 0.40 |
| 9:S:586:PHE:CZ | 9:S:592:LYS:HA | 2.56 | 0.40 |
| 2:Z:264:ILE:HG12 | 2:Z:347:VAL:H | 1.85 | 0.40 |
| 15:i:525:ILE:O | 15:i:525:ILE:HG22 | 2.21 | 0.40 |
| 19:m:612:ASN:HD21 | 20:n:659:PRO:HA | 1.85 | 0.40 |
| 14:a:397:ILE:HG22 | 14:a:526:ARG:HB2 | 2.03 | 0.40 |
| 1:0:375:SER:C | 1:0:420:ILE:CD1 | 2.95 | 0.40 |
| 2:1:1373:ASP:HB3 | 2:1:1374:PRO:HD2 | 2.04 | 0.40 |
| 4:J:727:SER:C | 7:O:746:LYS:HZ2 | 2.23 | 0.40 |
| 7:M:347:LEU:HD22 | 7:M:603:GLU:OE1 | 2.21 | 0.40 |
| 8:N:1277:ILE:O | 8:N:1277:ILE:CG1 | 2.70 | 0.40 |
| 8:P:439:LEU:HB3 | 8:P:441:PRO:HD2 | 2.03 | 0.40 |
| 8:P:710:GLN:HA | 8:P:713:LYS:HE2 | 2.02 | 0.40 |
| 8:P:1602:LEU:HD11 | 8:P:1647:LEU:HD22 | 2.03 | 0.40 |
| 9:T:257:TRP:HA | 9:T:257:TRP:CE3 | 2.57 | 0.40 |
| 11:X:282:ASN:OD1 | 11:X:300:VAL:HG12 | 2.21 | 0.40 |
| 2:Z:1254:GLY:HA2 | 2:Z:1301:SER:HB2 | 2.02 | 0.40 |
| 2:Z:1275:THR:O | 2:Z:1276:THR:HG23 | 2.21 | 0.40 |
| 14:h:443:LEU:HD22 | 14:h:443:LEU:H | 1.86 | 0.40 |
| 19:m:20:LYS:HD2 | 19:m:20:LYS:HA | 1.91 | 0.40 |
| 15:b:590:VAL:O | 15:b:590:VAL:HG23 | 2.21 | 0.40 |
| 19:f:249:SER:O | 19:f:253:GLN:HB2 | 2.21 | 0.40 |
| 19:f:392:LEU:HD23 | 19:f:392:LEU:HA | 1.88 | 0.40 |
| 19:f:659:TYR:O | 19:f:662:PHE:HB3 | 2.21 | 0.40 |
| 20:g:587:LEU:H | 20:g:587:LEU:HD23 | 1.86 | 0.40 |
| 1:0:411:PRO:HB2 | 1:0:517:LEU:HD11 | 2.01 | 0.40 |
| 2:1:768:ILE:O | 2:1:768:ILE:HG22 | 2.21 | 0.40 |
| 5:H:308:LEU:HD12 | 5:H:309:ARG:H | 1.87 | 0.40 |
| 7:M:1211:GLU:HG2 | 7:M:1285:HIS:CD2 | 2.56 | 0.40 |
| 8:N:573:LEU:HD12 | 8:N:573:LEU:N | 2.36 | 0.40 |
| 8:N:803:LEU:HA | 8:N:807:LEU:HB2 | 2.04 | 0.40 |
| 7:O:3:TRP:CD2 | 7:O:41:LYS:HG2 | 2.56 | 0.40 |
| 7:O:483:LEU:HG | 7:O:487:PHE:CE2 | 2.57 | 0.40 |
| 7:O:1035:GLY:CA | 7:O:1041:PHE:CE1 | 3.02 | 0.40 |
| 8:P:107:SER:HB3 | 8:P:111:HIS:CE1 | 2.56 | 0.40 |
| 9:S:763:LEU:C | 9:S:765:ASP:H | 2.29 | 0.40 |
| 2:Z:538:LEU:HD12 | 2:Z:538:LEU:HA | 1.95 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:h:336:LEU:N | 14:h:336:LEU:HD23 | 2.36 | 0.40 |
| 15:i:573:TRP:CE2 | 15:i:577:GLU:HB2 | 2.57 | 0.40 |
| 19:m:341:HIS:CE1 | 19:m:343:ILE:HD12 | 2.56 | 0.40 |
| 20:n:860:LEU:HD13 | 20:n:860:LEU:HA | 1.98 | 0.40 |
| 20:n:1101:ARG:H | 20:n:1101:ARG:HD3 | 1.86 | 0.40 |
| 16:c:252:ASN:HD21 | 19:f:226:GLN:HE22 | 1.68 | 0.40 |
| 14:a:354:LEU:HD21 | 14:a:460:ALA:HB1 | 2.04 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | 0 | 1053/1502 (70%) | 857 (81%) | 118 (11%) | 78 (7%) | 1 10 |
| 1 | Y | 1054/1502 (70%) | 864 (82%) | 114 (11%) | 76 (7%) | 1 11 |
| 2 | 1 | 1087/1391 (78%) | 919 (84%) | 115 (11%) | 53 (5%) | 1 16 |
| 2 | Z | 1085/1391 (78%) | 918 (85%) | 113 (10%) | 54 (5%) | 1 16 |
| 4 | A | 156/823 (19%) | 150 (96%) | 2 (1%) | 4 (3%) | 4 25 |
| 4 | D | 157/823 (19%) | 150 (96%) | 6 (4%) | 1 (1%) | 21 59 |
| 4 | G | 158/823 (19%) | 151 (96%) | 1 (1%) | 6 (4%) | 2 19 |
| 4 | J | 158/823 (19%) | 150 (95%) | 6 (4%) | 2 (1%) | 9 42 |
| 4 | y | 180/823 (22%) | 180 (100%) | 0 | 0 | 100 100 |
| 4 | z | 183/823 (22%) | 181 (99%) | 2 (1%) | 0 | 100 100 |
| 5 | B | 211/541 (39%) | 189 (90%) | 9 (4%) | 13 (6%) | 1 13 |
| 5 | E | 211/541 (39%) | 189 (90%) | 17 (8%) | 5 (2%) | 4 27 |
| 5 | H | 211/541 (39%) | 179 (85%) | 21 (10%) | 11 (5%) | 1 15 |
| 5 | K | 211/541 (39%) | 193 (92%) | 11 (5%) | 7 (3%) | 3 21 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 6 | C | 160/472 (34%) | 149 (93%) | 8 (5%) | 3 (2%) | 6 32 |
| 6 | F | 161/472 (34%) | 153 (95%) | 6 (4%) | 2 (1%) | 10 44 |
| 6 | I | 160/472 (34%) | 151 (94%) | 6 (4%) | 3 (2%) | 6 32 |
| 6 | L | 161/472 (34%) | 152 (94%) | 5 (3%) | 4 (2%) | 4 26 |
| 7 | M | 1497/1683 (89%) | 1249 (83%) | 170 (11%) | 78 (5%) | 1 15 |
| 7 | O | 1496/1683 (89%) | 1245 (83%) | 173 (12%) | 78 (5%) | 1 15 |
| 8 | N | 1310/1655 (79%) | 994 (76%) | 208 (16%) | 108 (8%) | 0 9 |
| 8 | P | 1310/1655 (79%) | 1015 (78%) | 191 (15%) | 104 (8%) | 1 10 |
| 9 | Q | 670/839 (80%) | 576 (86%) | 63 (9%) | 31 (5%) | 2 17 |
| 9 | R | 692/839 (82%) | 590 (85%) | 60 (9%) | 42 (6%) | 1 13 |
| 9 | S | 672/839 (80%) | 584 (87%) | 66 (10%) | 22 (3%) | 3 21 |
| 9 | T | 692/839 (82%) | 588 (85%) | 68 (10%) | 36 (5%) | 1 15 |
| 10 | U | 90/475 (19%) | 78 (87%) | 6 (7%) | 6 (7%) | 1 12 |
| 10 | W | 90/475 (19%) | 74 (82%) | 9 (10%) | 7 (8%) | 1 10 |
| 11 | V | 90/528 (17%) | 70 (78%) | 15 (17%) | 5 (6%) | 1 14 |
| 11 | X | 90/528 (17%) | 74 (82%) | 9 (10%) | 7 (8%) | 1 10 |
| 12 | u | 569/713 (80%) | 500 (88%) | 38 (7%) | 31 (5%) | 1 15 |
| 12 | v | 546/713 (77%) | 481 (88%) | 40 (7%) | 25 (5%) | 2 17 |
| 13 | w | 179/1460 (12%) | 172 (96%) | 5 (3%) | 2 (1%) | 11 46 |
| 13 | x | 182/1460 (12%) | 177 (97%) | 4 (2%) | 1 (0%) | 24 63 |
| 14 | a | 996/1037 (96%) | 815 (82%) | 119 (12%) | 62 (6%) | 1 13 |
| 14 | h | 996/1037 (96%) | 825 (83%) | 107 (11%) | 64 (6%) | 1 12 |
| 15 | b | 667/744 (90%) | 532 (80%) | 92 (14%) | 43 (6%) | 1 12 |
| 15 | i | 655/744 (88%) | 522 (80%) | 91 (14%) | 42 (6%) | 1 12 |
| 16 | c | 551/712 (77%) | 472 (86%) | 51 (9%) | 28 (5%) | 1 15 |
| 16 | j | 551/712 (77%) | 475 (86%) | 52 (9%) | 24 (4%) | 2 17 |
| 17 | d | 270/297 (91%) | 233 (86%) | 29 (11%) | 8 (3%) | 3 23 |
| 17 | k | 270/297 (91%) | 230 (85%) | 28 (10%) | 12 (4%) | 2 17 |
| 18 | e | 297/349 (85%) | 262 (88%) | 25 (8%) | 10 (3%) | 3 21 |
| 18 | l | 303/349 (87%) | 261 (86%) | 28 (9%) | 14 (5%) | 2 17 |
| 19 | f | 635/726 (88%) | 539 (85%) | 68 (11%) | 28 (4%) | 2 17 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 19 | m | 635/726 (88%) | 548 (86%) | 61 (10%) | 26 (4%) | 2 18 |
| 20 | g | 1052/1157 (91%) | 864 (82%) | 126 (12%) | 62 (6%) | 1 13 |
| 20 | n | 1052/1157 (91%) | 844 (80%) | 142 (14%) | 66 (6%) | 1 13 |
| 21 | o | 84/92 (91%) | 78 (93%) | 4 (5%) | 2 (2%) | 4 27 |
| 21 | p | 84/92 (91%) | 80 (95%) | 3 (4%) | 1 (1%) | 10 44 |
| 21 | q | 84/92 (91%) | 78 (93%) | 4 (5%) | 2 (2%) | 4 27 |
| 21 | r | 84/92 (91%) | 76 (90%) | 5 (6%) | 3 (4%) | 2 20 |
| 21 | s | 84/92 (91%) | 79 (94%) | 4 (5%) | 1 (1%) | 10 44 |
| 21 | t | 84/92 (91%) | 77 (92%) | 5 (6%) | 2 (2%) | 4 27 |
| All | All | 26366/41756 (63%) | 22232 (84%) | 2729 (10%) | 1405 (5%) | 2 15 |

All (1405) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 180 | ASN |
| 1 | 0 | 250 | ALA |
| 1 | 0 | 293 | ILE |
| 1 | 0 | 420 | ILE |
| 1 | 0 | 517 | LEU |
| 1 | 0 | 523 | SER |
| 1 | 0 | 663 | ILE |
| 1 | 0 | 711 | VAL |
| 1 | 0 | 784 | ILE |
| 1 | 0 | 832 | VAL |
| 1 | 0 | 1030 | ASN |
| 1 | 0 | 1059 | TYR |
| 1 | 0 | 1061 | PRO |
| 1 | 0 | 1108 | VAL |
| 1 | 0 | 1154 | ASP |
| 1 | 0 | 1167 | SER |
| 1 | 0 | 1182 | ILE |
| 1 | 0 | 1258 | LEU |
| 1 | 0 | 1283 | ALA |
| 1 | 0 | 1305 | SER |
| 1 | 0 | 1308 | PHE |
| 1 | 0 | 1358 | GLU |
| 1 | 0 | 1361 | MET |
| 1 | 0 | 1380 | ASP |
| 1 | 0 | 1382 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 1440 | ASP |
| 1 | 0 | 1480 | ASP |
| 2 | 1 | 344 | GLN |
| 2 | 1 | 493 | ILE |
| 2 | 1 | 541 | SER |
| 2 | 1 | 608 | ALA |
| 2 | 1 | 913 | ALA |
| 2 | 1 | 1119 | ALA |
| 2 | 1 | 1198 | ARG |
| 2 | 1 | 1250 | SER |
| 2 | 1 | 1301 | SER |
| 2 | 1 | 1335 | ASN |
| 2 | 1 | 1356 | ASP |
| 2 | 1 | 1375 | ASN |
| 5 | B | 319 | THR |
| 5 | B | 321 | ALA |
| 5 | B | 393 | ASP |
| 5 | B | 434 | GLU |
| 6 | C | 342 | GLU |
| 4 | G | 726 | VAL |
| 4 | G | 744 | ALA |
| 5 | H | 309 | ARG |
| 5 | H | 344 | SER |
| 5 | H | 346 | GLN |
| 5 | H | 355 | PHE |
| 6 | I | 405 | LEU |
| 4 | J | 776 | PHE |
| 5 | K | 299 | TRP |
| 5 | K | 320 | GLU |
| 5 | K | 321 | ALA |
| 7 | M | 36 | ASN |
| 7 | M | 62 | SER |
| 7 | M | 127 | ASP |
| 7 | M | 137 | ASN |
| 7 | M | 505 | SER |
| 7 | M | 620 | THR |
| 7 | M | 686 | ASN |
| 7 | M | 761 | LEU |
| 7 | M | 792 | ASP |
| 7 | M | 815 | PHE |
| 7 | M | 835 | LYS |
| 7 | M | 886 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | M | 887 | PHE |
| 7 | M | 899 | PHE |
| 7 | M | 903 | ASN |
| 7 | M | 909 | LEU |
| 7 | M | 993 | ALA |
| 7 | M | 1188 | THR |
| 7 | M | 1189 | MET |
| 7 | M | 1193 | ARG |
| 7 | M | 1207 | CYS |
| 7 | M | 1470 | SER |
| 7 | M | 1506 | ILE |
| 7 | M | 1561 | LEU |
| 7 | M | 1576 | LEU |
| 8 | N | 71 | LEU |
| 8 | N | 278 | SER |
| 8 | N | 280 | ALA |
| 8 | N | 370 | SER |
| 8 | N | 442 | LEU |
| 8 | N | 650 | ASP |
| 8 | N | 748 | HIS |
| 8 | N | 794 | ILE |
| 8 | N | 810 | MET |
| 8 | N | 876 | LEU |
| 8 | N | 885 | VAL |
| 8 | N | 894 | VAL |
| 8 | N | 895 | HIS |
| 8 | N | 920 | LEU |
| 8 | N | 941 | SER |
| 8 | N | 965 | ASP |
| 8 | N | 968 | SER |
| 8 | N | 970 | LEU |
| 8 | N | 977 | ALA |
| 8 | N | 1030 | SER |
| 8 | N | 1042 | SER |
| 8 | N | 1049 | ASP |
| 8 | N | 1092 | SER |
| 8 | N | 1098 | ASN |
| 8 | N | 1162 | LEU |
| 8 | N | 1239 | ASP |
| 8 | N | 1290 | SER |
| 8 | N | 1320 | GLU |
| 8 | N | 1427 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | N | 1508 | SER |
| 8 | N | 1542 | ALA |
| 8 | N | 1594 | ASP |
| 7 | O | 36 | ASN |
| 7 | O | 62 | SER |
| 7 | O | 127 | ASP |
| 7 | O | 299 | THR |
| 7 | O | 518 | ASN |
| 7 | O | 667 | SER |
| 7 | O | 749 | ILE |
| 7 | O | 887 | PHE |
| 7 | O | 1037 | ASN |
| 7 | O | 1141 | SER |
| 7 | O | 1143 | SER |
| 7 | O | 1171 | SER |
| 7 | O | 1189 | MET |
| 7 | O | 1343 | ILE |
| 7 | O | 1365 | ASN |
| 7 | O | 1396 | LEU |
| 7 | O | 1495 | THR |
| 7 | O | 1566 | ASP |
| 7 | O | 1573 | SER |
| 7 | O | 1576 | LEU |
| 7 | O | 1665 | GLU |
| 8 | P | 49 | THR |
| 8 | P | 276 | ASN |
| 8 | P | 281 | GLN |
| 8 | P | 340 | SER |
| 8 | P | 358 | VAL |
| 8 | P | 359 | LEU |
| 8 | P | 416 | LEU |
| 8 | P | 442 | LEU |
| 8 | P | 448 | ILE |
| 8 | P | 658 | CYS |
| 8 | P | 668 | TYR |
| 8 | P | 691 | SER |
| 8 | P | 728 | ILE |
| 8 | P | 746 | ALA |
| 8 | P | 813 | ILE |
| 8 | P | 867 | ASP |
| 8 | P | 920 | LEU |
| 8 | P | 928 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | P | 964 | GLN |
| 8 | P | 1030 | SER |
| 8 | P | 1046 | LYS |
| 8 | P | 1095 | GLU |
| 8 | P | 1167 | LEU |
| 8 | P | 1288 | PHE |
| 8 | P | 1335 | GLN |
| 8 | P | 1482 | ASP |
| 8 | P | 1540 | LYS |
| 8 | P | 1542 | ALA |
| 8 | P | 1594 | ASP |
| 9 | Q | 43 | GLN |
| 9 | Q | 46 | ILE |
| 9 | Q | 49 | LEU |
| 9 | Q | 59 | LYS |
| 9 | Q | 421 | SER |
| 9 | Q | 442 | LEU |
| 9 | Q | 754 | ARG |
| 9 | R | 42 | ILE |
| 9 | R | 46 | ILE |
| 9 | R | 82 | ASP |
| 9 | R | 83 | VAL |
| 9 | R | 155 | VAL |
| 9 | R | 268 | ILE |
| 9 | R | 422 | ARG |
| 9 | R | 426 | PRO |
| 9 | R | 476 | ASN |
| 9 | R | 514 | LYS |
| 9 | R | 601 | PRO |
| 9 | R | 697 | PHE |
| 9 | R | 743 | ASP |
| 9 | R | 746 | PRO |
| 9 | S | 67 | THR |
| 9 | S | 82 | ASP |
| 9 | S | 298 | LEU |
| 9 | S | 456 | ARG |
| 9 | S | 766 | ASN |
| 9 | T | 44 | VAL |
| 9 | T | 45 | SER |
| 9 | T | 49 | LEU |
| 9 | T | 83 | VAL |
| 9 | T | 417 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | T | 472 | SER |
| 9 | T | 514 | LYS |
| 9 | T | 608 | GLN |
| 9 | T | 754 | ARG |
| 10 | U | 249 | ASP |
| 10 | U | 250 | ASP |
| 10 | U | 320 | SER |
| 10 | U | 345 | TYR |
| 11 | V | 281 | SER |
| 11 | V | 300 | VAL |
| 10 | W | 249 | ASP |
| 10 | W | 250 | ASP |
| 10 | W | 282 | VAL |
| 11 | X | 297 | ASP |
| 1 | Y | 206 | ASP |
| 1 | Y | 227 | ALA |
| 1 | Y | 250 | ALA |
| 1 | Y | 292 | ASN |
| 1 | Y | 416 | LYS |
| 1 | Y | 523 | SER |
| 1 | Y | 629 | ALA |
| 1 | Y | 711 | VAL |
| 1 | Y | 714 | LYS |
| 1 | Y | 832 | VAL |
| 1 | Y | 858 | ASP |
| 1 | Y | 1030 | ASN |
| 1 | Y | 1062 | LYS |
| 1 | Y | 1085 | ALA |
| 1 | Y | 1183 | LEU |
| 1 | Y | 1188 | GLU |
| 1 | Y | 1198 | ASN |
| 1 | Y | 1209 | LYS |
| 1 | Y | 1288 | ALA |
| 1 | Y | 1295 | LYS |
| 1 | Y | 1419 | ALA |
| 1 | Y | 1468 | TYR |
| 2 | Z | 577 | PHE |
| 2 | Z | 625 | ILE |
| 2 | Z | 650 | LYS |
| 2 | Z | 670 | PRO |
| 2 | Z | 922 | LYS |
| 2 | Z | 932 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Z | 960 | GLN |
| 2 | Z | 1124 | ASP |
| 2 | Z | 1277 | ARG |
| 2 | Z | 1360 | SER |
| 2 | Z | 1387 | HIS |
| 12 | u | 41 | ASN |
| 12 | u | 149 | ASP |
| 12 | u | 171 | ASN |
| 12 | u | 263 | TRP |
| 12 | u | 288 | ASN |
| 12 | u | 418 | ALA |
| 12 | v | 113 | HIS |
| 12 | v | 176 | ASP |
| 12 | v | 288 | ASN |
| 12 | v | 400 | SER |
| 13 | w | 1142 | VAL |
| 13 | w | 1150 | VAL |
| 13 | x | 1455 | ASN |
| 14 | h | 172 | GLN |
| 14 | h | 230 | HIS |
| 14 | h | 261 | SER |
| 14 | h | 276 | VAL |
| 14 | h | 295 | ASN |
| 14 | h | 427 | LEU |
| 14 | h | 490 | VAL |
| 14 | h | 559 | GLU |
| 14 | h | 606 | LYS |
| 14 | h | 716 | GLU |
| 14 | h | 797 | LEU |
| 14 | h | 798 | LYS |
| 14 | h | 806 | SER |
| 14 | h | 816 | THR |
| 14 | h | 884 | GLU |
| 14 | h | 897 | SER |
| 14 | h | 917 | ASP |
| 14 | h | 929 | HIS |
| 14 | h | 930 | SER |
| 14 | h | 993 | VAL |
| 14 | h | 1009 | SER |
| 14 | h | 1011 | ASP |
| 14 | h | 1013 | ALA |
| 15 | i | 191 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | i | 278 | CYS |
| 15 | i | 281 | SER |
| 15 | i | 403 | HIS |
| 15 | i | 492 | SER |
| 15 | i | 553 | ILE |
| 15 | i | 649 | LEU |
| 15 | i | 692 | ILE |
| 15 | i | 706 | SER |
| 16 | j | 147 | SER |
| 16 | j | 157 | SER |
| 16 | j | 317 | HIS |
| 16 | j | 323 | SER |
| 16 | j | 377 | SER |
| 17 | k | 219 | ARG |
| 17 | k | 285 | LEU |
| 18 | l | 189 | GLU |
| 18 | l | 217 | SER |
| 18 | l | 237 | ASP |
| 18 | l | 336 | SER |
| 18 | l | 337 | ASN |
| 19 | m | 228 | ALA |
| 19 | m | 605 | SER |
| 19 | m | 700 | LYS |
| 19 | m | 702 | TYR |
| 20 | n | 117 | THR |
| 20 | n | 148 | GLU |
| 20 | n | 151 | LEU |
| 20 | n | 164 | LEU |
| 20 | n | 343 | SER |
| 20 | n | 396 | LYS |
| 20 | n | 578 | LYS |
| 20 | n | 607 | SER |
| 20 | n | 655 | PHE |
| 20 | n | 713 | ASP |
| 20 | n | 940 | ASP |
| 20 | n | 1011 | ASP |
| 20 | n | 1015 | LEU |
| 20 | n | 1126 | ASP |
| 21 | p | 56 | THR |
| 21 | q | 56 | THR |
| 21 | t | 56 | THR |
| 15 | b | 124 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | b | 426 | ALA |
| 15 | b | 516 | ASN |
| 15 | b | 594 | ILE |
| 15 | b | 615 | VAL |
| 15 | b | 675 | PHE |
| 15 | b | 703 | ASP |
| 16 | c | 157 | SER |
| 16 | c | 323 | SER |
| 16 | c | 499 | ASP |
| 16 | c | 520 | ALA |
| 16 | c | 569 | GLU |
| 16 | c | 635 | ASP |
| 16 | c | 650 | HIS |
| 16 | c | 761 | SER |
| 16 | c | 781 | TYR |
| 17 | d | 30 | ASP |
| 17 | d | 217 | LEU |
| 17 | d | 219 | ARG |
| 18 | e | 57 | SER |
| 18 | e | 79 | LYS |
| 18 | e | 106 | ASP |
| 18 | e | 212 | LYS |
| 18 | e | 325 | ASP |
| 18 | e | 338 | GLU |
| 19 | f | 439 | SER |
| 19 | f | 559 | CYS |
| 19 | f | 560 | LYS |
| 19 | f | 612 | ASN |
| 19 | f | 627 | THR |
| 19 | f | 644 | ALA |
| 19 | f | 674 | ALA |
| 19 | f | 702 | TYR |
| 20 | g | 81 | SER |
| 20 | g | 393 | THR |
| 20 | g | 396 | LYS |
| 20 | g | 422 | ASN |
| 20 | g | 448 | SER |
| 20 | g | 625 | GLN |
| 20 | g | 688 | THR |
| 20 | g | 761 | ASN |
| 20 | g | 819 | GLN |
| 20 | g | 936 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | g | 1007 | SER |
| 20 | g | 1015 | LEU |
| 20 | g | 1083 | LEU |
| 14 | a | 115 | GLN |
| 14 | a | 156 | TYR |
| 14 | a | 382 | VAL |
| 14 | a | 456 | ALA |
| 14 | a | 490 | VAL |
| 14 | a | 559 | GLU |
| 14 | a | 884 | GLU |
| 14 | a | 897 | SER |
| 14 | a | 917 | ASP |
| 14 | a | 966 | CYS |
| 14 | a | 993 | VAL |
| 14 | a | 1011 | ASP |
| 14 | a | 1013 | ALA |
| 1 | 0 | 140 | ASN |
| 1 | 0 | 266 | GLN |
| 1 | 0 | 419 | LYS |
| 1 | 0 | 432 | ASN |
| 1 | 0 | 1153 | ASN |
| 1 | 0 | 1198 | ASN |
| 1 | 0 | 1296 | THR |
| 1 | 0 | 1379 | GLN |
| 1 | 0 | 1463 | ARG |
| 2 | 1 | 149 | GLU |
| 2 | 1 | 152 | SER |
| 2 | 1 | 287 | GLN |
| 2 | 1 | 416 | GLU |
| 2 | 1 | 679 | SER |
| 2 | 1 | 724 | TRP |
| 2 | 1 | 745 | ILE |
| 2 | 1 | 922 | LYS |
| 2 | 1 | 931 | ALA |
| 2 | 1 | 975 | ASP |
| 2 | 1 | 1106 | GLU |
| 2 | 1 | 1317 | SER |
| 4 | A | 744 | ALA |
| 4 | A | 754 | ASN |
| 5 | B | 320 | GLU |
| 5 | B | 324 | TYR |
| 6 | C | 353 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | C | 370 | ASP |
| 4 | D | 754 | ASN |
| 5 | E | 332 | GLN |
| 5 | E | 346 | GLN |
| 5 | E | 393 | ASP |
| 6 | F | 353 | LEU |
| 4 | G | 752 | ASP |
| 5 | H | 305 | LYS |
| 5 | H | 324 | TYR |
| 5 | H | 327 | PRO |
| 5 | H | 434 | GLU |
| 6 | I | 438 | ALA |
| 4 | J | 752 | ASP |
| 5 | K | 319 | THR |
| 5 | K | 332 | GLN |
| 5 | K | 507 | ASN |
| 6 | L | 370 | ASP |
| 7 | M | 298 | ASP |
| 7 | M | 307 | ASP |
| 7 | M | 346 | SER |
| 7 | M | 666 | SER |
| 7 | M | 667 | SER |
| 7 | M | 730 | VAL |
| 7 | M | 749 | ILE |
| 7 | M | 963 | ASN |
| 7 | M | 1036 | PRO |
| 7 | M | 1323 | THR |
| 7 | M | 1435 | LYS |
| 7 | M | 1609 | SER |
| 7 | M | 1665 | GLU |
| 8 | N | 32 | VAL |
| 8 | N | 67 | ASP |
| 8 | N | 70 | LYS |
| 8 | N | 203 | LYS |
| 8 | N | 221 | VAL |
| 8 | N | 257 | LEU |
| 8 | N | 277 | THR |
| 8 | N | 325 | TRP |
| 8 | N | 358 | VAL |
| 8 | N | 360 | GLN |
| 8 | N | 409 | GLU |
| 8 | N | 421 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | N | 659 | GLU |
| 8 | N | 668 | TYR |
| 8 | N | 683 | ASP |
| 8 | N | 754 | TYR |
| 8 | N | 828 | LEU |
| 8 | N | 870 | PRO |
| 8 | N | 878 | PHE |
| 8 | N | 915 | ASP |
| 8 | N | 930 | ALA |
| 8 | N | 931 | PHE |
| 8 | N | 948 | LEU |
| 8 | N | 1060 | LEU |
| 8 | N | 1252 | LEU |
| 8 | N | 1403 | ASN |
| 7 | O | 22 | PHE |
| 7 | O | 205 | ALA |
| 7 | O | 307 | ASP |
| 7 | O | 342 | TYR |
| 7 | O | 351 | HIS |
| 7 | O | 470 | ASP |
| 7 | O | 499 | PHE |
| 7 | O | 682 | ASP |
| 7 | O | 761 | LEU |
| 7 | O | 762 | ALA |
| 7 | O | 795 | VAL |
| 7 | O | 821 | GLU |
| 7 | O | 835 | LYS |
| 7 | O | 885 | GLU |
| 7 | O | 951 | ARG |
| 7 | O | 993 | ALA |
| 7 | O | 995 | VAL |
| 7 | O | 1030 | ASN |
| 7 | O | 1064 | THR |
| 7 | O | 1138 | PHE |
| 7 | O | 1188 | THR |
| 7 | O | 1482 | THR |
| 7 | O | 1483 | THR |
| 7 | O | 1516 | THR |
| 8 | P | 57 | THR |
| 8 | P | 132 | ASN |
| 8 | P | 161 | ALA |
| 8 | P | 257 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | P | 275 | LEU |
| 8 | P | 278 | SER |
| 8 | P | 425 | LEU |
| 8 | P | 457 | LEU |
| 8 | P | 650 | ASP |
| 8 | P | 763 | GLN |
| 8 | P | 870 | PRO |
| 8 | P | 871 | SER |
| 8 | P | 874 | GLU |
| 8 | P | 875 | LYS |
| 8 | P | 892 | SER |
| 8 | P | 897 | LYS |
| 8 | P | 926 | ALA |
| 8 | P | 941 | SER |
| 8 | P | 968 | SER |
| 8 | P | 1032 | ILE |
| 8 | P | 1050 | SER |
| 8 | P | 1051 | LYS |
| 8 | P | 1092 | SER |
| 8 | P | 1250 | ILE |
| 8 | P | 1320 | GLU |
| 8 | P | 1398 | VAL |
| 8 | P | 1512 | ILE |
| 8 | P | 1566 | TYR |
| 9 | Q | 45 | SER |
| 9 | Q | 47 | ASN |
| 9 | Q | 79 | SER |
| 9 | Q | 83 | VAL |
| 9 | Q | 229 | ASN |
| 9 | Q | 270 | ILE |
| 9 | Q | 316 | ALA |
| 9 | Q | 318 | LYS |
| 9 | Q | 427 | ALA |
| 9 | Q | 615 | ASP |
| 9 | R | 47 | ASN |
| 9 | R | 79 | SER |
| 9 | R | 111 | PHE |
| 9 | R | 294 | MET |
| 9 | R | 307 | SER |
| 9 | R | 324 | ASN |
| 9 | R | 669 | ASP |
| 9 | R | 681 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | R | 765 | ASP |
| 9 | S | 324 | ASN |
| 9 | S | 604 | ILE |
| 9 | S | 697 | PHE |
| 9 | S | 775 | LEU |
| 9 | T | 46 | ILE |
| 9 | T | 78 | LEU |
| 9 | T | 107 | GLU |
| 9 | T | 149 | ALA |
| 9 | T | 155 | VAL |
| 9 | T | 316 | ALA |
| 9 | T | 319 | SER |
| 9 | T | 457 | TYR |
| 9 | T | 476 | ASN |
| 9 | T | 596 | ASP |
| 9 | T | 681 | SER |
| 9 | T | 732 | TRP |
| 10 | U | 261 | THR |
| 10 | U | 354 | ALA |
| 11 | V | 270 | ALA |
| 11 | V | 373 | ASN |
| 11 | X | 279 | SER |
| 11 | X | 282 | ASN |
| 1 | Y | 139 | LYS |
| 1 | Y | 293 | ILE |
| 1 | Y | 522 | ALA |
| 1 | Y | 710 | VAL |
| 1 | Y | 784 | ILE |
| 1 | Y | 1108 | VAL |
| 1 | Y | 1169 | ASN |
| 1 | Y | 1258 | LEU |
| 1 | Y | 1303 | SER |
| 1 | Y | 1350 | GLU |
| 2 | Z | 128 | GLU |
| 2 | Z | 134 | ALA |
| 2 | Z | 220 | ASN |
| 2 | Z | 361 | SER |
| 2 | Z | 513 | LYS |
| 2 | Z | 668 | GLY |
| 2 | Z | 672 | VAL |
| 2 | Z | 679 | SER |
| 2 | Z | 788 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Z | 878 | GLY |
| 2 | Z | 901 | ILE |
| 2 | Z | 988 | CYS |
| 2 | Z | 1186 | ASP |
| 2 | Z | 1198 | ARG |
| 2 | Z | 1210 | ALA |
| 2 | Z | 1382 | TYR |
| 2 | Z | 1386 | ARG |
| 2 | Z | 1390 | LEU |
| 12 | u | 49 | LEU |
| 12 | u | 52 | SER |
| 12 | u | 66 | ASP |
| 12 | u | 75 | THR |
| 12 | u | 85 | ASP |
| 12 | u | 136 | SER |
| 12 | u | 139 | ASP |
| 12 | u | 176 | ASP |
| 12 | u | 239 | SER |
| 12 | u | 275 | GLU |
| 12 | u | 333 | MET |
| 12 | u | 338 | ASP |
| 12 | v | 75 | THR |
| 12 | v | 76 | SER |
| 12 | v | 85 | ASP |
| 12 | v | 129 | LYS |
| 12 | v | 171 | ASN |
| 12 | v | 239 | SER |
| 12 | v | 243 | VAL |
| 12 | v | 283 | GLY |
| 12 | v | 295 | TYR |
| 14 | h | 55 | GLU |
| 14 | h | 155 | PRO |
| 14 | h | 190 | ASP |
| 14 | h | 219 | ASP |
| 14 | h | 241 | CYS |
| 14 | h | 326 | SER |
| 14 | h | 424 | GLN |
| 14 | h | 456 | ALA |
| 14 | h | 494 | PHE |
| 14 | h | 601 | PHE |
| 14 | h | 805 | ASP |
| 14 | h | 967 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | h | 1003 | VAL |
| 15 | i | 57 | PRO |
| 15 | i | 86 | ASP |
| 15 | i | 122 | ARG |
| 15 | i | 273 | TYR |
| 15 | i | 348 | GLN |
| 15 | i | 369 | GLU |
| 15 | i | 390 | TRP |
| 15 | i | 593 | ALA |
| 15 | i | 660 | LYS |
| 15 | i | 677 | LEU |
| 15 | i | 686 | ASP |
| 15 | i | 689 | ALA |
| 15 | i | 718 | LYS |
| 15 | i | 721 | PRO |
| 15 | i | 723 | SER |
| 16 | j | 301 | ASN |
| 16 | j | 345 | THR |
| 16 | j | 366 | PHE |
| 16 | j | 520 | ALA |
| 16 | j | 649 | LYS |
| 16 | j | 778 | GLU |
| 16 | j | 781 | TYR |
| 17 | k | 65 | LYS |
| 17 | k | 144 | HIS |
| 17 | k | 217 | LEU |
| 17 | k | 276 | ASN |
| 18 | l | 78 | ASP |
| 18 | l | 158 | SER |
| 18 | l | 163 | ASN |
| 19 | m | 218 | TYR |
| 19 | m | 319 | SER |
| 19 | m | 433 | ALA |
| 19 | m | 451 | SER |
| 19 | m | 515 | GLU |
| 19 | m | 548 | GLN |
| 19 | m | 635 | LEU |
| 20 | n | 144 | ALA |
| 20 | n | 247 | LEU |
| 20 | n | 251 | PRO |
| 20 | n | 451 | ASN |
| 20 | n | 714 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | n | 733 | GLY |
| 20 | n | 819 | GLN |
| 20 | n | 856 | LYS |
| 20 | n | 885 | VAL |
| 20 | n | 1074 | ASN |
| 20 | n | 1083 | LEU |
| 21 | o | 56 | THR |
| 21 | q | 55 | ASN |
| 21 | r | 55 | ASN |
| 21 | r | 69 | VAL |
| 15 | b | 56 | GLN |
| 15 | b | 216 | ASP |
| 15 | b | 251 | GLN |
| 15 | b | 272 | PRO |
| 15 | b | 350 | SER |
| 15 | b | 381 | ALA |
| 15 | b | 387 | THR |
| 15 | b | 521 | TRP |
| 15 | b | 621 | ARG |
| 15 | b | 681 | LYS |
| 15 | b | 742 | ALA |
| 16 | c | 583 | SER |
| 16 | c | 607 | ARG |
| 16 | c | 609 | LYS |
| 16 | c | 632 | GLU |
| 17 | d | 9 | ASN |
| 17 | d | 286 | GLU |
| 18 | e | 176 | SER |
| 19 | f | 142 | SER |
| 19 | f | 144 | TRP |
| 19 | f | 320 | HIS |
| 19 | f | 453 | GLU |
| 19 | f | 542 | ARG |
| 19 | f | 699 | ASP |
| 20 | g | 144 | ALA |
| 20 | g | 152 | ALA |
| 20 | g | 217 | ALA |
| 20 | g | 274 | PRO |
| 20 | g | 313 | TYR |
| 20 | g | 370 | SER |
| 20 | g | 441 | ARG |
| 20 | g | 575 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | g | 578 | LYS |
| 20 | g | 639 | PRO |
| 20 | g | 705 | LYS |
| 20 | g | 1084 | LEU |
| 20 | g | 1150 | TYR |
| 14 | a | 55 | GLU |
| 14 | a | 155 | PRO |
| 14 | a | 172 | GLN |
| 14 | a | 192 | VAL |
| 14 | a | 219 | ASP |
| 14 | a | 295 | ASN |
| 14 | a | 326 | SER |
| 14 | a | 346 | ALA |
| 14 | a | 404 | VAL |
| 14 | a | 424 | GLN |
| 14 | a | 885 | VAL |
| 14 | a | 957 | ASP |
| 14 | a | 965 | TYR |
| 14 | a | 1028 | THR |
| 14 | a | 1035 | ARG |
| 1 | 0 | 122 | ASP |
| 1 | 0 | 261 | LEU |
| 1 | 0 | 522 | ALA |
| 1 | 0 | 617 | ALA |
| 1 | 0 | 693 | GLU |
| 1 | 0 | 710 | VAL |
| 1 | 0 | 885 | ALA |
| 1 | 0 | 1006 | ALA |
| 1 | 0 | 1022 | ASP |
| 1 | 0 | 1058 | ASN |
| 1 | 0 | 1292 | GLU |
| 1 | 0 | 1312 | ALA |
| 1 | 0 | 1332 | ASP |
| 1 | 0 | 1381 | SER |
| 2 | 1 | 160 | LYS |
| 2 | 1 | 195 | ASP |
| 2 | 1 | 341 | THR |
| 2 | 1 | 351 | ARG |
| 2 | 1 | 371 | ASN |
| 2 | 1 | 376 | PRO |
| 2 | 1 | 415 | CYS |
| 2 | 1 | 419 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1 | 706 | SER |
| 2 | 1 | 721 | SER |
| 2 | 1 | 925 | ARG |
| 2 | 1 | 1385 | ASP |
| 5 | B | 329 | HIS |
| 6 | F | 370 | ASP |
| 4 | G | 755 | LEU |
| 4 | G | 776 | PHE |
| 5 | H | 316 | VAL |
| 6 | I | 300 | ASP |
| 5 | K | 318 | GLU |
| 6 | L | 405 | LEU |
| 7 | M | 3 | TRP |
| 7 | M | 83 | LEU |
| 7 | M | 518 | ASN |
| 7 | M | 603 | GLU |
| 7 | M | 997 | ALA |
| 7 | M | 998 | LEU |
| 7 | M | 1064 | THR |
| 7 | M | 1069 | ASP |
| 7 | M | 1205 | ASN |
| 7 | M | 1221 | LEU |
| 7 | M | 1273 | LYS |
| 7 | M | 1396 | LEU |
| 7 | M | 1448 | GLY |
| 7 | M | 1500 | ASN |
| 7 | M | 1577 | LYS |
| 8 | N | 26 | ALA |
| 8 | N | 42 | GLN |
| 8 | N | 59 | ARG |
| 8 | N | 132 | ASN |
| 8 | N | 410 | GLN |
| 8 | N | 457 | LEU |
| 8 | N | 474 | ASP |
| 8 | N | 516 | CYS |
| 8 | N | 604 | PRO |
| 8 | N | 826 | SER |
| 8 | N | 829 | ASN |
| 8 | N | 871 | SER |
| 8 | N | 886 | ASP |
| 8 | N | 986 | SER |
| 8 | N | 987 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | N | 991 | LYS |
| 8 | N | 1028 | THR |
| 8 | N | 1061 | THR |
| 8 | N | 1164 | ASP |
| 8 | N | 1172 | SER |
| 8 | N | 1344 | PHE |
| 7 | O | 137 | ASN |
| 7 | O | 353 | PRO |
| 7 | O | 603 | GLU |
| 7 | O | 620 | THR |
| 7 | O | 705 | ASP |
| 7 | O | 736 | PHE |
| 7 | O | 739 | ARG |
| 7 | O | 1045 | GLY |
| 7 | O | 1069 | ASP |
| 7 | O | 1214 | SER |
| 7 | O | 1273 | LYS |
| 7 | O | 1435 | LYS |
| 7 | O | 1505 | HIS |
| 7 | O | 1559 | LEU |
| 7 | O | 1577 | LYS |
| 7 | O | 1598 | PHE |
| 8 | P | 23 | ASN |
| 8 | P | 24 | ASP |
| 8 | P | 164 | TYR |
| 8 | P | 337 | SER |
| 8 | P | 360 | GLN |
| 8 | P | 372 | ASP |
| 8 | P | 411 | PHE |
| 8 | P | 417 | THR |
| 8 | P | 426 | SER |
| 8 | P | 473 | LEU |
| 8 | P | 517 | LEU |
| 8 | P | 523 | SER |
| 8 | P | 587 | GLN |
| 8 | P | 647 | GLN |
| 8 | P | 796 | SER |
| 8 | P | 992 | SER |
| 8 | P | 1237 | ASN |
| 8 | P | 1333 | SER |
| 9 | Q | 62 | ALA |
| 9 | Q | 65 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | Q | 299 | ALA |
| 9 | Q | 678 | ASP |
| 9 | Q | 765 | ASP |
| 9 | R | 65 | ASP |
| 9 | R | 84 | ASP |
| 9 | R | 154 | GLU |
| 9 | R | 419 | ASP |
| 9 | R | 546 | ARG |
| 9 | R | 547 | TYR |
| 9 | R | 677 | PRO |
| 9 | R | 730 | LYS |
| 9 | R | 754 | ARG |
| 9 | R | 766 | ASN |
| 9 | S | 65 | ASP |
| 9 | S | 230 | GLY |
| 9 | S | 472 | SER |
| 9 | S | 707 | HIS |
| 9 | T | 39 | LEU |
| 9 | T | 105 | GLU |
| 9 | T | 356 | ASN |
| 10 | W | 305 | TYR |
| 10 | W | 306 | PRO |
| 10 | W | 324 | LYS |
| 11 | X | 269 | SER |
| 1 | Y | 147 | PRO |
| 1 | Y | 266 | GLN |
| 1 | Y | 291 | LEU |
| 1 | Y | 514 | SER |
| 1 | Y | 709 | GLY |
| 1 | Y | 766 | LEU |
| 1 | Y | 914 | TYR |
| 1 | Y | 1080 | ALA |
| 1 | Y | 1093 | ASP |
| 1 | Y | 1277 | SER |
| 1 | Y | 1292 | GLU |
| 1 | Y | 1305 | SER |
| 1 | Y | 1313 | VAL |
| 2 | Z | 115 | ASP |
| 2 | Z | 168 | GLU |
| 2 | Z | 179 | LYS |
| 2 | Z | 280 | GLY |
| 2 | Z | 403 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Z | 415 | CYS |
| 2 | Z | 499 | SER |
| 2 | Z | 551 | TYR |
| 2 | Z | 925 | ARG |
| 2 | Z | 927 | HIS |
| 2 | Z | 1040 | LYS |
| 2 | Z | 1156 | LEU |
| 2 | Z | 1187 | TYR |
| 12 | u | 76 | SER |
| 12 | u | 129 | LYS |
| 12 | u | 243 | VAL |
| 12 | u | 295 | TYR |
| 12 | v | 52 | SER |
| 12 | v | 134 | PRO |
| 12 | v | 177 | ALA |
| 12 | v | 238 | ASP |
| 12 | v | 308 | ASP |
| 14 | h | 207 | SER |
| 14 | h | 232 | ARG |
| 14 | h | 357 | SER |
| 14 | h | 398 | VAL |
| 14 | h | 454 | LYS |
| 14 | h | 744 | VAL |
| 14 | h | 935 | LEU |
| 14 | h | 975 | ARG |
| 14 | h | 1004 | ILE |
| 15 | i | 268 | SER |
| 15 | i | 507 | LEU |
| 15 | i | 544 | ASN |
| 15 | i | 607 | ILE |
| 15 | i | 657 | TYR |
| 15 | i | 662 | TYR |
| 15 | i | 685 | GLU |
| 16 | j | 485 | GLN |
| 16 | j | 499 | ASP |
| 16 | j | 636 | SER |
| 16 | j | 647 | GLN |
| 16 | j | 651 | CYS |
| 16 | j | 761 | SER |
| 18 | l | 168 | ASP |
| 18 | l | 177 | ARG |
| 18 | l | 291 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | m | 98 | PRO |
| 19 | m | 429 | ILE |
| 19 | m | 559 | CYS |
| 19 | m | 678 | LEU |
| 20 | n | 73 | GLN |
| 20 | n | 154 | ASN |
| 20 | n | 159 | ASP |
| 20 | n | 357 | ASN |
| 20 | n | 371 | SER |
| 20 | n | 496 | SER |
| 20 | n | 509 | ALA |
| 20 | n | 540 | HIS |
| 20 | n | 705 | LYS |
| 20 | n | 712 | PHE |
| 20 | n | 822 | ASP |
| 20 | n | 1016 | PHE |
| 20 | n | 1031 | PHE |
| 20 | n | 1055 | ASP |
| 15 | b | 51 | MET |
| 15 | b | 88 | TYR |
| 15 | b | 168 | ARG |
| 15 | b | 199 | GLU |
| 15 | b | 229 | SER |
| 15 | b | 460 | GLY |
| 15 | b | 678 | ASP |
| 15 | b | 741 | GLN |
| 16 | c | 147 | SER |
| 16 | c | 247 | PRO |
| 16 | c | 317 | HIS |
| 16 | c | 321 | LEU |
| 16 | c | 364 | SER |
| 16 | c | 651 | CYS |
| 17 | d | 131 | LYS |
| 18 | e | 188 | LEU |
| 19 | f | 230 | GLU |
| 19 | f | 576 | ASN |
| 19 | f | 605 | SER |
| 19 | f | 611 | SER |
| 20 | g | 146 | MET |
| 20 | g | 148 | GLU |
| 20 | g | 343 | SER |
| 20 | g | 509 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | g | 633 | THR |
| 20 | g | 713 | ASP |
| 20 | g | 716 | ASN |
| 20 | g | 835 | PHE |
| 20 | g | 863 | ARG |
| 20 | g | 884 | HIS |
| 20 | g | 893 | ASP |
| 20 | g | 937 | ASP |
| 20 | g | 1016 | PHE |
| 14 | a | 77 | THR |
| 14 | a | 114 | GLU |
| 14 | a | 207 | SER |
| 14 | a | 250 | SER |
| 14 | a | 283 | TYR |
| 14 | a | 328 | ILE |
| 14 | a | 469 | GLU |
| 14 | a | 750 | LEU |
| 14 | a | 816 | THR |
| 14 | a | 881 | MET |
| 1 | 0 | 260 | HIS |
| 1 | 0 | 270 | VAL |
| 1 | 0 | 386 | SER |
| 1 | 0 | 629 | ALA |
| 1 | 0 | 636 | THR |
| 1 | 0 | 669 | PHE |
| 1 | 0 | 714 | LYS |
| 1 | 0 | 1080 | ALA |
| 1 | 0 | 1081 | CYS |
| 1 | 0 | 1165 | LEU |
| 2 | 1 | 136 | THR |
| 2 | 1 | 178 | ASN |
| 2 | 1 | 281 | VAL |
| 2 | 1 | 405 | LYS |
| 2 | 1 | 1357 | LEU |
| 2 | 1 | 1387 | HIS |
| 5 | B | 297 | GLU |
| 5 | B | 318 | GLU |
| 5 | B | 346 | GLN |
| 5 | E | 331 | LEU |
| 6 | L | 342 | GLU |
| 6 | L | 406 | PHE |
| 7 | M | 351 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | M | 425 | ASP |
| 7 | M | 704 | SER |
| 7 | M | 989 | SER |
| 7 | M | 1143 | SER |
| 7 | M | 1343 | ILE |
| 7 | M | 1600 | LEU |
| 7 | M | 1666 | MET |
| 8 | N | 341 | PHE |
| 8 | N | 417 | THR |
| 8 | N | 450 | THR |
| 8 | N | 611 | SER |
| 8 | N | 663 | MET |
| 8 | N | 780 | HIS |
| 8 | N | 783 | PHE |
| 8 | N | 1120 | LYS |
| 7 | O | 725 | ASN |
| 7 | O | 742 | GLN |
| 7 | O | 859 | LYS |
| 7 | O | 989 | SER |
| 7 | O | 1013 | TYR |
| 7 | O | 1239 | PHE |
| 8 | P | 27 | ALA |
| 8 | P | 59 | ARG |
| 8 | P | 86 | ASP |
| 8 | P | 89 | PHE |
| 8 | P | 119 | ASN |
| 8 | P | 192 | LEU |
| 8 | P | 343 | ASP |
| 8 | P | 604 | PRO |
| 8 | P | 805 | LEU |
| 8 | P | 1059 | ASN |
| 8 | P | 1240 | PHE |
| 8 | P | 1336 | LEU |
| 8 | P | 1432 | ARG |
| 9 | Q | 78 | LEU |
| 9 | Q | 84 | ASP |
| 9 | Q | 677 | PRO |
| 9 | Q | 756 | LYS |
| 9 | Q | 760 | PHE |
| 9 | R | 106 | SER |
| 9 | R | 264 | LYS |
| 9 | R | 321 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | R | 672 | GLN |
| 9 | R | 834 | ASN |
| 9 | S | 370 | TYR |
| 9 | S | 550 | PRO |
| 9 | S | 615 | ASP |
| 9 | S | 698 | ASP |
| 9 | S | 774 | LEU |
| 9 | S | 791 | GLU |
| 9 | T | 79 | SER |
| 9 | T | 102 | LYS |
| 9 | T | 109 | LEU |
| 9 | T | 269 | ASN |
| 9 | T | 430 | LEU |
| 9 | T | 546 | ARG |
| 9 | T | 678 | ASP |
| 11 | V | 354 | SER |
| 10 | W | 357 | LYS |
| 11 | X | 293 | HIS |
| 11 | X | 299 | GLN |
| 1 | Y | 122 | ASP |
| 1 | Y | 170 | LYS |
| 1 | Y | 186 | ILE |
| 1 | Y | 187 | ASP |
| 1 | Y | 210 | THR |
| 1 | Y | 270 | VAL |
| 1 | Y | 464 | SER |
| 1 | Y | 636 | THR |
| 1 | Y | 693 | GLU |
| 1 | Y | 1061 | PRO |
| 1 | Y | 1107 | LEU |
| 1 | Y | 1110 | ASP |
| 1 | Y | 1224 | ASN |
| 1 | Y | 1361 | MET |
| 1 | Y | 1475 | LYS |
| 2 | Z | 161 | SER |
| 2 | Z | 340 | GLU |
| 2 | Z | 352 | GLY |
| 2 | Z | 537 | LYS |
| 2 | Z | 706 | SER |
| 12 | u | 177 | ALA |
| 12 | u | 182 | ILE |
| 12 | u | 291 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | v | 41 | ASN |
| 14 | h | 77 | THR |
| 14 | h | 266 | ASP |
| 14 | h | 346 | ALA |
| 14 | h | 504 | SER |
| 14 | h | 750 | LEU |
| 14 | h | 817 | VAL |
| 15 | i | 134 | SER |
| 15 | i | 270 | LEU |
| 15 | i | 454 | LEU |
| 15 | i | 543 | GLY |
| 15 | i | 646 | LEU |
| 16 | j | 176 | PRO |
| 16 | j | 612 | VAL |
| 17 | k | 30 | ASP |
| 17 | k | 51 | GLY |
| 17 | k | 151 | ALA |
| 19 | m | 315 | LEU |
| 19 | m | 335 | HIS |
| 19 | m | 470 | LEU |
| 19 | m | 683 | PHE |
| 19 | m | 687 | ALA |
| 20 | n | 152 | ALA |
| 20 | n | 156 | ASN |
| 20 | n | 181 | ILE |
| 20 | n | 209 | ASP |
| 20 | n | 346 | LEU |
| 20 | n | 355 | SER |
| 20 | n | 444 | GLU |
| 20 | n | 510 | ASN |
| 20 | n | 575 | PHE |
| 20 | n | 760 | ILE |
| 20 | n | 868 | HIS |
| 21 | s | 56 | THR |
| 15 | b | 48 | LEU |
| 15 | b | 403 | HIS |
| 15 | b | 458 | ARG |
| 15 | b | 555 | SER |
| 15 | b | 587 | ASP |
| 15 | b | 591 | LEU |
| 15 | b | 608 | PRO |
| 15 | b | 661 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | b | 664 | VAL |
| 15 | b | 687 | SER |
| 16 | c | 370 | PHE |
| 16 | c | 579 | ARG |
| 16 | c | 649 | LYS |
| 19 | f | 154 | LYS |
| 19 | f | 228 | ALA |
| 19 | f | 708 | SER |
| 20 | g | 76 | TYR |
| 20 | g | 94 | ILE |
| 20 | g | 159 | ASP |
| 20 | g | 314 | GLU |
| 20 | g | 374 | SER |
| 20 | g | 404 | MET |
| 20 | g | 510 | ASN |
| 20 | g | 546 | ILE |
| 20 | g | 581 | PRO |
| 20 | g | 795 | VAL |
| 20 | g | 813 | GLY |
| 20 | g | 856 | LYS |
| 20 | g | 1031 | PHE |
| 14 | a | 65 | SER |
| 14 | a | 190 | ASP |
| 14 | a | 230 | HIS |
| 14 | a | 357 | SER |
| 14 | a | 427 | LEU |
| 14 | a | 543 | SER |
| 14 | a | 671 | ASP |
| 14 | a | 736 | ASN |
| 14 | a | 751 | ARG |
| 14 | a | 798 | LYS |
| 14 | a | 817 | VAL |
| 14 | a | 837 | SER |
| 14 | a | 996 | LYS |
| 14 | a | 1010 | PHE |
| 1 | 0 | 209 | HIS |
| 1 | 0 | 527 | SER |
| 1 | 0 | 947 | LEU |
| 1 | 0 | 1186 | LEU |
| 1 | 0 | 1200 | LEU |
| 1 | 0 | 1401 | THR |
| 2 | 1 | 141 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1 | 177 | ASP |
| 2 | 1 | 676 | LYS |
| 2 | 1 | 746 | SER |
| 2 | 1 | 960 | GLN |
| 2 | 1 | 1123 | PHE |
| 2 | 1 | 1227 | GLN |
| 2 | 1 | 1334 | GLY |
| 2 | 1 | 1364 | GLU |
| 4 | A | 723 | SER |
| 5 | B | 446 | ARG |
| 4 | G | 723 | SER |
| 7 | M | 619 | VAL |
| 7 | M | 790 | SER |
| 7 | M | 1030 | ASN |
| 7 | M | 1141 | SER |
| 7 | M | 1612 | LEU |
| 7 | M | 1663 | LEU |
| 7 | M | 1664 | ASN |
| 8 | N | 54 | SER |
| 8 | N | 66 | GLY |
| 8 | N | 80 | GLN |
| 8 | N | 223 | PHE |
| 8 | N | 290 | MET |
| 8 | N | 552 | LEU |
| 8 | N | 609 | GLU |
| 8 | N | 746 | ALA |
| 8 | N | 938 | ASP |
| 8 | N | 1027 | TRP |
| 8 | N | 1254 | ARG |
| 8 | N | 1277 | ILE |
| 7 | O | 293 | PRO |
| 7 | O | 463 | SER |
| 7 | O | 623 | VAL |
| 7 | O | 726 | SER |
| 7 | O | 791 | PHE |
| 7 | O | 899 | PHE |
| 7 | O | 1500 | ASN |
| 7 | O | 1535 | ALA |
| 8 | P | 42 | GLN |
| 8 | P | 58 | ILE |
| 8 | P | 162 | HIS |
| 8 | P | 443 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | P | 471 | ASN |
| 8 | P | 602 | VAL |
| 8 | P | 613 | GLU |
| 8 | P | 1249 | GLN |
| 9 | Q | 534 | PHE |
| 9 | R | 44 | VAL |
| 9 | R | 295 | ASN |
| 9 | R | 358 | ALA |
| 9 | R | 671 | ASP |
| 9 | S | 44 | VAL |
| 9 | S | 60 | ASN |
| 9 | T | 84 | ASP |
| 9 | T | 604 | ILE |
| 11 | X | 354 | SER |
| 1 | Y | 126 | TYR |
| 1 | Y | 261 | LEU |
| 1 | Y | 527 | SER |
| 1 | Y | 616 | ASN |
| 1 | Y | 978 | GLY |
| 1 | Y | 1045 | GLU |
| 1 | Y | 1154 | ASP |
| 1 | Y | 1332 | ASP |
| 1 | Y | 1349 | MET |
| 1 | Y | 1403 | PRO |
| 1 | Y | 1466 | ILE |
| 2 | Z | 991 | ALA |
| 12 | u | 111 | ILE |
| 12 | u | 378 | ASP |
| 12 | v | 167 | ASN |
| 12 | v | 289 | PRO |
| 12 | v | 309 | ASN |
| 14 | h | 408 | PHE |
| 14 | h | 751 | ARG |
| 14 | h | 788 | ASP |
| 14 | h | 836 | ASN |
| 14 | h | 837 | SER |
| 14 | h | 918 | PHE |
| 14 | h | 1015 | ASP |
| 14 | h | 1017 | TRP |
| 15 | i | 222 | GLU |
| 15 | i | 594 | ILE |
| 15 | i | 641 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | j | 567 | LEU |
| 16 | j | 769 | PRO |
| 18 | l | 146 | ARG |
| 19 | m | 454 | ASP |
| 19 | m | 627 | THR |
| 20 | n | 66 | ARG |
| 20 | n | 94 | ILE |
| 20 | n | 437 | TYR |
| 20 | n | 472 | MET |
| 20 | n | 511 | PRO |
| 20 | n | 546 | ILE |
| 20 | n | 716 | ASN |
| 20 | n | 833 | GLU |
| 20 | n | 835 | PHE |
| 20 | n | 899 | ALA |
| 20 | n | 912 | LYS |
| 21 | o | 75 | HIS |
| 21 | r | 56 | THR |
| 21 | t | 65 | PHE |
| 15 | b | 201 | ARG |
| 15 | b | 463 | SER |
| 15 | b | 595 | VAL |
| 15 | b | 723 | SER |
| 16 | c | 288 | SER |
| 16 | c | 366 | PHE |
| 16 | c | 568 | ALA |
| 16 | c | 584 | ASN |
| 19 | f | 452 | LEU |
| 19 | f | 633 | THR |
| 19 | f | 687 | ALA |
| 20 | g | 70 | LYS |
| 20 | g | 170 | SER |
| 20 | g | 733 | GLY |
| 14 | a | 435 | ALA |
| 14 | a | 689 | GLY |
| 14 | a | 992 | ASP |
| 1 | 0 | 529 | GLY |
| 1 | 0 | 1083 | TYR |
| 1 | 0 | 1085 | ALA |
| 1 | 0 | 1405 | GLU |
| 1 | 0 | 1437 | SER |
| 2 | 1 | 945 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | B | 332 | GLN |
| 5 | H | 291 | GLN |
| 7 | M | 353 | PRO |
| 7 | M | 744 | TYR |
| 7 | M | 990 | ILE |
| 7 | M | 1594 | GLY |
| 8 | N | 89 | PHE |
| 8 | N | 135 | PHE |
| 8 | N | 276 | ASN |
| 8 | N | 686 | GLY |
| 8 | N | 919 | LEU |
| 8 | N | 1171 | ARG |
| 7 | O | 23 | ASP |
| 7 | O | 790 | SER |
| 8 | P | 277 | THR |
| 8 | P | 419 | ASP |
| 8 | P | 588 | HIS |
| 8 | P | 917 | PRO |
| 8 | P | 965 | ASP |
| 8 | P | 1277 | ILE |
| 9 | Q | 269 | ASN |
| 9 | Q | 443 | ILE |
| 9 | Q | 544 | SER |
| 9 | T | 115 | THR |
| 1 | Y | 238 | MET |
| 1 | Y | 383 | THR |
| 1 | Y | 1059 | TYR |
| 2 | Z | 226 | THR |
| 2 | Z | 958 | ASN |
| 12 | u | 201 | GLU |
| 12 | u | 312 | ASN |
| 12 | u | 341 | ASN |
| 12 | u | 381 | ILE |
| 12 | v | 381 | ILE |
| 12 | v | 433 | ASP |
| 14 | h | 325 | ALA |
| 14 | h | 736 | ASN |
| 14 | h | 996 | LYS |
| 15 | i | 413 | ASP |
| 15 | i | 671 | LEU |
| 16 | j | 326 | GLY |
| 16 | j | 650 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | k | 9 | ASN |
| 17 | k | 254 | PRO |
| 18 | l | 118 | PRO |
| 19 | m | 142 | SER |
| 19 | m | 612 | ASN |
| 20 | n | 810 | ASP |
| 20 | n | 941 | ILE |
| 15 | b | 413 | ASP |
| 15 | b | 658 | LEU |
| 16 | c | 365 | PRO |
| 16 | c | 413 | PRO |
| 17 | d | 18 | ASP |
| 18 | e | 119 | ALA |
| 18 | e | 304 | ASN |
| 19 | f | 279 | TYR |
| 19 | f | 613 | ILE |
| 20 | g | 239 | LYS |
| 20 | g | 411 | ASN |
| 20 | g | 435 | SER |
| 20 | g | 576 | ASN |
| 20 | g | 631 | THR |
| 20 | g | 686 | GLU |
| 14 | a | 342 | LEU |
| 14 | a | 604 | ALA |
| 14 | a | 748 | PHE |
| 14 | a | 1017 | TRP |
| 1 | 0 | 177 | PRO |
| 1 | 0 | 186 | ILE |
| 4 | A | 725 | VAL |
| 5 | E | 343 | PRO |
| 7 | M | 796 | ILE |
| 7 | M | 1441 | ILE |
| 8 | N | 601 | VAL |
| 9 | T | 746 | PRO |
| 2 | Z | 627 | ASN |
| 14 | h | 791 | PRO |
| 5 | H | 322 | ILE |
| 7 | M | 1611 | VAL |
| 8 | N | 863 | GLY |
| 1 | Y | 1385 | PHE |
| 2 | Z | 598 | PRO |
| 12 | v | 182 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | i | 605 | VAL |
| 19 | m | 318 | PRO |
| 20 | n | 707 | PRO |
| 15 | b | 383 | VAL |
| 19 | f | 272 | PRO |
| 14 | a | 945 | VAL |
| 14 | a | 1025 | VAL |
| 1 | 0 | 1384 | ILE |
| 7 | M | 1090 | PRO |
| 7 | M | 1595 | VAL |
| 9 | T | 603 | VAL |
| 2 | Z | 676 | LYS |
| 14 | h | 192 | VAL |
| 18 | l | 66 | PRO |
| 19 | m | 35 | PRO |
| 20 | n | 277 | GLY |
| 17 | d | 97 | VAL |
| 20 | g | 154 | ASN |
| 1 | 0 | 147 | PRO |
| 1 | 0 | 515 | VAL |
| 1 | 0 | 1216 | ILE |
| 1 | 0 | 1279 | VAL |
| 2 | 1 | 150 | VAL |
| 7 | M | 1560 | GLY |
| 7 | O | 344 | ILE |
| 8 | P | 321 | ILE |
| 8 | P | 440 | ILE |
| 9 | S | 416 | GLY |
| 1 | Y | 221 | PRO |
| 17 | k | 55 | PRO |
| 20 | n | 494 | VAL |
| 14 | a | 791 | PRO |
| 5 | B | 343 | PRO |
| 8 | N | 391 | PRO |
| 2 | Z | 376 | PRO |
| 19 | f | 471 | PRO |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | 0 | 978/1353 (72%) | 924 (94%) | 54 (6%) | 19 | 41 |
| 1 | Y | 979/1353 (72%) | 918 (94%) | 61 (6%) | 16 | 38 |
| 2 | 1 | 1008/1250 (81%) | 929 (92%) | 79 (8%) | 11 | 32 |
| 2 | Z | 1007/1250 (81%) | 942 (94%) | 65 (6%) | 15 | 37 |
| 4 | A | 154/674 (23%) | 148 (96%) | 6 (4%) | 28 | 49 |
| 4 | D | 154/674 (23%) | 147 (96%) | 7 (4%) | 24 | 46 |
| 4 | G | 155/674 (23%) | 143 (92%) | 12 (8%) | 12 | 32 |
| 4 | J | 155/674 (23%) | 148 (96%) | 7 (4%) | 24 | 46 |
| 5 | B | 196/439 (45%) | 182 (93%) | 14 (7%) | 13 | 35 |
| 5 | E | 196/439 (45%) | 181 (92%) | 15 (8%) | 12 | 32 |
| 5 | H | 196/439 (45%) | 181 (92%) | 15 (8%) | 12 | 32 |
| 5 | K | 196/439 (45%) | 184 (94%) | 12 (6%) | 17 | 38 |
| 6 | C | 155/377 (41%) | 146 (94%) | 9 (6%) | 18 | 40 |
| 6 | F | 155/377 (41%) | 146 (94%) | 9 (6%) | 18 | 40 |
| 6 | I | 155/377 (41%) | 148 (96%) | 7 (4%) | 24 | 46 |
| 6 | L | 155/377 (41%) | 146 (94%) | 9 (6%) | 18 | 40 |
| 7 | M | 1279/1538 (83%) | 1191 (93%) | 88 (7%) | 14 | 36 |
| 7 | O | 1278/1538 (83%) | 1197 (94%) | 81 (6%) | 16 | 37 |
| 8 | N | 1278/1557 (82%) | 1186 (93%) | 92 (7%) | 13 | 35 |
| 8 | P | 1278/1557 (82%) | 1178 (92%) | 100 (8%) | 11 | 32 |
| 9 | Q | 507/762 (66%) | 479 (94%) | 28 (6%) | 19 | 41 |
| 9 | R | 508/762 (67%) | 481 (95%) | 27 (5%) | 20 | 41 |
| 9 | S | 508/762 (67%) | 476 (94%) | 32 (6%) | 16 | 37 |
| 9 | T | 508/762 (67%) | 484 (95%) | 24 (5%) | 23 | 45 |
| 10 | U | 80/421 (19%) | 74 (92%) | 6 (8%) | 12 | 33 |
| 10 | W | 80/421 (19%) | 75 (94%) | 5 (6%) | 16 | 37 |
| 11 | V | 82/477 (17%) | 71 (87%) | 11 (13%) | 4 | 14 |
| 11 | X | 82/477 (17%) | 71 (87%) | 11 (13%) | 4 | 14 |
| 12 | u | 397/670 (59%) | 370 (93%) | 27 (7%) | 14 | 36 |
| 12 | v | 379/670 (57%) | 362 (96%) | 17 (4%) | 24 | 46 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 13 | w | 35/1290 (3%) | 33 (94%) | 2 (6%) | 18 | 40 |
| 13 | x | 36/1290 (3%) | 34 (94%) | 2 (6%) | 19 | 40 |
| 14 | a | 945/972 (97%) | 896 (95%) | 49 (5%) | 21 | 42 |
| 14 | h | 945/972 (97%) | 903 (96%) | 42 (4%) | 25 | 47 |
| 15 | b | 606/670 (90%) | 581 (96%) | 25 (4%) | 27 | 49 |
| 15 | i | 596/670 (89%) | 569 (96%) | 27 (4%) | 24 | 46 |
| 16 | c | 513/646 (79%) | 481 (94%) | 32 (6%) | 16 | 38 |
| 16 | j | 513/646 (79%) | 489 (95%) | 24 (5%) | 23 | 45 |
| 17 | d | 233/252 (92%) | 226 (97%) | 7 (3%) | 36 | 57 |
| 17 | k | 233/252 (92%) | 221 (95%) | 12 (5%) | 21 | 42 |
| 18 | e | 266/305 (87%) | 257 (97%) | 9 (3%) | 32 | 54 |
| 18 | l | 269/305 (88%) | 257 (96%) | 12 (4%) | 24 | 46 |
| 19 | f | 594/669 (89%) | 561 (94%) | 33 (6%) | 19 | 40 |
| 19 | m | 594/669 (89%) | 560 (94%) | 34 (6%) | 18 | 40 |
| 20 | g | 997/1088 (92%) | 956 (96%) | 41 (4%) | 27 | 49 |
| 20 | n | 997/1088 (92%) | 945 (95%) | 52 (5%) | 21 | 42 |
| 21 | o | 75/81 (93%) | 73 (97%) | 2 (3%) | 39 | 61 |
| 21 | p | 75/81 (93%) | 71 (95%) | 4 (5%) | 20 | 41 |
| 21 | q | 75/81 (93%) | 73 (97%) | 2 (3%) | 39 | 61 |
| 21 | r | 75/81 (93%) | 70 (93%) | 5 (7%) | 15 | 36 |
| 21 | s | 75/81 (93%) | 69 (92%) | 6 (8%) | 11 | 31 |
| 21 | t | 75/81 (93%) | 71 (95%) | 4 (5%) | 20 | 41 |
| All | All | 23060/35810 (64%) | 21704 (94%) | 1356 (6%) | 19 | 39 |

All (1356) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 124 | ARG |
| 1 | 0 | 183 | TRP |
| 1 | 0 | 184 | ILE |
| 1 | 0 | 209 | HIS |
| 1 | 0 | 273 | ILE |
| 1 | 0 | 274 | VAL |
| 1 | 0 | 284 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 296 | LEU |
| 1 | 0 | 316 | LYS |
| 1 | 0 | 376 | THR |
| 1 | 0 | 400 | ARG |
| 1 | 0 | 408 | ARG |
| 1 | 0 | 412 | ILE |
| 1 | 0 | 413 | LEU |
| 1 | 0 | 416 | LYS |
| 1 | 0 | 418 | LEU |
| 1 | 0 | 419 | LYS |
| 1 | 0 | 420 | ILE |
| 1 | 0 | 456 | ASN |
| 1 | 0 | 465 | ILE |
| 1 | 0 | 466 | LYS |
| 1 | 0 | 515 | VAL |
| 1 | 0 | 517 | LEU |
| 1 | 0 | 526 | ILE |
| 1 | 0 | 585 | ILE |
| 1 | 0 | 591 | LYS |
| 1 | 0 | 595 | ASN |
| 1 | 0 | 645 | THR |
| 1 | 0 | 788 | HIS |
| 1 | 0 | 832 | VAL |
| 1 | 0 | 884 | VAL |
| 1 | 0 | 897 | ILE |
| 1 | 0 | 904 | LYS |
| 1 | 0 | 953 | PHE |
| 1 | 0 | 962 | LEU |
| 1 | 0 | 976 | THR |
| 1 | 0 | 1012 | ARG |
| 1 | 0 | 1022 | ASP |
| 1 | 0 | 1065 | GLU |
| 1 | 0 | 1079 | LEU |
| 1 | 0 | 1096 | GLN |
| 1 | 0 | 1113 | ILE |
| 1 | 0 | 1200 | LEU |
| 1 | 0 | 1224 | ASN |
| 1 | 0 | 1285 | ILE |
| 1 | 0 | 1382 | GLU |
| 1 | 0 | 1415 | ILE |
| 1 | 0 | 1418 | THR |
| 1 | 0 | 1425 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 1446 | LYS |
| 1 | 0 | 1449 | THR |
| 1 | 0 | 1451 | LEU |
| 1 | 0 | 1475 | LYS |
| 1 | 0 | 1476 | GLU |
| 2 | 1 | 88 | SER |
| 2 | 1 | 89 | GLU |
| 2 | 1 | 110 | ILE |
| 2 | 1 | 144 | THR |
| 2 | 1 | 178 | ASN |
| 2 | 1 | 190 | GLU |
| 2 | 1 | 208 | LYS |
| 2 | 1 | 240 | ARG |
| 2 | 1 | 244 | LEU |
| 2 | 1 | 245 | ASN |
| 2 | 1 | 246 | ILE |
| 2 | 1 | 252 | LYS |
| 2 | 1 | 255 | VAL |
| 2 | 1 | 272 | ILE |
| 2 | 1 | 274 | PHE |
| 2 | 1 | 281 | VAL |
| 2 | 1 | 306 | LYS |
| 2 | 1 | 308 | ASN |
| 2 | 1 | 309 | LEU |
| 2 | 1 | 378 | LEU |
| 2 | 1 | 406 | ILE |
| 2 | 1 | 428 | THR |
| 2 | 1 | 431 | ARG |
| 2 | 1 | 438 | ILE |
| 2 | 1 | 440 | ARG |
| 2 | 1 | 457 | SER |
| 2 | 1 | 487 | LYS |
| 2 | 1 | 495 | THR |
| 2 | 1 | 509 | THR |
| 2 | 1 | 514 | ARG |
| 2 | 1 | 540 | VAL |
| 2 | 1 | 555 | VAL |
| 2 | 1 | 572 | PRO |
| 2 | 1 | 580 | THR |
| 2 | 1 | 603 | VAL |
| 2 | 1 | 604 | LEU |
| 2 | 1 | 609 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1 | 625 | ILE |
| 2 | 1 | 655 | GLU |
| 2 | 1 | 662 | LEU |
| 2 | 1 | 679 | SER |
| 2 | 1 | 723 | ILE |
| 2 | 1 | 745 | ILE |
| 2 | 1 | 762 | LEU |
| 2 | 1 | 765 | PHE |
| 2 | 1 | 774 | VAL |
| 2 | 1 | 824 | SER |
| 2 | 1 | 858 | LYS |
| 2 | 1 | 890 | GLU |
| 2 | 1 | 891 | ARG |
| 2 | 1 | 922 | LYS |
| 2 | 1 | 992 | ASP |
| 2 | 1 | 1002 | ILE |
| 2 | 1 | 1004 | VAL |
| 2 | 1 | 1040 | LYS |
| 2 | 1 | 1041 | LYS |
| 2 | 1 | 1049 | ASN |
| 2 | 1 | 1064 | VAL |
| 2 | 1 | 1078 | GLN |
| 2 | 1 | 1084 | LEU |
| 2 | 1 | 1090 | LYS |
| 2 | 1 | 1094 | ILE |
| 2 | 1 | 1122 | ASP |
| 2 | 1 | 1126 | LYS |
| 2 | 1 | 1127 | LEU |
| 2 | 1 | 1155 | GLN |
| 2 | 1 | 1156 | LEU |
| 2 | 1 | 1178 | ARG |
| 2 | 1 | 1202 | LEU |
| 2 | 1 | 1279 | THR |
| 2 | 1 | 1282 | VAL |
| 2 | 1 | 1292 | ILE |
| 2 | 1 | 1301 | SER |
| 2 | 1 | 1338 | LEU |
| 2 | 1 | 1343 | MET |
| 2 | 1 | 1347 | ILE |
| 2 | 1 | 1355 | SER |
| 2 | 1 | 1375 | ASN |
| 2 | 1 | 1379 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | A | 695 | GLN |
| 4 | A | 755 | LEU |
| 4 | A | 767 | VAL |
| 4 | A | 790 | ASN |
| 4 | A | 812 | THR |
| 4 | A | 823 | LYS |
| 5 | B | 293 | LEU |
| 5 | B | 306 | THR |
| 5 | B | 312 | VAL |
| 5 | B | 319 | THR |
| 5 | B | 322 | ILE |
| 5 | B | 324 | TYR |
| 5 | B | 331 | LEU |
| 5 | B | 361 | ARG |
| 5 | B | 421 | THR |
| 5 | B | 445 | GLN |
| 5 | B | 473 | ILE |
| 5 | B | 512 | ILE |
| 5 | B | 514 | THR |
| 5 | B | 523 | LEU |
| 6 | C | 347 | THR |
| 6 | C | 353 | LEU |
| 6 | C | 369 | LEU |
| 6 | C | 371 | LYS |
| 6 | C | 376 | LYS |
| 6 | C | 398 | VAL |
| 6 | C | 401 | ILE |
| 6 | C | 405 | LEU |
| 6 | C | 462 | GLN |
| 4 | D | 648 | LEU |
| 4 | D | 700 | ILE |
| 4 | D | 726 | VAL |
| 4 | D | 742 | GLN |
| 4 | D | 758 | LEU |
| 4 | D | 762 | LEU |
| 4 | D | 817 | GLN |
| 5 | E | 297 | GLU |
| 5 | E | 305 | LYS |
| 5 | E | 320 | GLU |
| 5 | E | 322 | ILE |
| 5 | E | 323 | LEU |
| 5 | E | 324 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | E | 325 | THR |
| 5 | E | 326 | LYS |
| 5 | E | 356 | GLU |
| 5 | E | 366 | THR |
| 5 | E | 398 | ILE |
| 5 | E | 413 | LEU |
| 5 | E | 435 | LYS |
| 5 | E | 455 | LYS |
| 5 | E | 458 | GLU |
| 6 | F | 276 | GLU |
| 6 | F | 290 | ILE |
| 6 | F | 292 | HIS |
| 6 | F | 318 | SER |
| 6 | F | 349 | THR |
| 6 | F | 370 | ASP |
| 6 | F | 382 | LYS |
| 6 | F | 383 | LYS |
| 6 | F | 440 | VAL |
| 4 | G | 659 | THR |
| 4 | G | 669 | LEU |
| 4 | G | 678 | GLN |
| 4 | G | 695 | GLN |
| 4 | G | 727 | SER |
| 4 | G | 755 | LEU |
| 4 | G | 790 | ASN |
| 4 | G | 791 | ILE |
| 4 | G | 811 | SER |
| 4 | G | 814 | LEU |
| 4 | G | 817 | GLN |
| 4 | G | 821 | ILE |
| 5 | H | 296 | LYS |
| 5 | H | 316 | VAL |
| 5 | H | 318 | GLU |
| 5 | H | 322 | ILE |
| 5 | H | 323 | LEU |
| 5 | H | 324 | TYR |
| 5 | H | 363 | GLN |
| 5 | H | 366 | THR |
| 5 | H | 392 | LEU |
| 5 | H | 446 | ARG |
| 5 | H | 463 | LEU |
| 5 | H | 466 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | H | 514 | THR |
| 5 | H | 517 | GLN |
| 5 | H | 536 | LYS |
| 6 | I | 280 | LEU |
| 6 | I | 345 | LEU |
| 6 | I | 356 | GLN |
| 6 | I | 370 | ASP |
| 6 | I | 390 | ILE |
| 6 | I | 457 | ILE |
| 6 | I | 462 | GLN |
| 4 | J | 660 | LYS |
| 4 | J | 718 | THR |
| 4 | J | 727 | SER |
| 4 | J | 776 | PHE |
| 4 | J | 793 | LEU |
| 4 | J | 817 | GLN |
| 4 | J | 819 | ASN |
| 5 | K | 319 | THR |
| 5 | K | 323 | LEU |
| 5 | K | 326 | LYS |
| 5 | K | 347 | THR |
| 5 | K | 351 | GLN |
| 5 | K | 387 | GLN |
| 5 | K | 392 | LEU |
| 5 | K | 405 | ASN |
| 5 | K | 414 | LYS |
| 5 | K | 442 | THR |
| 5 | K | 471 | LYS |
| 5 | K | 516 | GLN |
| 6 | L | 282 | GLN |
| 6 | L | 347 | THR |
| 6 | L | 353 | LEU |
| 6 | L | 370 | ASP |
| 6 | L | 371 | LYS |
| 6 | L | 382 | LYS |
| 6 | L | 396 | THR |
| 6 | L | 405 | LEU |
| 6 | L | 449 | LEU |
| 7 | M | 33 | GLN |
| 7 | M | 39 | THR |
| 7 | M | 42 | LEU |
| 7 | M | 48 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | M | 56 | ILE |
| 7 | M | 67 | ASN |
| 7 | M | 103 | LYS |
| 7 | M | 126 | GLU |
| 7 | M | 145 | LEU |
| 7 | M | 190 | TYR |
| 7 | M | 193 | LEU |
| 7 | M | 203 | LYS |
| 7 | M | 226 | ASN |
| 7 | M | 231 | ILE |
| 7 | M | 233 | TYR |
| 7 | M | 234 | THR |
| 7 | M | 247 | LEU |
| 7 | M | 273 | VAL |
| 7 | M | 277 | LEU |
| 7 | M | 288 | TRP |
| 7 | M | 309 | PRO |
| 7 | M | 323 | LEU |
| 7 | M | 336 | LYS |
| 7 | M | 360 | LEU |
| 7 | M | 418 | TYR |
| 7 | M | 441 | THR |
| 7 | M | 449 | LEU |
| 7 | M | 461 | LEU |
| 7 | M | 511 | ILE |
| 7 | M | 532 | SER |
| 7 | M | 553 | ILE |
| 7 | M | 571 | ASN |
| 7 | M | 655 | LYS |
| 7 | M | 672 | TRP |
| 7 | M | 701 | THR |
| 7 | M | 702 | LYS |
| 7 | M | 707 | LEU |
| 7 | M | 712 | LEU |
| 7 | M | 733 | LYS |
| 7 | M | 739 | ARG |
| 7 | M | 780 | ILE |
| 7 | M | 848 | VAL |
| 7 | M | 859 | LYS |
| 7 | M | 890 | VAL |
| 7 | M | 910 | ARG |
| 7 | M | 923 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | M | 932 | VAL |
| 7 | M | 942 | LEU |
| 7 | M | 964 | LYS |
| 7 | M | 998 | LEU |
| 7 | M | 1023 | LEU |
| 7 | M | 1041 | PHE |
| 7 | M | 1084 | LEU |
| 7 | M | 1091 | LEU |
| 7 | M | 1117 | THR |
| 7 | M | 1121 | THR |
| 7 | M | 1138 | PHE |
| 7 | M | 1140 | GLU |
| 7 | M | 1161 | LEU |
| 7 | M | 1165 | ILE |
| 7 | M | 1183 | TYR |
| 7 | M | 1189 | MET |
| 7 | M | 1215 | ILE |
| 7 | M | 1224 | GLU |
| 7 | M | 1225 | GLN |
| 7 | M | 1242 | MET |
| 7 | M | 1253 | ARG |
| 7 | M | 1273 | LYS |
| 7 | M | 1283 | LYS |
| 7 | M | 1294 | LYS |
| 7 | M | 1318 | LYS |
| 7 | M | 1323 | THR |
| 7 | M | 1325 | SER |
| 7 | M | 1347 | ILE |
| 7 | M | 1401 | LEU |
| 7 | M | 1402 | ARG |
| 7 | M | 1408 | LEU |
| 7 | M | 1415 | ARG |
| 7 | M | 1437 | LEU |
| 7 | M | 1451 | THR |
| 7 | M | 1460 | LEU |
| 7 | M | 1464 | ILE |
| 7 | M | 1482 | THR |
| 7 | M | 1525 | LEU |
| 7 | M | 1527 | ARG |
| 7 | M | 1532 | ARG |
| 7 | M | 1544 | PHE |
| 7 | M | 1555 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | N | 22 | MET |
| 8 | N | 40 | ILE |
| 8 | N | 44 | LEU |
| 8 | N | 52 | ILE |
| 8 | N | 70 | LYS |
| 8 | N | 72 | ARG |
| 8 | N | 110 | LEU |
| 8 | N | 132 | ASN |
| 8 | N | 137 | VAL |
| 8 | N | 166 | ASN |
| 8 | N | 176 | LEU |
| 8 | N | 202 | THR |
| 8 | N | 203 | LYS |
| 8 | N | 208 | ILE |
| 8 | N | 214 | LEU |
| 8 | N | 217 | GLN |
| 8 | N | 257 | LEU |
| 8 | N | 271 | LEU |
| 8 | N | 281 | GLN |
| 8 | N | 288 | LEU |
| 8 | N | 318 | HIS |
| 8 | N | 359 | LEU |
| 8 | N | 360 | GLN |
| 8 | N | 378 | VAL |
| 8 | N | 380 | THR |
| 8 | N | 391 | PRO |
| 8 | N | 393 | THR |
| 8 | N | 406 | LYS |
| 8 | N | 412 | ILE |
| 8 | N | 447 | LEU |
| 8 | N | 466 | THR |
| 8 | N | 467 | LYS |
| 8 | N | 470 | LEU |
| 8 | N | 473 | LEU |
| 8 | N | 507 | PRO |
| 8 | N | 520 | ILE |
| 8 | N | 522 | LYS |
| 8 | N | 524 | THR |
| 8 | N | 528 | ILE |
| 8 | N | 552 | LEU |
| 8 | N | 564 | LEU |
| 8 | N | 568 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | N | 577 | MET |
| 8 | N | 597 | LEU |
| 8 | N | 605 | LYS |
| 8 | N | 648 | ARG |
| 8 | N | 691 | SER |
| 8 | N | 706 | THR |
| 8 | N | 720 | ARG |
| 8 | N | 784 | THR |
| 8 | N | 794 | ILE |
| 8 | N | 803 | LEU |
| 8 | N | 825 | ILE |
| 8 | N | 875 | LYS |
| 8 | N | 892 | SER |
| 8 | N | 903 | LEU |
| 8 | N | 920 | LEU |
| 8 | N | 934 | GLU |
| 8 | N | 988 | ILE |
| 8 | N | 998 | LEU |
| 8 | N | 1008 | THR |
| 8 | N | 1021 | THR |
| 8 | N | 1031 | LYS |
| 8 | N | 1053 | LEU |
| 8 | N | 1056 | LYS |
| 8 | N | 1057 | LYS |
| 8 | N | 1060 | LEU |
| 8 | N | 1095 | GLU |
| 8 | N | 1096 | ILE |
| 8 | N | 1162 | LEU |
| 8 | N | 1163 | LEU |
| 8 | N | 1186 | GLU |
| 8 | N | 1210 | LEU |
| 8 | N | 1234 | LEU |
| 8 | N | 1249 | GLN |
| 8 | N | 1254 | ARG |
| 8 | N | 1276 | LYS |
| 8 | N | 1277 | ILE |
| 8 | N | 1278 | ILE |
| 8 | N | 1281 | MET |
| 8 | N | 1290 | SER |
| 8 | N | 1303 | LEU |
| 8 | N | 1304 | LYS |
| 8 | N | 1319 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | N | 1352 | LEU |
| 8 | N | 1389 | LEU |
| 8 | N | 1398 | VAL |
| 8 | N | 1423 | ASN |
| 8 | N | 1459 | LYS |
| 8 | N | 1475 | SER |
| 8 | N | 1497 | ASN |
| 8 | N | 1527 | LYS |
| 7 | O | 83 | LEU |
| 7 | O | 98 | THR |
| 7 | O | 103 | LYS |
| 7 | O | 116 | ILE |
| 7 | O | 121 | VAL |
| 7 | O | 141 | VAL |
| 7 | O | 145 | LEU |
| 7 | O | 172 | ASN |
| 7 | O | 234 | THR |
| 7 | O | 270 | THR |
| 7 | O | 277 | LEU |
| 7 | O | 309 | PRO |
| 7 | O | 329 | THR |
| 7 | O | 331 | ILE |
| 7 | O | 334 | GLN |
| 7 | O | 336 | LYS |
| 7 | O | 350 | ARG |
| 7 | O | 360 | LEU |
| 7 | O | 418 | TYR |
| 7 | O | 430 | PHE |
| 7 | O | 431 | PHE |
| 7 | O | 438 | VAL |
| 7 | O | 441 | THR |
| 7 | O | 449 | LEU |
| 7 | O | 488 | PHE |
| 7 | O | 512 | GLU |
| 7 | O | 553 | ILE |
| 7 | O | 569 | ILE |
| 7 | O | 602 | ASN |
| 7 | O | 603 | GLU |
| 7 | O | 608 | PHE |
| 7 | O | 623 | VAL |
| 7 | O | 634 | VAL |
| 7 | O | 697 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | O | 714 | HIS |
| 7 | O | 719 | ILE |
| 7 | O | 725 | ASN |
| 7 | O | 730 | VAL |
| 7 | O | 770 | ILE |
| 7 | O | 836 | ILE |
| 7 | O | 838 | LYS |
| 7 | O | 916 | ILE |
| 7 | O | 925 | HIS |
| 7 | O | 978 | ILE |
| 7 | O | 991 | THR |
| 7 | O | 1042 | ILE |
| 7 | O | 1046 | THR |
| 7 | O | 1065 | LYS |
| 7 | O | 1084 | LEU |
| 7 | O | 1092 | THR |
| 7 | O | 1112 | LEU |
| 7 | O | 1126 | PRO |
| 7 | O | 1138 | PHE |
| 7 | O | 1154 | ARG |
| 7 | O | 1158 | THR |
| 7 | O | 1174 | LYS |
| 7 | O | 1183 | TYR |
| 7 | O | 1189 | MET |
| 7 | O | 1202 | ASN |
| 7 | O | 1214 | SER |
| 7 | O | 1224 | GLU |
| 7 | O | 1225 | GLN |
| 7 | O | 1235 | ASN |
| 7 | O | 1250 | LYS |
| 7 | O | 1272 | LEU |
| 7 | O | 1273 | LYS |
| 7 | O | 1274 | ASP |
| 7 | O | 1308 | GLN |
| 7 | O | 1312 | ILE |
| 7 | O | 1319 | LEU |
| 7 | O | 1320 | GLU |
| 7 | O | 1347 | ILE |
| 7 | O | 1396 | LEU |
| 7 | O | 1399 | VAL |
| 7 | O | 1406 | TYR |
| 7 | O | 1430 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | O | 1464 | ILE |
| 7 | O | 1498 | LEU |
| 7 | O | 1525 | LEU |
| 7 | O | 1526 | ILE |
| 7 | O | 1531 | THR |
| 8 | P | 23 | ASN |
| 8 | P | 32 | VAL |
| 8 | P | 40 | ILE |
| 8 | P | 41 | ARG |
| 8 | P | 42 | GLN |
| 8 | P | 45 | LYS |
| 8 | P | 55 | LEU |
| 8 | P | 70 | LYS |
| 8 | P | 73 | SER |
| 8 | P | 74 | THR |
| 8 | P | 75 | ILE |
| 8 | P | 78 | LEU |
| 8 | P | 103 | MET |
| 8 | P | 131 | ASP |
| 8 | P | 141 | LEU |
| 8 | P | 178 | GLN |
| 8 | P | 193 | GLN |
| 8 | P | 199 | ILE |
| 8 | P | 202 | THR |
| 8 | P | 214 | LEU |
| 8 | P | 257 | LEU |
| 8 | P | 266 | THR |
| 8 | P | 272 | ILE |
| 8 | P | 275 | LEU |
| 8 | P | 281 | GLN |
| 8 | P | 359 | LEU |
| 8 | P | 361 | LYS |
| 8 | P | 378 | VAL |
| 8 | P | 379 | ILE |
| 8 | P | 396 | THR |
| 8 | P | 399 | VAL |
| 8 | P | 466 | THR |
| 8 | P | 499 | LEU |
| 8 | P | 522 | LYS |
| 8 | P | 552 | LEU |
| 8 | P | 553 | ILE |
| 8 | P | 577 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | P | 597 | LEU |
| 8 | P | 603 | ASP |
| 8 | P | 605 | LYS |
| 8 | P | 608 | ILE |
| 8 | P | 639 | PHE |
| 8 | P | 767 | ILE |
| 8 | P | 773 | LEU |
| 8 | P | 778 | VAL |
| 8 | P | 793 | LEU |
| 8 | P | 795 | ILE |
| 8 | P | 815 | LEU |
| 8 | P | 821 | THR |
| 8 | P | 830 | THR |
| 8 | P | 835 | LEU |
| 8 | P | 853 | LYS |
| 8 | P | 868 | LEU |
| 8 | P | 869 | LYS |
| 8 | P | 879 | ILE |
| 8 | P | 881 | SER |
| 8 | P | 897 | LYS |
| 8 | P | 944 | GLN |
| 8 | P | 963 | LYS |
| 8 | P | 972 | LEU |
| 8 | P | 988 | ILE |
| 8 | P | 994 | ILE |
| 8 | P | 996 | THR |
| 8 | P | 999 | GLN |
| 8 | P | 1018 | GLU |
| 8 | P | 1024 | LEU |
| 8 | P | 1031 | LYS |
| 8 | P | 1046 | LYS |
| 8 | P | 1053 | LEU |
| 8 | P | 1055 | GLN |
| 8 | P | 1060 | LEU |
| 8 | P | 1061 | THR |
| 8 | P | 1095 | GLU |
| 8 | P | 1160 | ILE |
| 8 | P | 1178 | LYS |
| 8 | P | 1181 | THR |
| 8 | P | 1194 | LEU |
| 8 | P | 1220 | VAL |
| 8 | P | 1249 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | P | 1257 | LEU |
| 8 | P | 1278 | ILE |
| 8 | P | 1280 | LEU |
| 8 | P | 1288 | PHE |
| 8 | P | 1303 | LEU |
| 8 | P | 1304 | LYS |
| 8 | P | 1306 | ASN |
| 8 | P | 1334 | ASP |
| 8 | P | 1335 | GLN |
| 8 | P | 1391 | LEU |
| 8 | P | 1400 | PRO |
| 8 | P | 1429 | HIS |
| 8 | P | 1438 | ILE |
| 8 | P | 1441 | GLN |
| 8 | P | 1442 | ILE |
| 8 | P | 1527 | LYS |
| 8 | P | 1541 | LEU |
| 8 | P | 1566 | TYR |
| 8 | P | 1595 | LYS |
| 8 | P | 1617 | ILE |
| 8 | P | 1647 | LEU |
| 9 | Q | 208 | LEU |
| 9 | Q | 222 | PHE |
| 9 | Q | 231 | ASN |
| 9 | Q | 277 | TYR |
| 9 | Q | 298 | LEU |
| 9 | Q | 334 | TRP |
| 9 | Q | 347 | LYS |
| 9 | Q | 355 | GLU |
| 9 | Q | 414 | LEU |
| 9 | Q | 437 | TRP |
| 9 | Q | 484 | LEU |
| 9 | Q | 495 | THR |
| 9 | Q | 501 | MET |
| 9 | Q | 513 | LEU |
| 9 | Q | 514 | LYS |
| 9 | Q | 570 | GLU |
| 9 | Q | 576 | LEU |
| 9 | Q | 590 | LEU |
| 9 | Q | 672 | GLN |
| 9 | Q | 698 | ASP |
| 9 | Q | 709 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | Q | 755 | LYS |
| 9 | Q | 763 | LEU |
| 9 | Q | 766 | ASN |
| 9 | Q | 772 | PRO |
| 9 | Q | 825 | PRO |
| 9 | Q | 829 | TYR |
| 9 | Q | 833 | ILE |
| 9 | R | 227 | GLN |
| 9 | R | 229 | ASN |
| 9 | R | 234 | ILE |
| 9 | R | 241 | ILE |
| 9 | R | 258 | LYS |
| 9 | R | 266 | LYS |
| 9 | R | 312 | LYS |
| 9 | R | 314 | LYS |
| 9 | R | 322 | ILE |
| 9 | R | 360 | ILE |
| 9 | R | 428 | VAL |
| 9 | R | 480 | GLN |
| 9 | R | 481 | THR |
| 9 | R | 515 | LEU |
| 9 | R | 554 | VAL |
| 9 | R | 562 | LEU |
| 9 | R | 596 | ASP |
| 9 | R | 599 | ARG |
| 9 | R | 604 | ILE |
| 9 | R | 617 | LYS |
| 9 | R | 654 | ILE |
| 9 | R | 709 | LYS |
| 9 | R | 726 | LEU |
| 9 | R | 733 | GLN |
| 9 | R | 754 | ARG |
| 9 | R | 755 | LYS |
| 9 | R | 788 | ILE |
| 9 | S | 232 | PHE |
| 9 | S | 248 | THR |
| 9 | S | 287 | ASP |
| 9 | S | 333 | ILE |
| 9 | S | 356 | ASN |
| 9 | S | 357 | LYS |
| 9 | S | 372 | LYS |
| 9 | S | 459 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | S | 471 | PRO |
| 9 | S | 480 | GLN |
| 9 | S | 514 | LYS |
| 9 | S | 515 | LEU |
| 9 | S | 537 | ILE |
| 9 | S | 547 | TYR |
| 9 | S | 552 | VAL |
| 9 | S | 583 | THR |
| 9 | S | 592 | LYS |
| 9 | S | 603 | VAL |
| 9 | S | 672 | GLN |
| 9 | S | 675 | VAL |
| 9 | S | 691 | ARG |
| 9 | S | 695 | ILE |
| 9 | S | 706 | ILE |
| 9 | S | 713 | ILE |
| 9 | S | 720 | ILE |
| 9 | S | 754 | ARG |
| 9 | S | 755 | LYS |
| 9 | S | 756 | LYS |
| 9 | S | 771 | ILE |
| 9 | S | 777 | ILE |
| 9 | S | 798 | THR |
| 9 | S | 814 | MET |
| 9 | T | 241 | ILE |
| 9 | T | 260 | LEU |
| 9 | T | 270 | ILE |
| 9 | T | 276 | GLN |
| 9 | T | 300 | THR |
| 9 | T | 312 | LYS |
| 9 | T | 315 | LYS |
| 9 | T | 353 | LEU |
| 9 | T | 356 | ASN |
| 9 | T | 432 | ILE |
| 9 | T | 506 | LEU |
| 9 | T | 515 | LEU |
| 9 | T | 542 | THR |
| 9 | T | 557 | LEU |
| 9 | T | 633 | GLU |
| 9 | T | 637 | ILE |
| 9 | T | 673 | PRO |
| 9 | T | 713 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | T | 729 | ASN |
| 9 | T | 732 | TRP |
| 9 | T | 754 | ARG |
| 9 | T | 768 | VAL |
| 9 | T | 770 | ASN |
| 9 | T | 826 | ARG |
| 10 | U | 249 | ASP |
| 10 | U | 283 | ILE |
| 10 | U | 304 | LYS |
| 10 | U | 324 | LYS |
| 10 | U | 334 | ILE |
| 10 | U | 351 | LYS |
| 11 | V | 271 | ILE |
| 11 | V | 294 | ILE |
| 11 | V | 300 | VAL |
| 11 | V | 301 | LEU |
| 11 | V | 302 | ARG |
| 11 | V | 348 | PRO |
| 11 | V | 351 | THR |
| 11 | V | 359 | THR |
| 11 | V | 373 | ASN |
| 11 | V | 392 | VAL |
| 11 | V | 402 | ASN |
| 10 | W | 249 | ASP |
| 10 | W | 255 | ILE |
| 10 | W | 279 | ASP |
| 10 | W | 304 | LYS |
| 10 | W | 305 | TYR |
| 11 | X | 276 | TYR |
| 11 | X | 277 | PRO |
| 11 | X | 280 | ILE |
| 11 | X | 285 | ILE |
| 11 | X | 300 | VAL |
| 11 | X | 301 | LEU |
| 11 | X | 302 | ARG |
| 11 | X | 346 | LYS |
| 11 | X | 351 | THR |
| 11 | X | 373 | ASN |
| 11 | X | 399 | LYS |
| 1 | Y | 120 | VAL |
| 1 | Y | 124 | ARG |
| 1 | Y | 126 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 193 | TRP |
| 1 | Y | 201 | TYR |
| 1 | Y | 216 | LEU |
| 1 | Y | 228 | VAL |
| 1 | Y | 271 | ILE |
| 1 | Y | 273 | ILE |
| 1 | Y | 394 | GLU |
| 1 | Y | 404 | THR |
| 1 | Y | 406 | THR |
| 1 | Y | 412 | ILE |
| 1 | Y | 413 | LEU |
| 1 | Y | 418 | LEU |
| 1 | Y | 432 | ASN |
| 1 | Y | 512 | LYS |
| 1 | Y | 577 | PHE |
| 1 | Y | 580 | VAL |
| 1 | Y | 583 | TYR |
| 1 | Y | 586 | LEU |
| 1 | Y | 588 | THR |
| 1 | Y | 597 | THR |
| 1 | Y | 599 | LEU |
| 1 | Y | 618 | THR |
| 1 | Y | 656 | ASP |
| 1 | Y | 686 | THR |
| 1 | Y | 766 | LEU |
| 1 | Y | 832 | VAL |
| 1 | Y | 835 | SER |
| 1 | Y | 860 | ILE |
| 1 | Y | 886 | ASN |
| 1 | Y | 942 | LYS |
| 1 | Y | 968 | LEU |
| 1 | Y | 1016 | ILE |
| 1 | Y | 1079 | LEU |
| 1 | Y | 1096 | GLN |
| 1 | Y | 1105 | TYR |
| 1 | Y | 1157 | PHE |
| 1 | Y | 1158 | HIS |
| 1 | Y | 1179 | THR |
| 1 | Y | 1196 | ILE |
| 1 | Y | 1222 | THR |
| 1 | Y | 1224 | ASN |
| 1 | Y | 1257 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 1258 | LEU |
| 1 | Y | 1281 | THR |
| 1 | Y | 1296 | THR |
| 1 | Y | 1300 | LYS |
| 1 | Y | 1314 | PRO |
| 1 | Y | 1378 | VAL |
| 1 | Y | 1384 | ILE |
| 1 | Y | 1390 | LEU |
| 1 | Y | 1393 | ILE |
| 1 | Y | 1405 | GLU |
| 1 | Y | 1437 | SER |
| 1 | Y | 1441 | ASN |
| 1 | Y | 1451 | LEU |
| 1 | Y | 1462 | PHE |
| 1 | Y | 1466 | ILE |
| 1 | Y | 1483 | PRO |
| 2 | Z | 88 | SER |
| 2 | Z | 107 | ASN |
| 2 | Z | 144 | THR |
| 2 | Z | 166 | PHE |
| 2 | Z | 168 | GLU |
| 2 | Z | 178 | ASN |
| 2 | Z | 185 | ILE |
| 2 | Z | 194 | ILE |
| 2 | Z | 218 | VAL |
| 2 | Z | 224 | VAL |
| 2 | Z | 245 | ASN |
| 2 | Z | 246 | ILE |
| 2 | Z | 284 | TRP |
| 2 | Z | 289 | ASN |
| 2 | Z | 301 | LYS |
| 2 | Z | 306 | LYS |
| 2 | Z | 345 | LEU |
| 2 | Z | 364 | ARG |
| 2 | Z | 457 | SER |
| 2 | Z | 496 | THR |
| 2 | Z | 502 | ILE |
| 2 | Z | 511 | VAL |
| 2 | Z | 513 | LYS |
| 2 | Z | 514 | ARG |
| 2 | Z | 548 | LEU |
| 2 | Z | 561 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | Z | 563 | THR |
| 2 | Z | 590 | PHE |
| 2 | Z | 599 | LEU |
| 2 | Z | 609 | LEU |
| 2 | Z | 670 | PRO |
| 2 | Z | 679 | SER |
| 2 | Z | 724 | TRP |
| 2 | Z | 768 | ILE |
| 2 | Z | 786 | THR |
| 2 | Z | 806 | LYS |
| 2 | Z | 858 | LYS |
| 2 | Z | 883 | TYR |
| 2 | Z | 888 | LEU |
| 2 | Z | 889 | LYS |
| 2 | Z | 902 | LEU |
| 2 | Z | 904 | TYR |
| 2 | Z | 916 | PHE |
| 2 | Z | 932 | ILE |
| 2 | Z | 949 | ARG |
| 2 | Z | 976 | LYS |
| 2 | Z | 990 | THR |
| 2 | Z | 1008 | ILE |
| 2 | Z | 1013 | LYS |
| 2 | Z | 1040 | LYS |
| 2 | Z | 1043 | VAL |
| 2 | Z | 1078 | GLN |
| 2 | Z | 1092 | LEU |
| 2 | Z | 1155 | GLN |
| 2 | Z | 1156 | LEU |
| 2 | Z | 1177 | VAL |
| 2 | Z | 1218 | ILE |
| 2 | Z | 1220 | LEU |
| 2 | Z | 1229 | LYS |
| 2 | Z | 1233 | VAL |
| 2 | Z | 1241 | LEU |
| 2 | Z | 1255 | SER |
| 2 | Z | 1277 | ARG |
| 2 | Z | 1300 | SER |
| 2 | Z | 1301 | SER |
| 12 | u | 25 | TYR |
| 12 | u | 27 | PHE |
| 12 | u | 49 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | u | 65 | LEU |
| 12 | u | 86 | ASN |
| 12 | u | 151 | ILE |
| 12 | u | 152 | THR |
| 12 | u | 157 | LEU |
| 12 | u | 159 | SER |
| 12 | u | 199 | THR |
| 12 | u | 216 | LEU |
| 12 | u | 298 | THR |
| 12 | u | 317 | VAL |
| 12 | u | 329 | LYS |
| 12 | u | 358 | ARG |
| 12 | u | 363 | LEU |
| 12 | u | 365 | THR |
| 12 | u | 366 | LEU |
| 12 | u | 367 | PRO |
| 12 | u | 379 | ASN |
| 12 | u | 381 | ILE |
| 12 | u | 404 | PRO |
| 12 | u | 439 | LEU |
| 12 | u | 442 | ASN |
| 12 | u | 443 | LYS |
| 12 | u | 444 | THR |
| 12 | u | 447 | PHE |
| 12 | v | 49 | LEU |
| 12 | v | 90 | VAL |
| 12 | v | 131 | LEU |
| 12 | v | 156 | ILE |
| 12 | v | 182 | ILE |
| 12 | v | 241 | THR |
| 12 | v | 300 | THR |
| 12 | v | 301 | ASN |
| 12 | v | 304 | THR |
| 12 | v | 309 | ASN |
| 12 | v | 335 | MET |
| 12 | v | 351 | ILE |
| 12 | v | 363 | LEU |
| 12 | v | 379 | ASN |
| 12 | v | 386 | PHE |
| 12 | v | 392 | THR |
| 12 | v | 439 | LEU |
| 13 | w | 1122 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 13 | w | 1431 | MET |
| 13 | x | 1122 | ILE |
| 13 | x | 1445 | THR |
| 14 | h | 23 | THR |
| 14 | h | 58 | ASN |
| 14 | h | 67 | TYR |
| 14 | h | 105 | ARG |
| 14 | h | 130 | THR |
| 14 | h | 174 | SER |
| 14 | h | 186 | LEU |
| 14 | h | 278 | GLU |
| 14 | h | 283 | TYR |
| 14 | h | 293 | LEU |
| 14 | h | 336 | LEU |
| 14 | h | 338 | ARG |
| 14 | h | 339 | PRO |
| 14 | h | 340 | LEU |
| 14 | h | 351 | LEU |
| 14 | h | 376 | TYR |
| 14 | h | 395 | LEU |
| 14 | h | 398 | VAL |
| 14 | h | 427 | LEU |
| 14 | h | 464 | THR |
| 14 | h | 472 | LEU |
| 14 | h | 555 | LYS |
| 14 | h | 580 | PRO |
| 14 | h | 602 | ILE |
| 14 | h | 618 | SER |
| 14 | h | 640 | PHE |
| 14 | h | 646 | ILE |
| 14 | h | 694 | ASN |
| 14 | h | 728 | ILE |
| 14 | h | 751 | ARG |
| 14 | h | 787 | ASN |
| 14 | h | 811 | LEU |
| 14 | h | 842 | LEU |
| 14 | h | 876 | LEU |
| 14 | h | 878 | HIS |
| 14 | h | 894 | GLU |
| 14 | h | 935 | LEU |
| 14 | h | 944 | ILE |
| 14 | h | 968 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | h | 991 | LEU |
| 14 | h | 1006 | VAL |
| 14 | h | 1023 | LYS |
| 15 | i | 58 | ILE |
| 15 | i | 94 | ARG |
| 15 | i | 123 | VAL |
| 15 | i | 143 | THR |
| 15 | i | 144 | VAL |
| 15 | i | 168 | ARG |
| 15 | i | 200 | ASN |
| 15 | i | 208 | LEU |
| 15 | i | 249 | LEU |
| 15 | i | 310 | VAL |
| 15 | i | 322 | THR |
| 15 | i | 365 | ILE |
| 15 | i | 405 | ILE |
| 15 | i | 454 | LEU |
| 15 | i | 488 | LEU |
| 15 | i | 507 | LEU |
| 15 | i | 515 | THR |
| 15 | i | 544 | ASN |
| 15 | i | 553 | ILE |
| 15 | i | 586 | LEU |
| 15 | i | 608 | PRO |
| 15 | i | 629 | VAL |
| 15 | i | 647 | ARG |
| 15 | i | 662 | TYR |
| 15 | i | 724 | MET |
| 15 | i | 726 | THR |
| 15 | i | 738 | LYS |
| 16 | j | 167 | LYS |
| 16 | j | 182 | LYS |
| 16 | j | 183 | PHE |
| 16 | j | 197 | VAL |
| 16 | j | 198 | THR |
| 16 | j | 211 | SER |
| 16 | j | 233 | LEU |
| 16 | j | 243 | PRO |
| 16 | j | 318 | LEU |
| 16 | j | 332 | ILE |
| 16 | j | 334 | ASP |
| 16 | j | 335 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | j | 404 | GLN |
| 16 | j | 420 | VAL |
| 16 | j | 433 | LYS |
| 16 | j | 511 | VAL |
| 16 | j | 564 | SER |
| 16 | j | 569 | GLU |
| 16 | j | 578 | PRO |
| 16 | j | 580 | LEU |
| 16 | j | 605 | SER |
| 16 | j | 614 | ILE |
| 16 | j | 652 | ARG |
| 16 | j | 777 | PRO |
| 17 | k | 31 | LYS |
| 17 | k | 42 | THR |
| 17 | k | 66 | PHE |
| 17 | k | 86 | ASN |
| 17 | k | 91 | GLN |
| 17 | k | 110 | HIS |
| 17 | k | 125 | VAL |
| 17 | k | 193 | THR |
| 17 | k | 210 | VAL |
| 17 | k | 219 | ARG |
| 17 | k | 238 | ASN |
| 17 | k | 285 | LEU |
| 18 | l | 51 | TRP |
| 18 | l | 80 | THR |
| 18 | l | 90 | GLN |
| 18 | l | 202 | LEU |
| 18 | l | 213 | SER |
| 18 | l | 215 | ILE |
| 18 | l | 230 | LEU |
| 18 | l | 237 | ASP |
| 18 | l | 240 | ILE |
| 18 | l | 289 | GLN |
| 18 | l | 291 | ASN |
| 18 | l | 345 | ILE |
| 19 | m | 7 | TYR |
| 19 | m | 8 | GLN |
| 19 | m | 20 | LYS |
| 19 | m | 29 | GLU |
| 19 | m | 140 | PRO |
| 19 | m | 149 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | m | 153 | LEU |
| 19 | m | 184 | ILE |
| 19 | m | 207 | SER |
| 19 | m | 216 | GLN |
| 19 | m | 226 | GLN |
| 19 | m | 237 | ILE |
| 19 | m | 246 | THR |
| 19 | m | 277 | LEU |
| 19 | m | 347 | MET |
| 19 | m | 350 | VAL |
| 19 | m | 355 | LEU |
| 19 | m | 373 | THR |
| 19 | m | 415 | THR |
| 19 | m | 431 | ILE |
| 19 | m | 459 | LYS |
| 19 | m | 473 | SER |
| 19 | m | 479 | THR |
| 19 | m | 481 | GLN |
| 19 | m | 482 | ARG |
| 19 | m | 543 | VAL |
| 19 | m | 575 | GLU |
| 19 | m | 585 | THR |
| 19 | m | 614 | PRO |
| 19 | m | 667 | LEU |
| 19 | m | 676 | LYS |
| 19 | m | 703 | LEU |
| 19 | m | 704 | LEU |
| 19 | m | 717 | LEU |
| 20 | n | 64 | ASN |
| 20 | n | 71 | THR |
| 20 | n | 85 | GLU |
| 20 | n | 117 | THR |
| 20 | n | 128 | ASP |
| 20 | n | 159 | ASP |
| 20 | n | 161 | THR |
| 20 | n | 168 | LYS |
| 20 | n | 173 | ILE |
| 20 | n | 182 | ASN |
| 20 | n | 198 | LEU |
| 20 | n | 210 | LEU |
| 20 | n | 223 | THR |
| 20 | n | 256 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | n | 285 | ILE |
| 20 | n | 293 | GLN |
| 20 | n | 390 | ILE |
| 20 | n | 427 | THR |
| 20 | n | 429 | VAL |
| 20 | n | 461 | ASP |
| 20 | n | 466 | TYR |
| 20 | n | 512 | ILE |
| 20 | n | 516 | LEU |
| 20 | n | 538 | ILE |
| 20 | n | 566 | ASN |
| 20 | n | 594 | LEU |
| 20 | n | 598 | ILE |
| 20 | n | 624 | THR |
| 20 | n | 633 | THR |
| 20 | n | 652 | HIS |
| 20 | n | 663 | GLN |
| 20 | n | 688 | THR |
| 20 | n | 698 | PRO |
| 20 | n | 699 | MET |
| 20 | n | 703 | THR |
| 20 | n | 704 | SER |
| 20 | n | 723 | PHE |
| 20 | n | 772 | ASP |
| 20 | n | 775 | ILE |
| 20 | n | 817 | THR |
| 20 | n | 827 | THR |
| 20 | n | 846 | THR |
| 20 | n | 851 | LEU |
| 20 | n | 853 | LYS |
| 20 | n | 889 | GLN |
| 20 | n | 906 | ILE |
| 20 | n | 917 | LEU |
| 20 | n | 918 | SER |
| 20 | n | 943 | THR |
| 20 | n | 1037 | LEU |
| 20 | n | 1084 | LEU |
| 20 | n | 1101 | ARG |
| 21 | o | 56 | THR |
| 21 | o | 91 | THR |
| 21 | p | 55 | ASN |
| 21 | p | 56 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | p | 70 | THR |
| 21 | p | 91 | THR |
| 21 | q | 55 | ASN |
| 21 | q | 56 | THR |
| 21 | r | 8 | THR |
| 21 | r | 12 | LYS |
| 21 | r | 46 | LYS |
| 21 | r | 51 | VAL |
| 21 | r | 56 | THR |
| 21 | s | 7 | SER |
| 21 | s | 10 | ILE |
| 21 | s | 44 | THR |
| 21 | s | 56 | THR |
| 21 | s | 60 | ILE |
| 21 | s | 69 | VAL |
| 21 | t | 17 | THR |
| 21 | t | 21 | LYS |
| 21 | t | 55 | ASN |
| 21 | t | 56 | THR |
| 15 | b | 52 | THR |
| 15 | b | 58 | ILE |
| 15 | b | 64 | LYS |
| 15 | b | 122 | ARG |
| 15 | b | 200 | ASN |
| 15 | b | 238 | LYS |
| 15 | b | 265 | ILE |
| 15 | b | 271 | LEU |
| 15 | b | 396 | ASP |
| 15 | b | 397 | ILE |
| 15 | b | 463 | SER |
| 15 | b | 503 | VAL |
| 15 | b | 506 | GLU |
| 15 | b | 544 | ASN |
| 15 | b | 547 | LEU |
| 15 | b | 598 | ASN |
| 15 | b | 599 | SER |
| 15 | b | 626 | PRO |
| 15 | b | 657 | TYR |
| 15 | b | 659 | PRO |
| 15 | b | 672 | TYR |
| 15 | b | 681 | LYS |
| 15 | b | 692 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | b | 698 | LYS |
| 15 | b | 744 | MET |
| 16 | c | 136 | LYS |
| 16 | c | 170 | VAL |
| 16 | c | 183 | PHE |
| 16 | c | 197 | VAL |
| 16 | c | 233 | LEU |
| 16 | c | 256 | LYS |
| 16 | c | 261 | LYS |
| 16 | c | 325 | LEU |
| 16 | c | 328 | ASN |
| 16 | c | 332 | ILE |
| 16 | c | 335 | LEU |
| 16 | c | 354 | ILE |
| 16 | c | 366 | PHE |
| 16 | c | 369 | LEU |
| 16 | c | 407 | LEU |
| 16 | c | 441 | ARG |
| 16 | c | 455 | GLN |
| 16 | c | 515 | ILE |
| 16 | c | 544 | LEU |
| 16 | c | 560 | LEU |
| 16 | c | 564 | SER |
| 16 | c | 567 | LEU |
| 16 | c | 584 | ASN |
| 16 | c | 594 | THR |
| 16 | c | 610 | TRP |
| 16 | c | 612 | VAL |
| 16 | c | 620 | TYR |
| 16 | c | 648 | TYR |
| 16 | c | 652 | ARG |
| 16 | c | 661 | MET |
| 16 | c | 781 | TYR |
| 16 | c | 782 | LEU |
| 17 | d | 33 | ILE |
| 17 | d | 105 | VAL |
| 17 | d | 175 | THR |
| 17 | d | 180 | ASN |
| 17 | d | 193 | THR |
| 17 | d | 227 | GLN |
| 17 | d | 230 | THR |
| 18 | e | 11 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | e | 72 | ILE |
| 18 | e | 118 | PRO |
| 18 | e | 133 | ILE |
| 18 | e | 140 | LEU |
| 18 | e | 151 | THR |
| 18 | e | 170 | CYS |
| 18 | e | 212 | LYS |
| 18 | e | 236 | LYS |
| 19 | f | 8 | GLN |
| 19 | f | 29 | GLU |
| 19 | f | 74 | PHE |
| 19 | f | 80 | LEU |
| 19 | f | 114 | LYS |
| 19 | f | 136 | PRO |
| 19 | f | 139 | VAL |
| 19 | f | 143 | LYS |
| 19 | f | 169 | LEU |
| 19 | f | 172 | LYS |
| 19 | f | 216 | GLN |
| 19 | f | 226 | GLN |
| 19 | f | 237 | ILE |
| 19 | f | 246 | THR |
| 19 | f | 277 | LEU |
| 19 | f | 317 | LEU |
| 19 | f | 363 | VAL |
| 19 | f | 373 | THR |
| 19 | f | 374 | GLU |
| 19 | f | 419 | LEU |
| 19 | f | 434 | THR |
| 19 | f | 457 | VAL |
| 19 | f | 473 | SER |
| 19 | f | 522 | LEU |
| 19 | f | 543 | VAL |
| 19 | f | 551 | GLU |
| 19 | f | 560 | LYS |
| 19 | f | 575 | GLU |
| 19 | f | 576 | ASN |
| 19 | f | 577 | GLU |
| 19 | f | 678 | LEU |
| 19 | f | 716 | ASP |
| 19 | f | 717 | LEU |
| 20 | g | 68 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | g | 74 | THR |
| 20 | g | 107 | ILE |
| 20 | g | 110 | ILE |
| 20 | g | 134 | VAL |
| 20 | g | 198 | LEU |
| 20 | g | 201 | ASN |
| 20 | g | 219 | ILE |
| 20 | g | 263 | THR |
| 20 | g | 267 | VAL |
| 20 | g | 308 | ILE |
| 20 | g | 380 | THR |
| 20 | g | 424 | VAL |
| 20 | g | 430 | ASN |
| 20 | g | 449 | LEU |
| 20 | g | 463 | LYS |
| 20 | g | 469 | THR |
| 20 | g | 538 | ILE |
| 20 | g | 595 | ASN |
| 20 | g | 622 | ASN |
| 20 | g | 623 | LEU |
| 20 | g | 631 | THR |
| 20 | g | 643 | PRO |
| 20 | g | 703 | THR |
| 20 | g | 772 | ASP |
| 20 | g | 797 | LEU |
| 20 | g | 802 | ILE |
| 20 | g | 814 | LEU |
| 20 | g | 820 | THR |
| 20 | g | 889 | GLN |
| 20 | g | 903 | LEU |
| 20 | g | 907 | THR |
| 20 | g | 917 | LEU |
| 20 | g | 934 | VAL |
| 20 | g | 960 | ILE |
| 20 | g | 1078 | LEU |
| 20 | g | 1089 | LEU |
| 20 | g | 1091 | THR |
| 20 | g | 1095 | ILE |
| 20 | g | 1098 | THR |
| 20 | g | 1142 | LYS |
| 14 | a | 1 | MET |
| 14 | a | 58 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | a | 77 | THR |
| 14 | a | 130 | THR |
| 14 | a | 150 | PHE |
| 14 | a | 161 | ARG |
| 14 | a | 210 | ARG |
| 14 | a | 272 | LYS |
| 14 | a | 298 | PHE |
| 14 | a | 314 | THR |
| 14 | a | 330 | SER |
| 14 | a | 338 | ARG |
| 14 | a | 340 | LEU |
| 14 | a | 356 | LYS |
| 14 | a | 359 | THR |
| 14 | a | 363 | LEU |
| 14 | a | 376 | TYR |
| 14 | a | 397 | ILE |
| 14 | a | 419 | ILE |
| 14 | a | 426 | ILE |
| 14 | a | 429 | GLU |
| 14 | a | 454 | LYS |
| 14 | a | 463 | ILE |
| 14 | a | 464 | THR |
| 14 | a | 472 | LEU |
| 14 | a | 501 | THR |
| 14 | a | 513 | LEU |
| 14 | a | 545 | THR |
| 14 | a | 555 | LYS |
| 14 | a | 714 | ILE |
| 14 | a | 716 | GLU |
| 14 | a | 719 | PHE |
| 14 | a | 720 | PHE |
| 14 | a | 724 | PHE |
| 14 | a | 741 | LEU |
| 14 | a | 751 | ARG |
| 14 | a | 787 | ASN |
| 14 | a | 809 | LYS |
| 14 | a | 842 | LEU |
| 14 | a | 864 | PHE |
| 14 | a | 876 | LEU |
| 14 | a | 896 | LEU |
| 14 | a | 901 | ARG |
| 14 | a | 913 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 14 | a | 939 | THR |
| 14 | a | 959 | GLU |
| 14 | a | 972 | LYS |
| 14 | a | 981 | LEU |
| 14 | a | 1035 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (744) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 0 | 112 | GLN |
| 1 | 0 | 113 | HIS |
| 1 | 0 | 194 | ASN |
| 1 | 0 | 196 | ASN |
| 1 | 0 | 230 | HIS |
| 1 | 0 | 363 | GLN |
| 1 | 0 | 456 | ASN |
| 1 | 0 | 862 | GLN |
| 1 | 0 | 924 | ASN |
| 1 | 0 | 972 | ASN |
| 1 | 0 | 1027 | HIS |
| 1 | 0 | 1082 | GLN |
| 1 | 0 | 1096 | GLN |
| 1 | 0 | 1160 | HIS |
| 1 | 0 | 1257 | GLN |
| 1 | 0 | 1365 | ASN |
| 1 | 0 | 1377 | ASN |
| 1 | 0 | 1379 | GLN |
| 1 | 0 | 1424 | ASN |
| 1 | 0 | 1445 | ASN |
| 2 | 1 | 92 | GLN |
| 2 | 1 | 139 | GLN |
| 2 | 1 | 192 | HIS |
| 2 | 1 | 199 | HIS |
| 2 | 1 | 238 | ASN |
| 2 | 1 | 262 | ASN |
| 2 | 1 | 282 | ASN |
| 2 | 1 | 287 | GLN |
| 2 | 1 | 308 | ASN |
| 2 | 1 | 355 | HIS |
| 2 | 1 | 418 | ASN |
| 2 | 1 | 722 | GLN |
| 2 | 1 | 796 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 1 | 856 | ASN |
| 2 | 1 | 927 | HIS |
| 2 | 1 | 1003 | ASN |
| 2 | 1 | 1049 | ASN |
| 2 | 1 | 1159 | ASN |
| 2 | 1 | 1161 | HIS |
| 2 | 1 | 1175 | ASN |
| 2 | 1 | 1190 | GLN |
| 2 | 1 | 1196 | ASN |
| 2 | 1 | 1239 | ASN |
| 2 | 1 | 1290 | ASN |
| 2 | 1 | 1375 | ASN |
| 4 | A | 654 | HIS |
| 4 | A | 663 | ASN |
| 4 | A | 703 | GLN |
| 4 | A | 761 | ASN |
| 4 | A | 770 | ASN |
| 4 | A | 771 | ASN |
| 4 | A | 774 | ASN |
| 4 | A | 792 | GLN |
| 4 | A | 800 | HIS |
| 5 | B | 289 | GLN |
| 5 | B | 314 | ASN |
| 5 | B | 317 | ASN |
| 5 | B | 329 | HIS |
| 5 | B | 363 | GLN |
| 5 | B | 365 | GLN |
| 5 | B | 378 | HIS |
| 5 | B | 387 | GLN |
| 5 | B | 441 | GLN |
| 5 | B | 457 | ASN |
| 5 | B | 507 | ASN |
| 5 | B | 516 | GLN |
| 5 | B | 524 | ASN |
| 6 | C | 279 | GLN |
| 6 | C | 301 | HIS |
| 6 | C | 355 | GLN |
| 6 | C | 462 | GLN |
| 4 | D | 646 | ASN |
| 4 | D | 647 | GLN |
| 4 | D | 654 | HIS |
| 4 | D | 663 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | D | 667 | GLN |
| 4 | D | 688 | HIS |
| 4 | D | 695 | GLN |
| 4 | D | 749 | GLN |
| 4 | D | 771 | ASN |
| 4 | D | 774 | ASN |
| 4 | D | 777 | ASN |
| 4 | D | 790 | ASN |
| 4 | D | 810 | ASN |
| 5 | E | 359 | ASN |
| 5 | E | 362 | ASN |
| 5 | E | 363 | GLN |
| 5 | E | 388 | GLN |
| 5 | E | 405 | ASN |
| 5 | E | 476 | GLN |
| 5 | E | 517 | GLN |
| 6 | F | 279 | GLN |
| 6 | F | 293 | HIS |
| 6 | F | 328 | GLN |
| 6 | F | 374 | GLN |
| 6 | F | 378 | HIS |
| 4 | G | 646 | ASN |
| 4 | G | 657 | GLN |
| 4 | G | 691 | ASN |
| 4 | G | 698 | GLN |
| 4 | G | 713 | ASN |
| 4 | G | 743 | GLN |
| 4 | G | 756 | ASN |
| 4 | G | 771 | ASN |
| 4 | G | 790 | ASN |
| 4 | G | 798 | ASN |
| 4 | G | 810 | ASN |
| 5 | H | 346 | GLN |
| 5 | H | 351 | GLN |
| 5 | H | 362 | ASN |
| 5 | H | 363 | GLN |
| 5 | H | 365 | GLN |
| 5 | H | 390 | HIS |
| 5 | H | 507 | ASN |
| 5 | H | 517 | GLN |
| 5 | H | 539 | ASN |
| 6 | I | 293 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | I | 355 | GLN |
| 6 | I | 356 | GLN |
| 6 | I | 378 | HIS |
| 6 | I | 462 | GLN |
| 4 | J | 646 | ASN |
| 4 | J | 654 | HIS |
| 4 | J | 688 | HIS |
| 4 | J | 691 | ASN |
| 4 | J | 749 | GLN |
| 4 | J | 774 | ASN |
| 4 | J | 817 | GLN |
| 4 | J | 819 | ASN |
| 5 | K | 291 | GLN |
| 5 | K | 362 | ASN |
| 5 | K | 390 | HIS |
| 5 | K | 457 | ASN |
| 5 | K | 472 | ASN |
| 5 | K | 507 | ASN |
| 5 | K | 515 | ASN |
| 5 | K | 516 | GLN |
| 5 | K | 517 | GLN |
| 6 | L | 279 | GLN |
| 6 | L | 292 | HIS |
| 6 | L | 355 | GLN |
| 7 | M | 9 | GLN |
| 7 | M | 38 | ASN |
| 7 | M | 68 | GLN |
| 7 | M | 101 | ASN |
| 7 | M | 152 | HIS |
| 7 | M | 166 | GLN |
| 7 | M | 219 | HIS |
| 7 | M | 258 | GLN |
| 7 | M | 506 | ASN |
| 7 | M | 520 | ASN |
| 7 | M | 539 | ASN |
| 7 | M | 542 | ASN |
| 7 | M | 573 | ASN |
| 7 | M | 622 | GLN |
| 7 | M | 659 | ASN |
| 7 | M | 714 | HIS |
| 7 | M | 715 | ASN |
| 7 | M | 742 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | M | 777 | GLN |
| 7 | M | 814 | ASN |
| 7 | M | 820 | GLN |
| 7 | M | 829 | ASN |
| 7 | M | 873 | ASN |
| 7 | M | 907 | HIS |
| 7 | M | 935 | GLN |
| 7 | M | 963 | ASN |
| 7 | M | 1009 | ASN |
| 7 | M | 1123 | ASN |
| 7 | M | 1235 | ASN |
| 7 | M | 1285 | HIS |
| 7 | M | 1311 | GLN |
| 7 | M | 1410 | ASN |
| 7 | M | 1411 | HIS |
| 7 | M | 1473 | ASN |
| 7 | M | 1542 | ASN |
| 8 | N | 23 | ASN |
| 8 | N | 82 | ASN |
| 8 | N | 85 | ASN |
| 8 | N | 111 | HIS |
| 8 | N | 132 | ASN |
| 8 | N | 150 | GLN |
| 8 | N | 166 | ASN |
| 8 | N | 190 | GLN |
| 8 | N | 196 | ASN |
| 8 | N | 201 | ASN |
| 8 | N | 211 | GLN |
| 8 | N | 218 | ASN |
| 8 | N | 304 | ASN |
| 8 | N | 322 | HIS |
| 8 | N | 356 | HIS |
| 8 | N | 444 | ASN |
| 8 | N | 574 | HIS |
| 8 | N | 667 | ASN |
| 8 | N | 670 | HIS |
| 8 | N | 677 | ASN |
| 8 | N | 745 | HIS |
| 8 | N | 760 | ASN |
| 8 | N | 770 | HIS |
| 8 | N | 780 | HIS |
| 8 | N | 800 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | N | 850 | ASN |
| 8 | N | 964 | GLN |
| 8 | N | 975 | GLN |
| 8 | N | 979 | ASN |
| 8 | N | 999 | GLN |
| 8 | N | 1041 | ASN |
| 8 | N | 1098 | ASN |
| 8 | N | 1195 | GLN |
| 8 | N | 1198 | ASN |
| 8 | N | 1282 | ASN |
| 8 | N | 1405 | ASN |
| 8 | N | 1413 | ASN |
| 8 | N | 1423 | ASN |
| 8 | N | 1429 | HIS |
| 8 | N | 1462 | ASN |
| 8 | N | 1480 | GLN |
| 8 | N | 1552 | ASN |
| 8 | N | 1624 | GLN |
| 7 | O | 9 | GLN |
| 7 | O | 36 | ASN |
| 7 | O | 82 | ASN |
| 7 | O | 122 | ASN |
| 7 | O | 152 | HIS |
| 7 | O | 172 | ASN |
| 7 | O | 176 | GLN |
| 7 | O | 195 | GLN |
| 7 | O | 219 | HIS |
| 7 | O | 239 | HIS |
| 7 | O | 334 | GLN |
| 7 | O | 428 | GLN |
| 7 | O | 560 | GLN |
| 7 | O | 602 | ASN |
| 7 | O | 622 | GLN |
| 7 | O | 646 | ASN |
| 7 | O | 694 | ASN |
| 7 | O | 715 | ASN |
| 7 | O | 777 | GLN |
| 7 | O | 820 | GLN |
| 7 | O | 842 | ASN |
| 7 | O | 860 | ASN |
| 7 | O | 907 | HIS |
| 7 | O | 935 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 7 | O | 953 | ASN |
| 7 | O | 1037 | ASN |
| 7 | O | 1061 | ASN |
| 7 | O | 1067 | ASN |
| 7 | O | 1123 | ASN |
| 7 | O | 1137 | ASN |
| 7 | O | 1155 | ASN |
| 7 | O | 1159 | GLN |
| 7 | O | 1187 | ASN |
| 7 | O | 1218 | ASN |
| 7 | O | 1235 | ASN |
| 7 | O | 1299 | ASN |
| 7 | O | 1304 | HIS |
| 7 | O | 1308 | GLN |
| 7 | O | 1326 | ASN |
| 7 | O | 1411 | HIS |
| 7 | O | 1428 | GLN |
| 7 | O | 1465 | GLN |
| 7 | O | 1468 | ASN |
| 7 | O | 1542 | ASN |
| 8 | P | 20 | ASN |
| 8 | P | 56 | ASN |
| 8 | P | 80 | GLN |
| 8 | P | 111 | HIS |
| 8 | P | 162 | HIS |
| 8 | P | 165 | ASN |
| 8 | P | 190 | GLN |
| 8 | P | 193 | GLN |
| 8 | P | 201 | ASN |
| 8 | P | 218 | ASN |
| 8 | P | 281 | GLN |
| 8 | P | 318 | HIS |
| 8 | P | 322 | HIS |
| 8 | P | 360 | GLN |
| 8 | P | 418 | ASN |
| 8 | P | 444 | ASN |
| 8 | P | 571 | ASN |
| 8 | P | 636 | GLN |
| 8 | P | 670 | HIS |
| 8 | P | 760 | ASN |
| 8 | P | 780 | HIS |
| 8 | P | 800 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 8 | P | 849 | ASN |
| 8 | P | 880 | ASN |
| 8 | P | 947 | ASN |
| 8 | P | 964 | GLN |
| 8 | P | 975 | GLN |
| 8 | P | 1055 | GLN |
| 8 | P | 1059 | ASN |
| 8 | P | 1098 | ASN |
| 8 | P | 1119 | ASN |
| 8 | P | 1127 | ASN |
| 8 | P | 1174 | ASN |
| 8 | P | 1182 | ASN |
| 8 | P | 1195 | GLN |
| 8 | P | 1249 | GLN |
| 8 | P | 1306 | ASN |
| 8 | P | 1383 | GLN |
| 8 | P | 1397 | ASN |
| 8 | P | 1399 | ASN |
| 8 | P | 1403 | ASN |
| 8 | P | 1429 | HIS |
| 8 | P | 1441 | GLN |
| 8 | P | 1492 | HIS |
| 8 | P | 1493 | ASN |
| 8 | P | 1509 | GLN |
| 8 | P | 1593 | HIS |
| 8 | P | 1608 | HIS |
| 8 | P | 1625 | GLN |
| 8 | P | 1626 | GLN |
| 9 | Q | 269 | ASN |
| 9 | Q | 276 | GLN |
| 9 | Q | 280 | GLN |
| 9 | Q | 281 | GLN |
| 9 | Q | 288 | ASN |
| 9 | Q | 359 | ASN |
| 9 | Q | 424 | ASN |
| 9 | Q | 536 | ASN |
| 9 | Q | 658 | ASN |
| 9 | Q | 699 | ASN |
| 9 | Q | 738 | GLN |
| 9 | Q | 808 | ASN |
| 9 | Q | 821 | GLN |
| 9 | R | 214 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | R | 224 | ASN |
| 9 | R | 252 | GLN |
| 9 | R | 269 | ASN |
| 9 | R | 281 | GLN |
| 9 | R | 288 | ASN |
| 9 | R | 293 | ASN |
| 9 | R | 324 | ASN |
| 9 | R | 329 | ASN |
| 9 | R | 359 | ASN |
| 9 | R | 505 | HIS |
| 9 | R | 573 | HIS |
| 9 | R | 608 | GLN |
| 9 | R | 626 | GLN |
| 9 | R | 658 | ASN |
| 9 | R | 684 | ASN |
| 9 | R | 699 | ASN |
| 9 | R | 719 | ASN |
| 9 | R | 784 | ASN |
| 9 | R | 790 | ASN |
| 9 | S | 205 | ASN |
| 9 | S | 214 | ASN |
| 9 | S | 227 | GLN |
| 9 | S | 231 | ASN |
| 9 | S | 246 | ASN |
| 9 | S | 280 | GLN |
| 9 | S | 281 | GLN |
| 9 | S | 288 | ASN |
| 9 | S | 293 | ASN |
| 9 | S | 301 | ASN |
| 9 | S | 303 | ASN |
| 9 | S | 324 | ASN |
| 9 | S | 351 | GLN |
| 9 | S | 356 | ASN |
| 9 | S | 439 | HIS |
| 9 | S | 476 | ASN |
| 9 | S | 563 | ASN |
| 9 | S | 573 | HIS |
| 9 | S | 645 | GLN |
| 9 | S | 672 | GLN |
| 9 | S | 680 | ASN |
| 9 | S | 705 | GLN |
| 9 | S | 733 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | S | 758 | GLN |
| 9 | S | 762 | ASN |
| 9 | S | 787 | HIS |
| 9 | S | 795 | GLN |
| 9 | S | 802 | GLN |
| 9 | T | 224 | ASN |
| 9 | T | 229 | ASN |
| 9 | T | 281 | GLN |
| 9 | T | 303 | ASN |
| 9 | T | 351 | GLN |
| 9 | T | 463 | GLN |
| 9 | T | 476 | ASN |
| 9 | T | 480 | GLN |
| 9 | T | 505 | HIS |
| 9 | T | 608 | GLN |
| 9 | T | 621 | HIS |
| 9 | T | 680 | ASN |
| 9 | T | 699 | ASN |
| 9 | T | 758 | GLN |
| 10 | U | 329 | GLN |
| 11 | V | 293 | HIS |
| 11 | V | 371 | GLN |
| 10 | W | 352 | GLN |
| 11 | X | 299 | GLN |
| 11 | X | 361 | ASN |
| 11 | X | 373 | ASN |
| 1 | Y | 112 | GLN |
| 1 | Y | 113 | HIS |
| 1 | Y | 128 | ASN |
| 1 | Y | 212 | GLN |
| 1 | Y | 230 | HIS |
| 1 | Y | 258 | ASN |
| 1 | Y | 260 | HIS |
| 1 | Y | 364 | GLN |
| 1 | Y | 449 | ASN |
| 1 | Y | 665 | ASN |
| 1 | Y | 672 | ASN |
| 1 | Y | 690 | ASN |
| 1 | Y | 698 | ASN |
| 1 | Y | 850 | ASN |
| 1 | Y | 887 | GLN |
| 1 | Y | 924 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 1224 | ASN |
| 1 | Y | 1333 | HIS |
| 1 | Y | 1379 | GLN |
| 1 | Y | 1406 | HIS |
| 1 | Y | 1441 | ASN |
| 1 | Y | 1445 | ASN |
| 2 | Z | 92 | GLN |
| 2 | Z | 99 | GLN |
| 2 | Z | 139 | GLN |
| 2 | Z | 141 | GLN |
| 2 | Z | 156 | ASN |
| 2 | Z | 184 | ASN |
| 2 | Z | 192 | HIS |
| 2 | Z | 238 | ASN |
| 2 | Z | 248 | ASN |
| 2 | Z | 271 | GLN |
| 2 | Z | 287 | GLN |
| 2 | Z | 344 | GLN |
| 2 | Z | 389 | ASN |
| 2 | Z | 494 | ASN |
| 2 | Z | 588 | ASN |
| 2 | Z | 607 | ASN |
| 2 | Z | 751 | GLN |
| 2 | Z | 796 | ASN |
| 2 | Z | 856 | ASN |
| 2 | Z | 872 | ASN |
| 2 | Z | 874 | ASN |
| 2 | Z | 909 | HIS |
| 2 | Z | 926 | ASN |
| 2 | Z | 958 | ASN |
| 2 | Z | 989 | ASN |
| 2 | Z | 1078 | GLN |
| 2 | Z | 1170 | GLN |
| 2 | Z | 1175 | ASN |
| 2 | Z | 1179 | ASN |
| 2 | Z | 1235 | GLN |
| 2 | Z | 1286 | HIS |
| 2 | Z | 1335 | ASN |
| 2 | Z | 1375 | ASN |
| 12 | u | 58 | ASN |
| 12 | u | 198 | ASN |
| 12 | u | 282 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | u | 311 | GLN |
| 12 | u | 369 | GLN |
| 12 | u | 398 | ASN |
| 12 | u | 425 | ASN |
| 12 | u | 432 | ASN |
| 12 | v | 39 | GLN |
| 12 | v | 180 | ASN |
| 12 | v | 219 | ASN |
| 12 | v | 260 | HIS |
| 12 | v | 288 | ASN |
| 12 | v | 301 | ASN |
| 12 | v | 398 | ASN |
| 12 | v | 432 | ASN |
| 12 | v | 442 | ASN |
| 13 | w | 1444 | ASN |
| 14 | h | 89 | HIS |
| 14 | h | 104 | GLN |
| 14 | h | 164 | HIS |
| 14 | h | 200 | ASN |
| 14 | h | 269 | HIS |
| 14 | h | 317 | ASN |
| 14 | h | 318 | ASN |
| 14 | h | 367 | ASN |
| 14 | h | 418 | GLN |
| 14 | h | 430 | ASN |
| 14 | h | 445 | ASN |
| 14 | h | 458 | ASN |
| 14 | h | 480 | ASN |
| 14 | h | 514 | ASN |
| 14 | h | 560 | ASN |
| 14 | h | 589 | ASN |
| 14 | h | 620 | HIS |
| 14 | h | 661 | GLN |
| 14 | h | 666 | ASN |
| 14 | h | 780 | HIS |
| 14 | h | 801 | ASN |
| 14 | h | 821 | HIS |
| 14 | h | 857 | GLN |
| 14 | h | 871 | HIS |
| 14 | h | 988 | GLN |
| 14 | h | 1016 | GLN |
| 15 | i | 61 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | i | 78 | ASN |
| 15 | i | 183 | ASN |
| 15 | i | 195 | GLN |
| 15 | i | 260 | GLN |
| 15 | i | 308 | ASN |
| 15 | i | 315 | GLN |
| 15 | i | 382 | ASN |
| 15 | i | 392 | GLN |
| 15 | i | 459 | ASN |
| 15 | i | 467 | ASN |
| 15 | i | 544 | ASN |
| 15 | i | 551 | ASN |
| 15 | i | 558 | ASN |
| 15 | i | 592 | ASN |
| 16 | j | 205 | ASN |
| 16 | j | 265 | HIS |
| 16 | j | 275 | GLN |
| 16 | j | 317 | HIS |
| 16 | j | 328 | ASN |
| 16 | j | 386 | ASN |
| 16 | j | 406 | HIS |
| 16 | j | 440 | GLN |
| 16 | j | 489 | HIS |
| 16 | j | 588 | GLN |
| 16 | j | 600 | ASN |
| 16 | j | 615 | ASN |
| 16 | j | 659 | ASN |
| 17 | k | 8 | HIS |
| 17 | k | 9 | ASN |
| 17 | k | 52 | HIS |
| 17 | k | 95 | HIS |
| 17 | k | 103 | ASN |
| 17 | k | 188 | ASN |
| 17 | k | 203 | HIS |
| 17 | k | 238 | ASN |
| 17 | k | 267 | ASN |
| 17 | k | 276 | ASN |
| 18 | l | 2 | GLN |
| 18 | l | 13 | HIS |
| 18 | l | 54 | HIS |
| 18 | l | 99 | ASN |
| 18 | l | 105 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 18 | l | 211 | HIS |
| 19 | m | 28 | ASN |
| 19 | m | 118 | GLN |
| 19 | m | 178 | HIS |
| 19 | m | 226 | GLN |
| 19 | m | 229 | ASN |
| 19 | m | 240 | HIS |
| 19 | m | 252 | GLN |
| 19 | m | 278 | GLN |
| 19 | m | 291 | ASN |
| 19 | m | 295 | GLN |
| 19 | m | 329 | ASN |
| 19 | m | 341 | HIS |
| 19 | m | 360 | HIS |
| 19 | m | 428 | ASN |
| 19 | m | 461 | GLN |
| 19 | m | 528 | HIS |
| 19 | m | 561 | ASN |
| 19 | m | 579 | GLN |
| 19 | m | 586 | GLN |
| 19 | m | 726 | ASN |
| 20 | n | 87 | ASN |
| 20 | n | 102 | HIS |
| 20 | n | 111 | HIS |
| 20 | n | 182 | ASN |
| 20 | n | 213 | ASN |
| 20 | n | 264 | ASN |
| 20 | n | 293 | GLN |
| 20 | n | 384 | ASN |
| 20 | n | 403 | GLN |
| 20 | n | 451 | ASN |
| 20 | n | 476 | GLN |
| 20 | n | 515 | ASN |
| 20 | n | 555 | GLN |
| 20 | n | 556 | HIS |
| 20 | n | 601 | ASN |
| 20 | n | 663 | GLN |
| 20 | n | 720 | GLN |
| 20 | n | 761 | ASN |
| 20 | n | 773 | ASN |
| 20 | n | 778 | ASN |
| 20 | n | 779 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | n | 796 | ASN |
| 20 | n | 816 | GLN |
| 20 | n | 824 | ASN |
| 20 | n | 854 | HIS |
| 20 | n | 858 | ASN |
| 20 | n | 884 | HIS |
| 20 | n | 948 | GLN |
| 20 | n | 950 | ASN |
| 20 | n | 962 | ASN |
| 20 | n | 977 | ASN |
| 20 | n | 985 | ASN |
| 20 | n | 998 | ASN |
| 20 | n | 1049 | ASN |
| 20 | n | 1119 | GLN |
| 20 | n | 1153 | ASN |
| 21 | o | 55 | ASN |
| 21 | p | 71 | HIS |
| 21 | q | 55 | ASN |
| 21 | r | 64 | ASN |
| 21 | r | 71 | HIS |
| 21 | s | 71 | HIS |
| 21 | t | 36 | GLN |
| 21 | t | 55 | ASN |
| 21 | t | 64 | ASN |
| 21 | t | 71 | HIS |
| 15 | b | 78 | ASN |
| 15 | b | 200 | ASN |
| 15 | b | 213 | ASN |
| 15 | b | 226 | GLN |
| 15 | b | 251 | GLN |
| 15 | b | 308 | ASN |
| 15 | b | 342 | ASN |
| 15 | b | 343 | GLN |
| 15 | b | 432 | ASN |
| 15 | b | 459 | ASN |
| 15 | b | 510 | HIS |
| 15 | b | 644 | GLN |
| 16 | c | 289 | ASN |
| 16 | c | 301 | ASN |
| 16 | c | 423 | GLN |
| 16 | c | 448 | GLN |
| 16 | c | 460 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | c | 480 | GLN |
| 16 | c | 485 | GLN |
| 16 | c | 489 | HIS |
| 16 | c | 525 | HIS |
| 16 | c | 557 | GLN |
| 16 | c | 584 | ASN |
| 16 | c | 589 | ASN |
| 16 | c | 600 | ASN |
| 16 | c | 647 | GLN |
| 16 | c | 650 | HIS |
| 16 | c | 767 | ASN |
| 17 | d | 8 | HIS |
| 17 | d | 106 | GLN |
| 17 | d | 149 | ASN |
| 17 | d | 188 | ASN |
| 17 | d | 227 | GLN |
| 17 | d | 236 | GLN |
| 17 | d | 238 | ASN |
| 17 | d | 284 | ASN |
| 18 | e | 190 | GLN |
| 18 | e | 211 | HIS |
| 18 | e | 291 | ASN |
| 18 | e | 337 | ASN |
| 19 | f | 8 | GLN |
| 19 | f | 27 | ASN |
| 19 | f | 28 | ASN |
| 19 | f | 48 | GLN |
| 19 | f | 100 | ASN |
| 19 | f | 216 | GLN |
| 19 | f | 226 | GLN |
| 19 | f | 240 | HIS |
| 19 | f | 273 | ASN |
| 19 | f | 274 | GLN |
| 19 | f | 287 | HIS |
| 19 | f | 292 | GLN |
| 19 | f | 307 | GLN |
| 19 | f | 341 | HIS |
| 19 | f | 360 | HIS |
| 19 | f | 391 | HIS |
| 19 | f | 428 | ASN |
| 19 | f | 437 | ASN |
| 19 | f | 576 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 19 | f | 668 | HIS |
| 19 | f | 696 | ASN |
| 19 | f | 706 | GLN |
| 20 | g | 102 | HIS |
| 20 | g | 111 | HIS |
| 20 | g | 129 | ASN |
| 20 | g | 201 | ASN |
| 20 | g | 224 | ASN |
| 20 | g | 288 | ASN |
| 20 | g | 303 | HIS |
| 20 | g | 408 | ASN |
| 20 | g | 430 | ASN |
| 20 | g | 451 | ASN |
| 20 | g | 476 | GLN |
| 20 | g | 529 | HIS |
| 20 | g | 551 | ASN |
| 20 | g | 556 | HIS |
| 20 | g | 566 | ASN |
| 20 | g | 574 | ASN |
| 20 | g | 595 | ASN |
| 20 | g | 626 | ASN |
| 20 | g | 651 | ASN |
| 20 | g | 752 | GLN |
| 20 | g | 761 | ASN |
| 20 | g | 773 | ASN |
| 20 | g | 778 | ASN |
| 20 | g | 784 | ASN |
| 20 | g | 796 | ASN |
| 20 | g | 800 | GLN |
| 20 | g | 854 | HIS |
| 20 | g | 858 | ASN |
| 20 | g | 867 | GLN |
| 20 | g | 873 | GLN |
| 20 | g | 884 | HIS |
| 20 | g | 948 | GLN |
| 20 | g | 950 | ASN |
| 20 | g | 959 | ASN |
| 20 | g | 970 | GLN |
| 20 | g | 998 | ASN |
| 20 | g | 1030 | ASN |
| 20 | g | 1124 | ASN |
| 20 | g | 1134 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | g | 1145 | ASN |
| 14 | a | 10 | ASN |
| 14 | a | 21 | ASN |
| 14 | a | 22 | ASN |
| 14 | a | 64 | ASN |
| 14 | a | 94 | ASN |
| 14 | a | 103 | ASN |
| 14 | a | 132 | GLN |
| 14 | a | 153 | GLN |
| 14 | a | 269 | HIS |
| 14 | a | 316 | GLN |
| 14 | a | 343 | ASN |
| 14 | a | 350 | ASN |
| 14 | a | 383 | ASN |
| 14 | a | 481 | HIS |
| 14 | a | 492 | ASN |
| 14 | a | 496 | ASN |
| 14 | a | 514 | ASN |
| 14 | a | 575 | ASN |
| 14 | a | 589 | ASN |
| 14 | a | 620 | HIS |
| 14 | a | 650 | HIS |
| 14 | a | 670 | GLN |
| 14 | a | 717 | ASN |
| 14 | a | 734 | HIS |
| 14 | a | 753 | ASN |
| 14 | a | 780 | HIS |
| 14 | a | 803 | HIS |
| 14 | a | 821 | HIS |
| 14 | a | 838 | GLN |
| 14 | a | 857 | GLN |
| 14 | a | 868 | GLN |
| 14 | a | 878 | HIS |
| 14 | a | 903 | ASN |
| 14 | a | 910 | GLN |
| 14 | a | 929 | HIS |
| 14 | a | 952 | ASN |
| 14 | a | 1005 | ASN |
| 14 | a | 1016 | GLN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 16 | j | 2 |
| 16 | c | 2 |
| 20 | n | 1 |
| 20 | g | 1 |
| 4 | A | 1 |
| 14 | a | 1 |
| 14 | h | 1 |
| 1 | 0 | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | n | 807:PHE | C | 808:TYR | N | 28.87 |
| 1 | g | 807:PHE | C | 808:TYR | N | 9.13 |
| 1 | j | 665:ILE | C | 760:VAL | N | 8.70 |
| 1 | A | 637:LEU | C | 638:ASP | N | 7.22 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | a | 486:LEU | C | 487:ASN | N | 6.29 |
| 1 | c | 665:ILE | C | 760:VAL | N | 5.59 |
| 1 | h | 486:LEU | C | 487:ASN | N | 4.92 |
| 1 | c | 533:PRO | C | 535:SER | N | 4.52 |
| 1 | j | 533:PRO | C | 535:SER | N | 3.50 |
| 1 | 0 | 393:ILE | C | 394:GLU | N | 1.13 |

# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24258. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

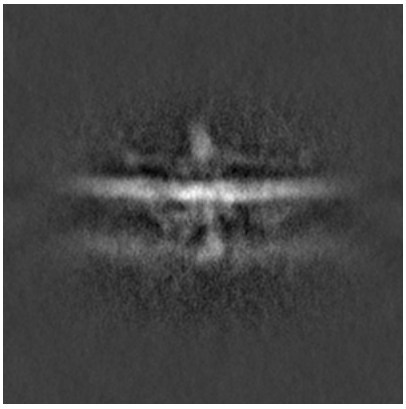
### 6.1.1 Primary map

X

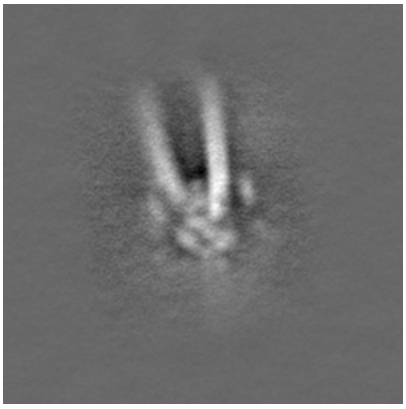
Y

Z

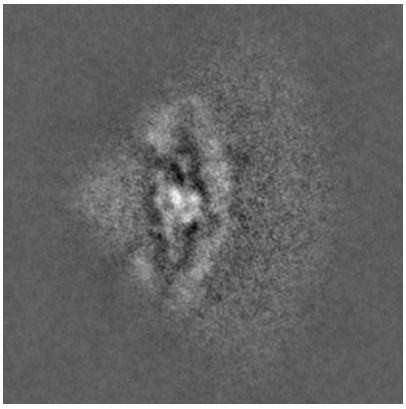
### 6.1.2 Raw map



X



Y

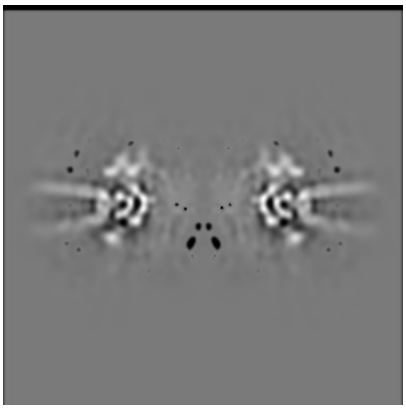


Z

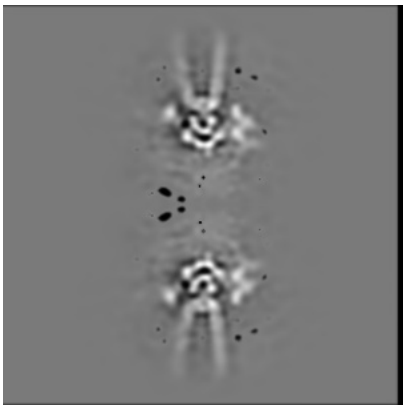
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

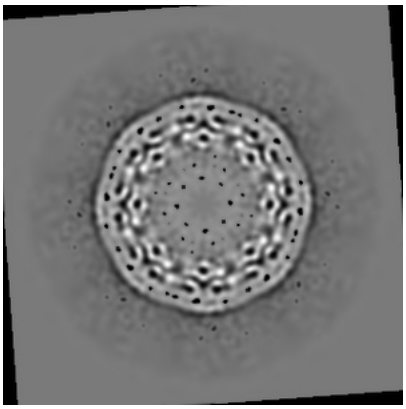
### 6.2.1 Primary map



X Index: 160

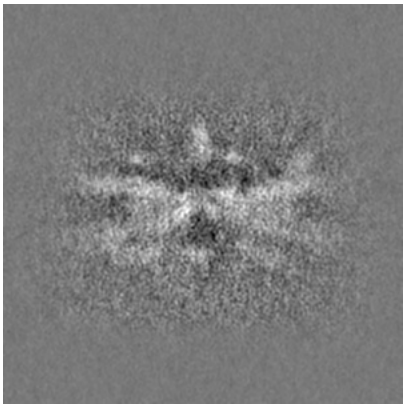


Y Index: 160

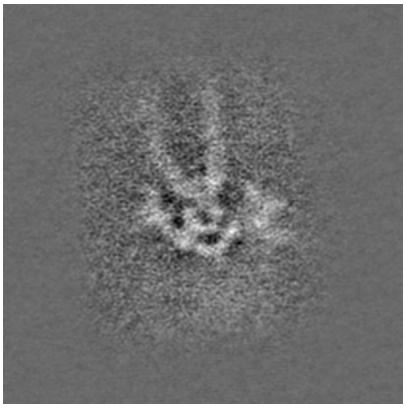


Z Index: 160

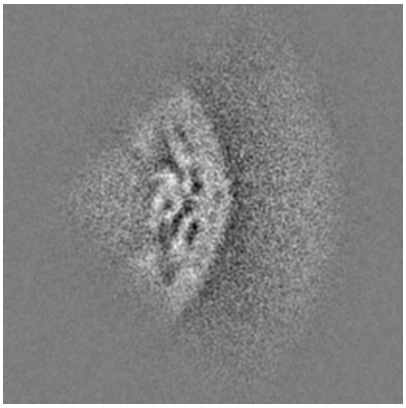
### 6.2.2 Raw map



X Index: 104



Y Index: 104

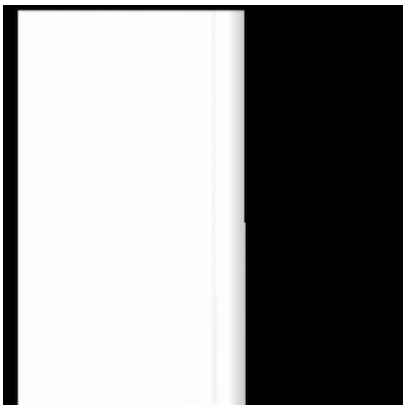


Z Index: 104

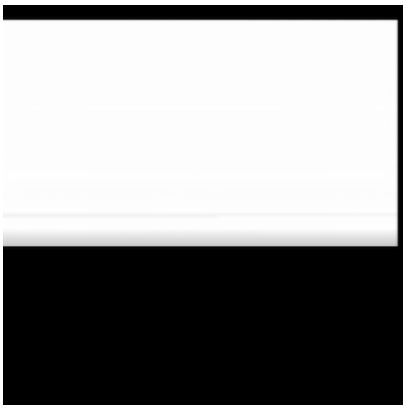
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

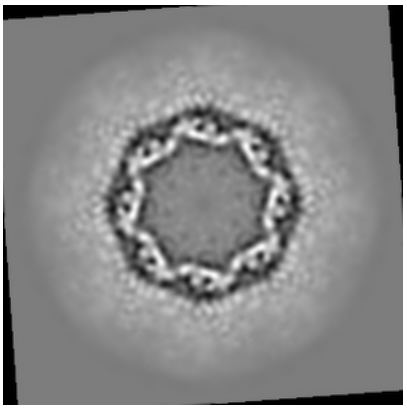
### 6.3.1 Primary map



X Index: 317

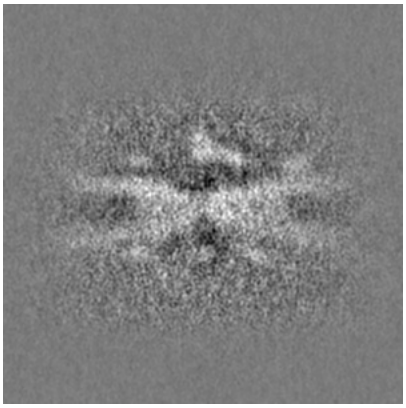


Y Index: 317

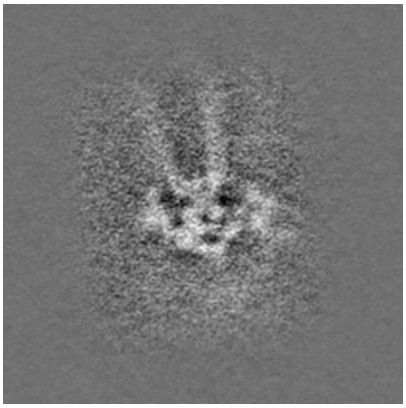


Z Index: 171

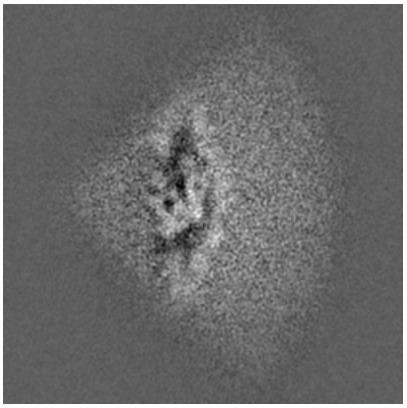
### 6.3.2 Raw map



X Index: 106



Y Index: 105

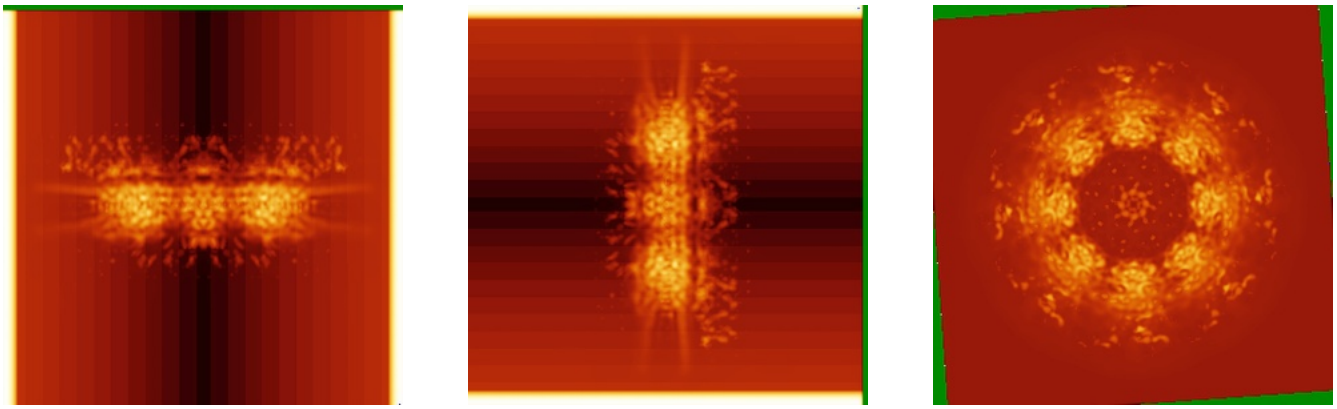


Z Index: 110

The images above show the largest variance slices of the map in three orthogonal directions.

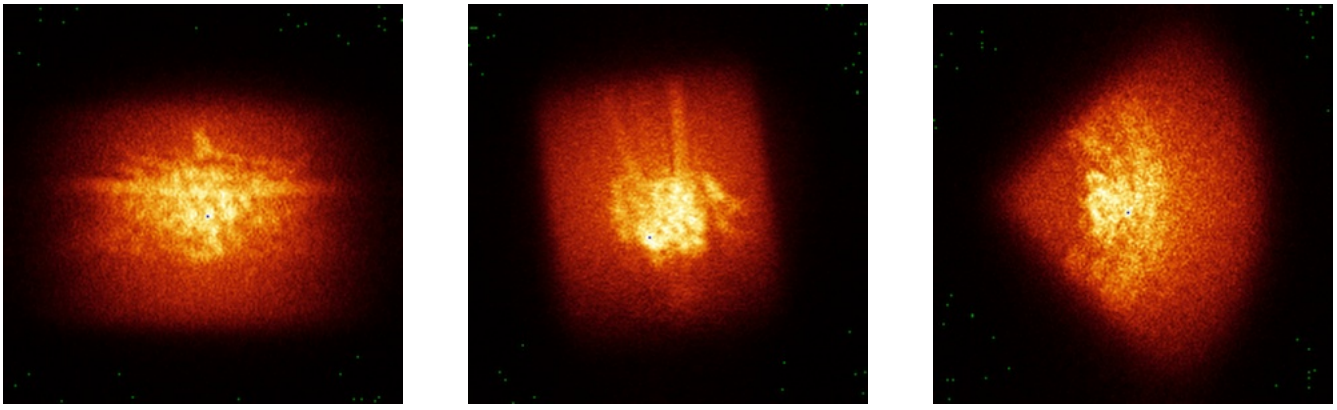
## 6.4 Orthogonal standard-deviation projections (False-color) (i)

### 6.4.1 Primary map



X Y Z

### 6.4.2 Raw map



X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1950.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation

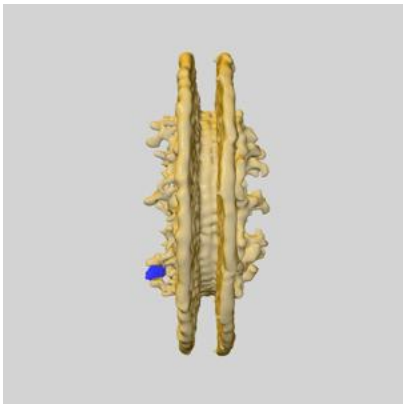
This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

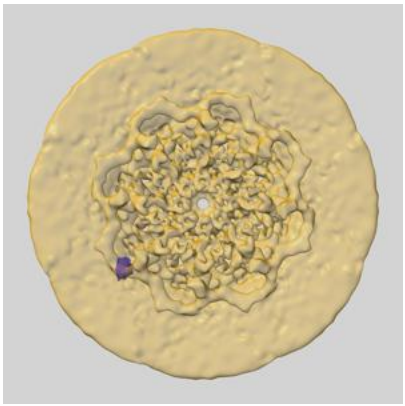
- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

### 6.6.1 emd_24258_msk_1.map

X



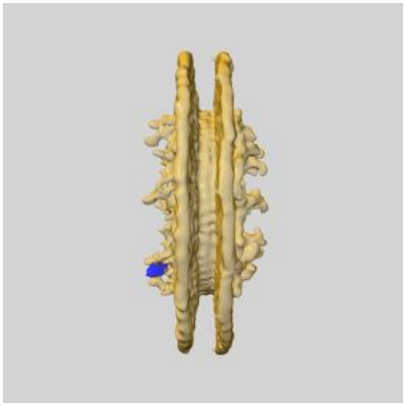
Y



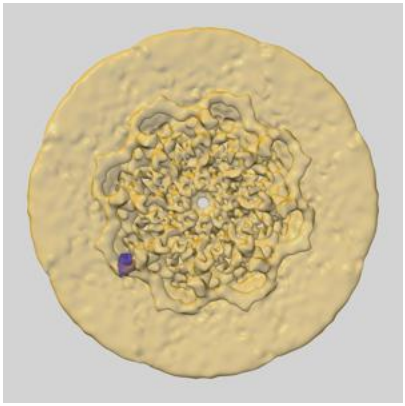
Z

### 6.6.2 emd_24258_msk_2.map

X



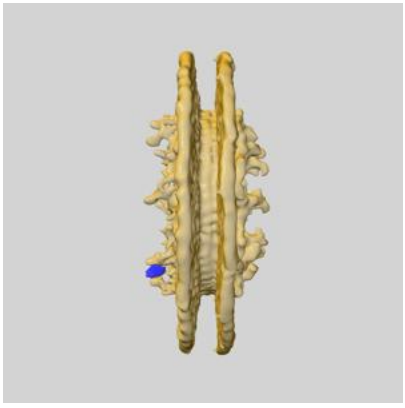
Y



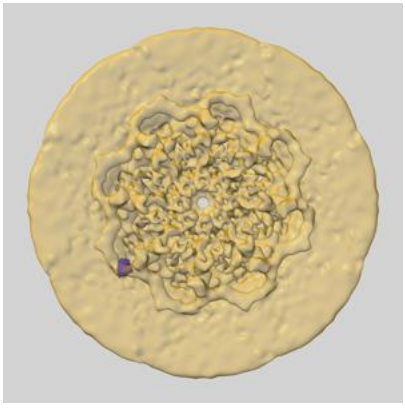
Z

### 6.6.3 emd_24258_msk_3.map

X



Y

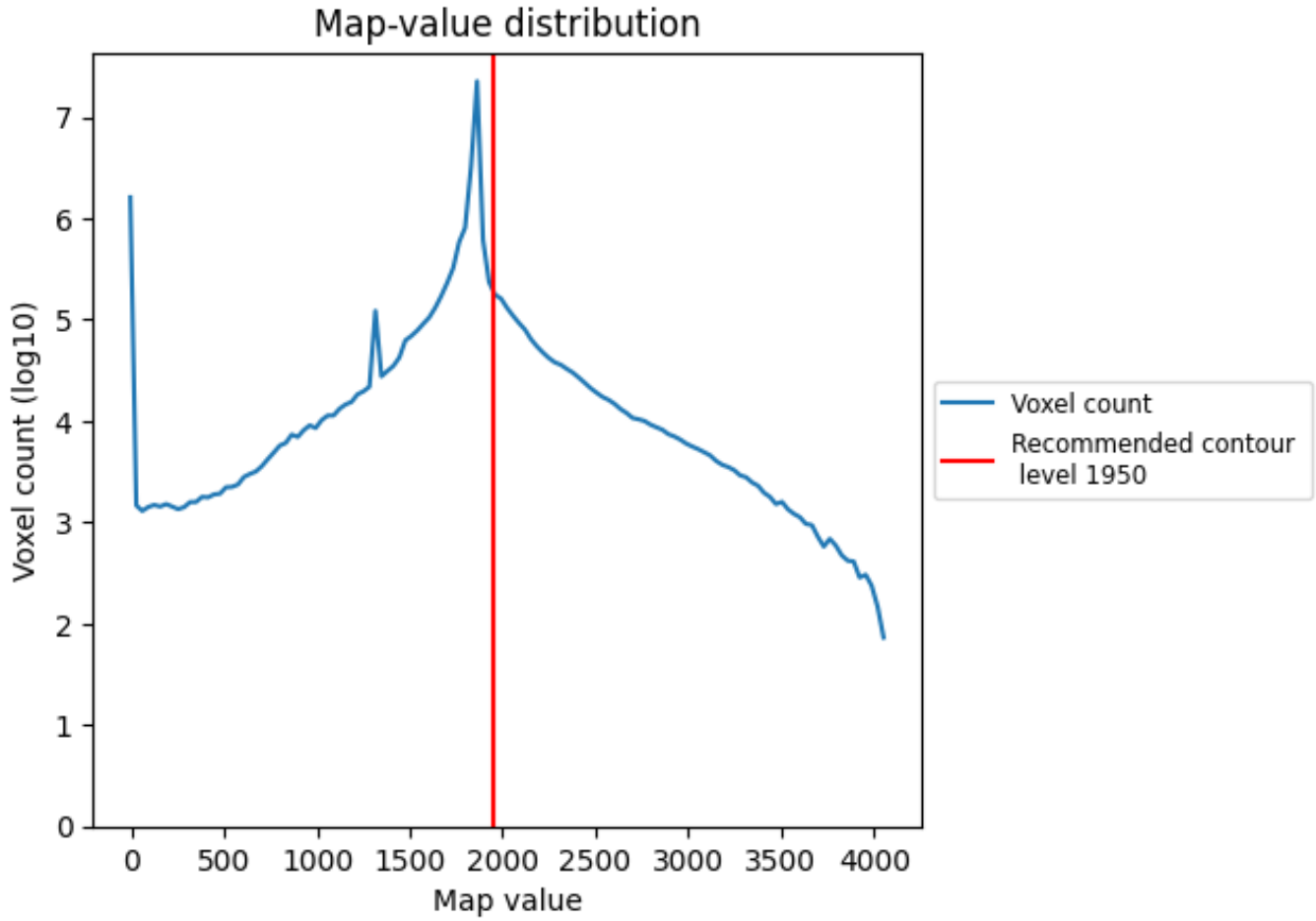


Z

# 7 Map analysis

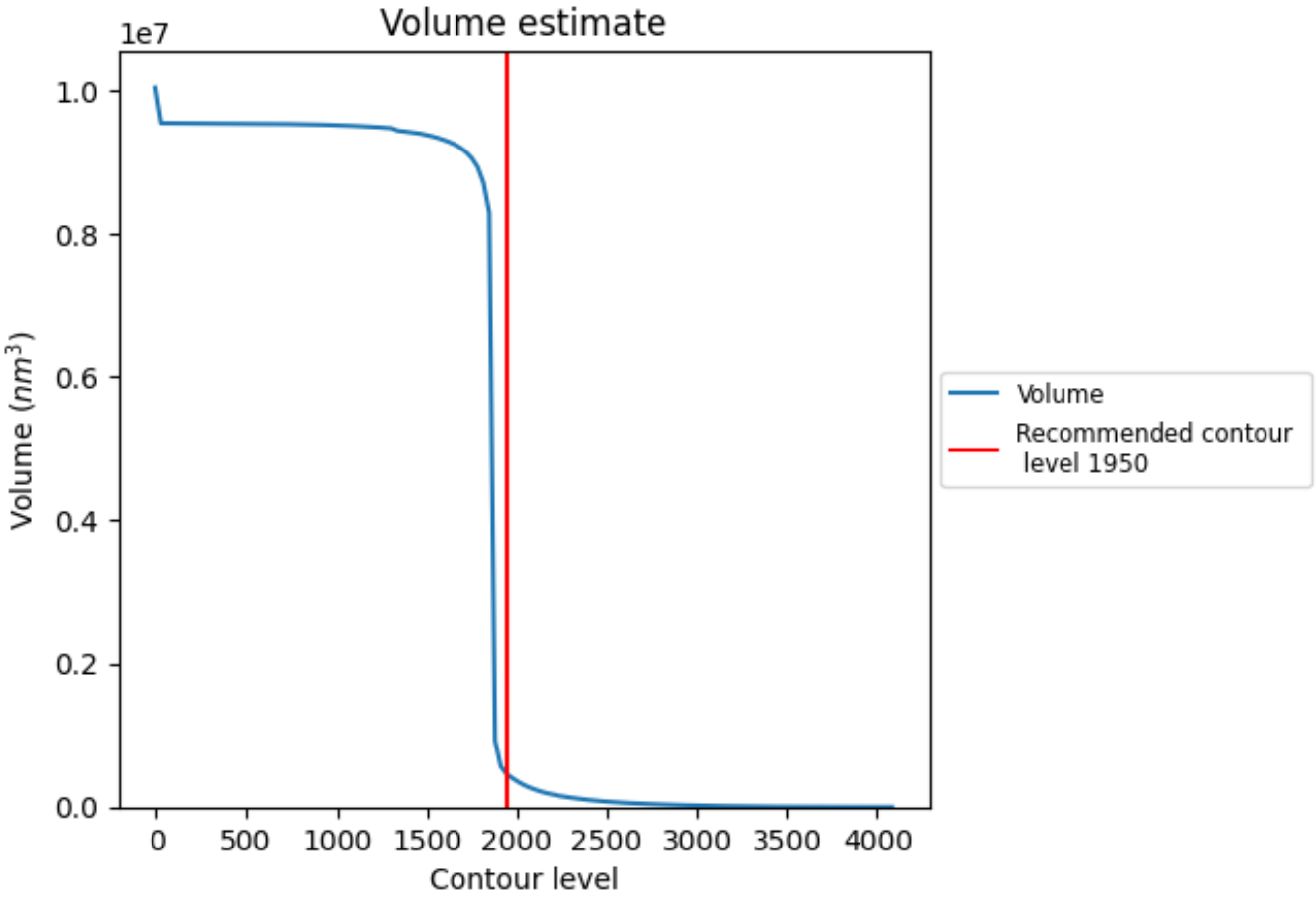
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

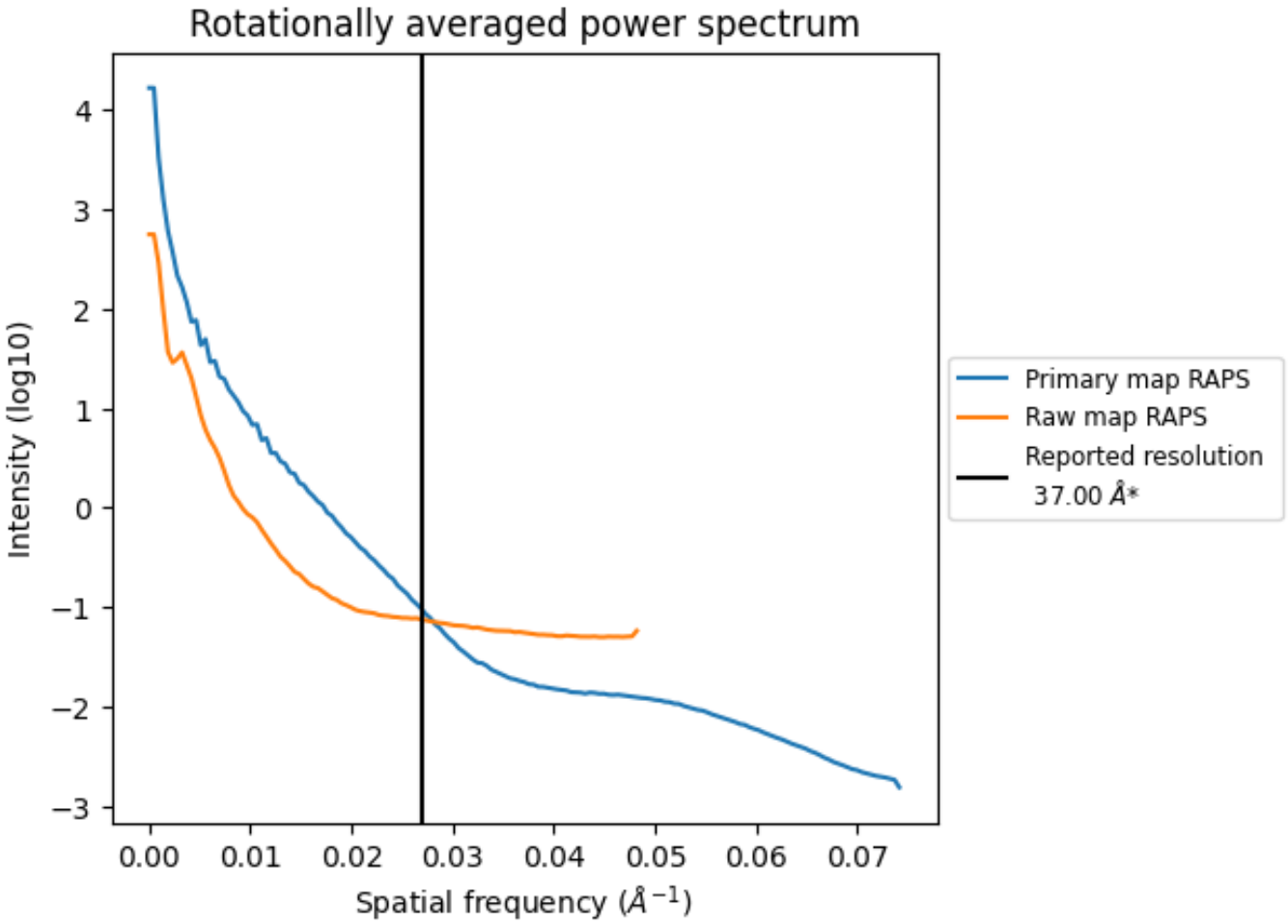
## 7.2 Volume estimate




The volume at the recommended contour level is 447442 $nm^3$; this corresponds to an approximate mass of 404186 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)

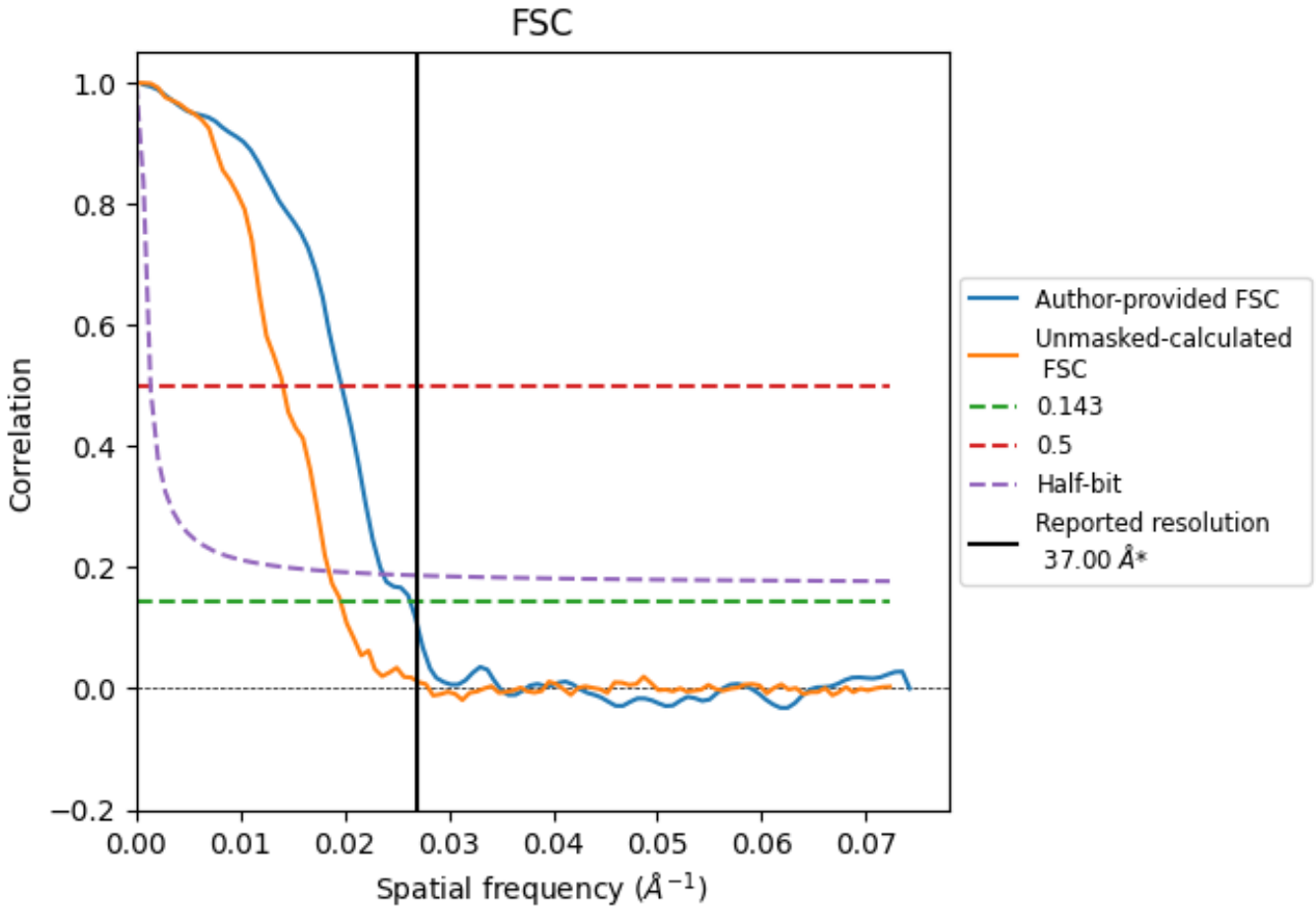



*Reported resolution corresponds to spatial frequency of 0.027 Å$^{-1}$

# 8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.027 Å$^{-1}$

## 8.2 Resolution estimates (i)

| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 37.00 | - | - |
| Author-provided FSC curve | 38.02 | 50.76 | 42.19 |
| Unmasked-calculated* | 51.02 | 70.92 | 54.05 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 51.02 differs from the reported value 37.0 by more than 10 %

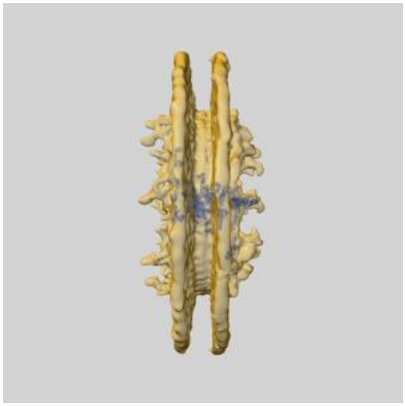
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24258 and PDB model 7N9F. Per-residue inclusion information can be found in section 3 on page 11.

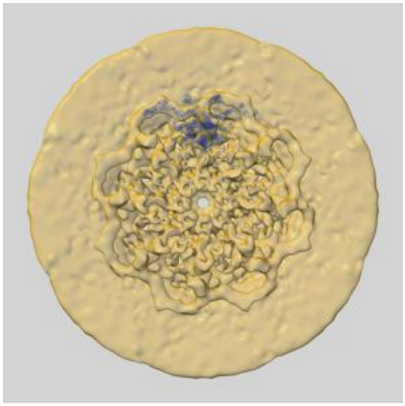
## 9.1 Map-model overlays

### 9.1.1 Map-model overlay

X

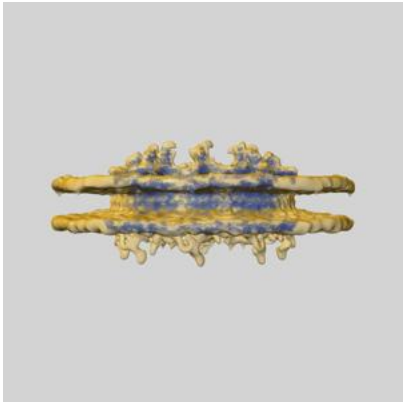


Y

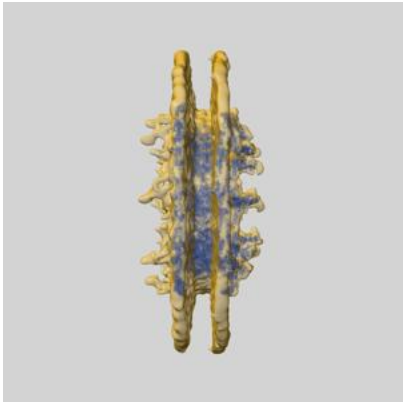


Z

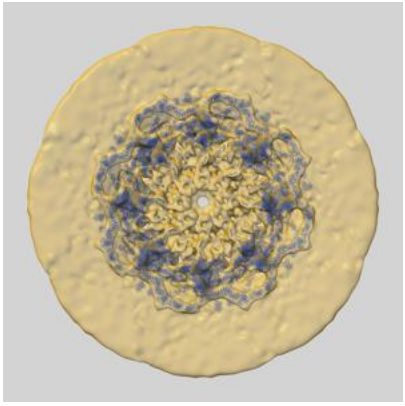
### 9.1.2 Map-model assembly overlay



X



Y



Z

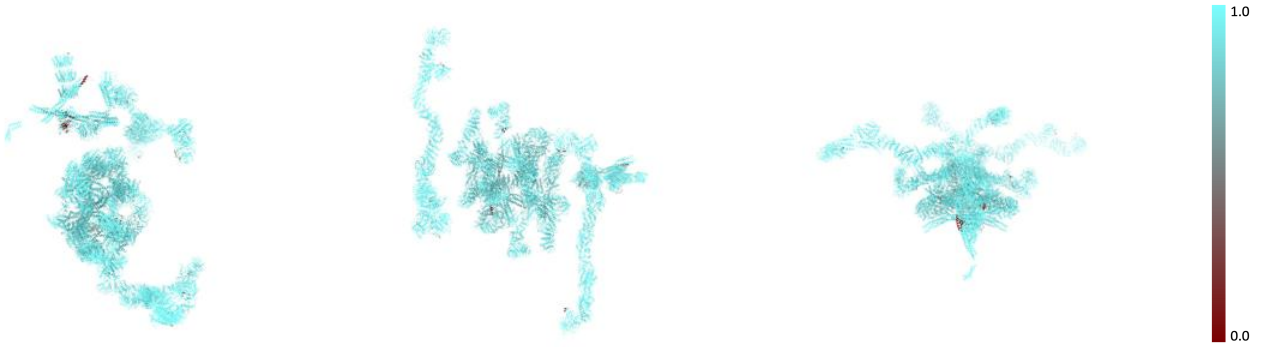
The images above show the 3D surface view of the map at the recommended contour level 1950.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

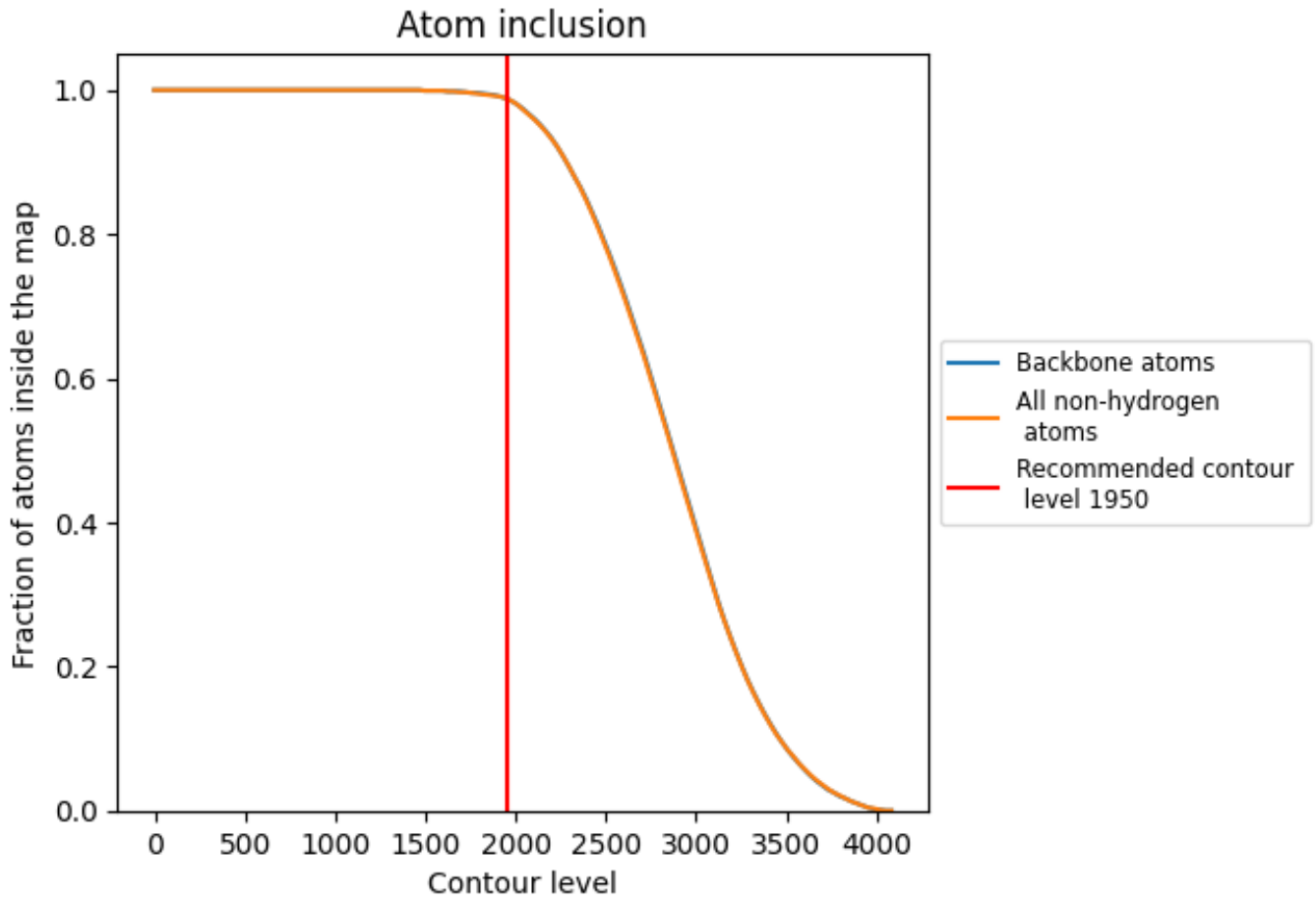
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1950).

## 9.4 Atom inclusion (i)




At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1950) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9880 | 0.0430 |
| 0 | 0.9750 | 0.0430 |
| 1 | 0.9920 | 0.0510 |
| 5 | 1.0000 | 0.0080 |
| 6 | 1.0000 | -0.0200 |
| A | 0.9980 | 0.0610 |
| B | 0.9770 | 0.0690 |
| C | 1.0000 | 0.0580 |
| D | 0.9750 | 0.0500 |
| E | 0.9860 | 0.0410 |
| F | 1.0000 | 0.0580 |
| G | 0.9830 | 0.0490 |
| H | 0.9860 | 0.0540 |
| I | 0.9990 | 0.0550 |
| J | 0.9460 | 0.0560 |
| K | 0.9770 | 0.0560 |
| L | 0.9990 | 0.0590 |
| M | 0.9960 | 0.0350 |
| N | 1.0000 | 0.0480 |
| O | 0.9840 | 0.0400 |
| P | 1.0000 | 0.0440 |
| Q | 1.0000 | 0.0580 |
| R | 0.9900 | 0.0440 |
| S | 1.0000 | 0.0440 |
| T | 0.9940 | 0.0520 |
| U | 1.0000 | 0.0560 |
| V | 1.0000 | 0.0100 |
| W | 1.0000 | 0.0550 |
| X | 1.0000 | 0.0650 |
| Y | 0.9930 | 0.0490 |
| Z | 0.9970 | 0.0450 |
| a | 0.9930 | 0.0390 |
| b | 1.0000 | 0.0480 |
| c | 0.9990 | 0.0400 |
| d | 1.0000 | 0.0400 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| e | 1.0000 | 0.0260 |
| f | 1.0000 | 0.0450 |
| g | 0.9880 | 0.0290 |
| h | 0.9820 | 0.0340 |
| i | 1.0000 | 0.0470 |
| j | 1.0000 | 0.0400 |
| k | 1.0000 | 0.0580 |
| l | 0.9660 | 0.0330 |
| m | 0.9990 | 0.0480 |
| n | 0.9910 | 0.0430 |
| o | 1.0000 | 0.0600 |
| p | 1.0000 | 0.0310 |
| q | 1.0000 | 0.0530 |
| r | 1.0000 | 0.0680 |
| s | 1.0000 | 0.0450 |
| t | 0.9930 | 0.0280 |
| u | 0.7990 | 0.0020 |
| v | 0.9870 | 0.0240 |
| w | 0.8960 | 0.0270 |
| x | 0.9820 | 0.0260 |
| y | 0.9150 | 0.0470 |
| z | 0.9230 | 0.0420 |