



Full wwPDB EM Validation Report ⓘ

Apr 29, 2026 – 12:46 am BST

PDB ID : 9RCD / pdb_00009rcd
EMDB ID : EMD-53917
Title : Sheathed flagellar filament in *Vibrio alginolyticus*
Authors : Qin, K.; Eikenkel, R.; Erhardt, M.; Bergeron, J.R.C.
Deposited on : 2025-05-27
Resolution : 3.60 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

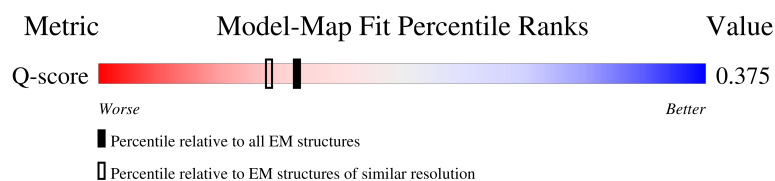
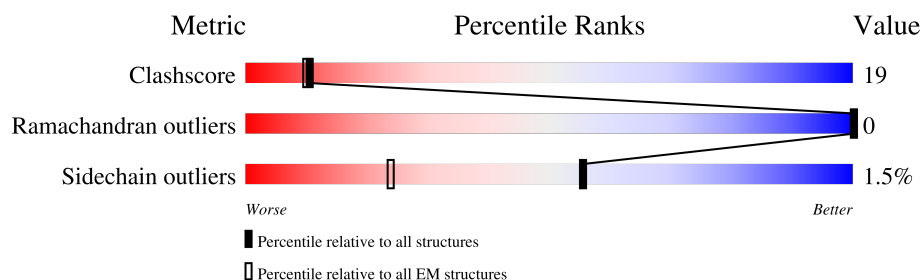
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 3.60 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.














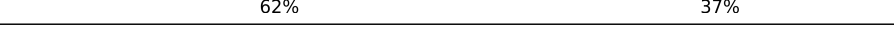







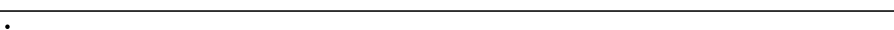

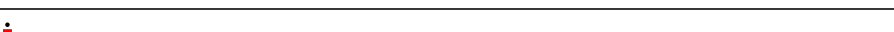
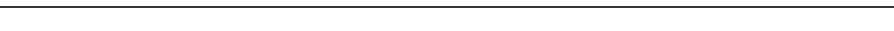


| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 12797 (3.10 - 4.10) |

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 $\leq 5\%$. 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 | 1 | 377 |  |
| 1 | 2 | 377 |  |
| 1 | 3 | 377 |  |
| 1 | A | 377 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | B | 377 |  66% 34% |
| 1 | C | 377 |  68% 31% |
| 1 | D | 377 |  67% 33% |
| 1 | E | 377 |  63% 36% |
| 1 | F | 377 |  66% 31% |
| 1 | G | 377 |  63% 36% |
| 1 | H | 377 |  64% 35% |
| 1 | I | 377 |  63% 36% |
| 1 | J | 377 |  67% 32% |
| 1 | K | 377 |  69% 29% |
| 1 | L | 377 |  63% 36% |
| 1 | M | 377 |  62% 37% |
| 1 | N | 377 |  62% 37% |
| 1 | O | 377 |  63% 37% |
| 1 | P | 377 |  64% 35% |
| 1 | Q | 377 |  67% 32% |
| 1 | R | 377 |  63% 35% |
| 1 | S | 377 |  62% 38% |
| 1 | T | 377 |  63% 37% |
| 1 | U | 377 |  66% 34% |
| 1 | V | 377 |  74% 25% |
| 1 | c | 377 |  62% 37% |
| 1 | h | 377 |  68% 31% |
| 1 | i | 377 |  63% 37% |
| 1 | j | 377 |  68% 31% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | k | 377 |  |
| 1 | l | 377 |  |
| 1 | m | 377 |  |
| 1 | n | 377 |  |
| 1 | o | 377 |  |
| 1 | p | 377 |  |
| 1 | q | 377 |  |
| 1 | r | 377 |  |
| 1 | s | 377 |  |
| 1 | t | 377 |  |
| 1 | u | 377 |  |
| 1 | v | 377 |  |
| 1 | w | 377 |  |
| 1 | x | 377 |  |
| 1 | z | 377 |  |

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 123112 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 Flagellin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1 | 1 | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | 2 | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | 3 | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | A | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | B | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | C | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | D | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | E | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | F | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | G | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | H | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | I | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | J | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | K | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | L | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | M | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |
| 1 | N | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2798 | 1692 | 503 | 594 | 9 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1 | O | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | P | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | Q | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | R | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | S | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | T | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | U | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | V | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | c | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | h | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | i | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | j | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | k | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | l | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | m | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | n | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | o | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | p | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | q | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | r | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | s | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |

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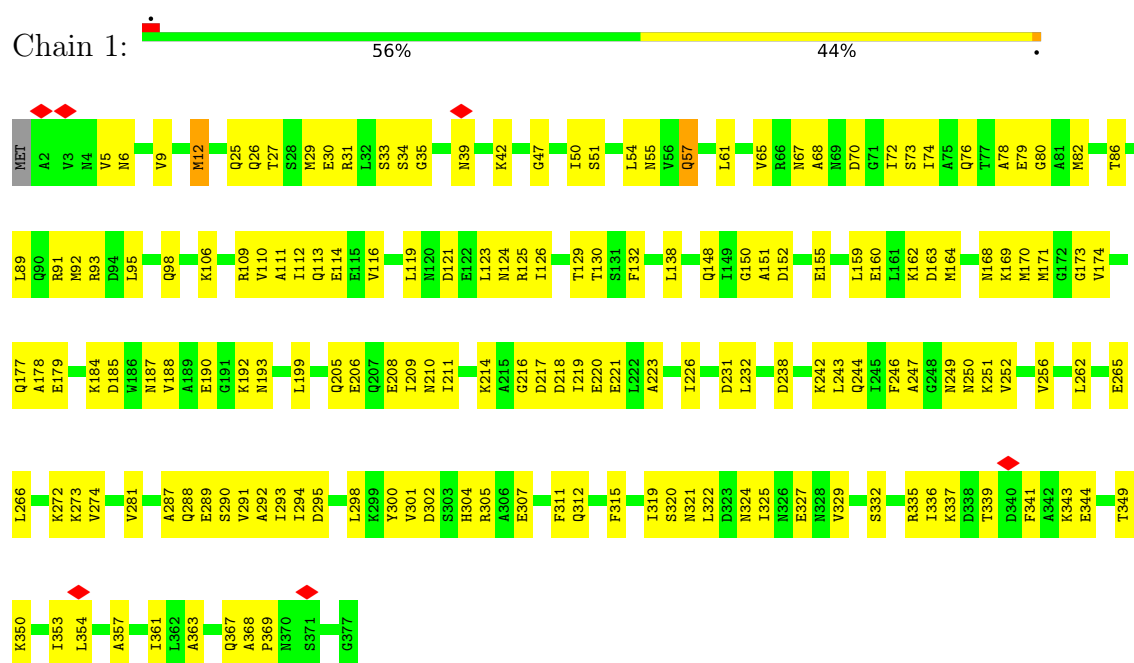
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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1 | t | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | u | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | v | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | w | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | x | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |
| 1 | z | 376 | Total 2798 | C 1692 | N 503 | O 594 | S 9 | 0 | 0 |

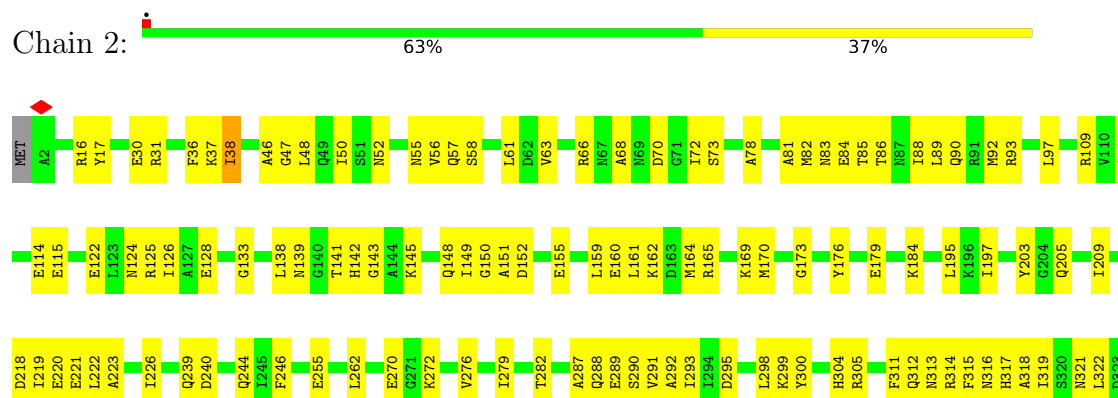
3 Residue-property plots [i](#)

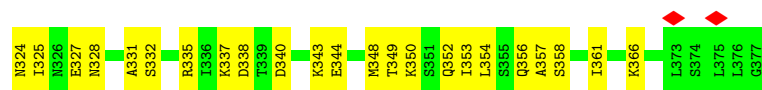
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Flagellin

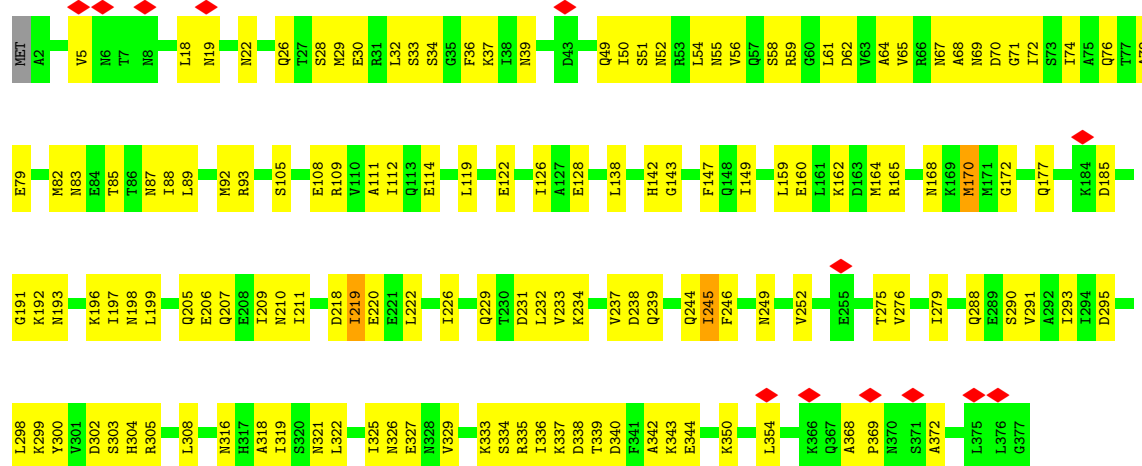


• Molecule 1: Flagellin

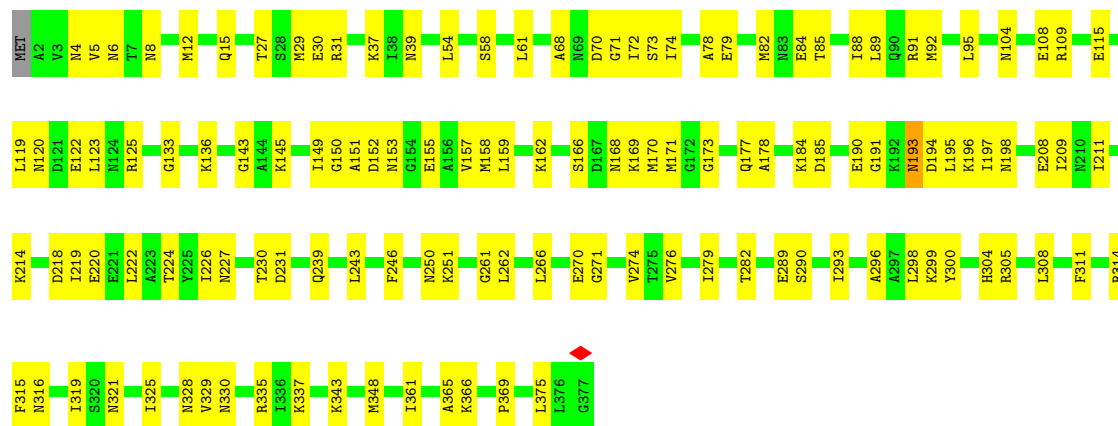




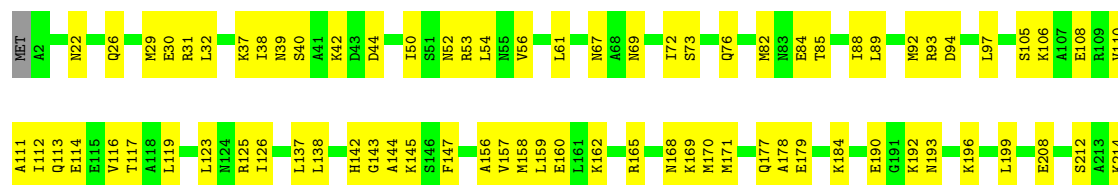
• Molecule 1: Flagellin

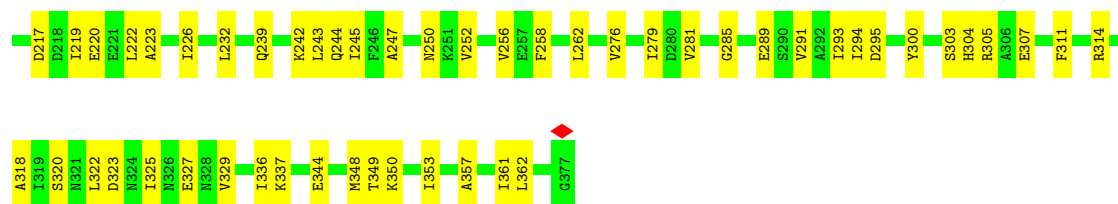


• Molecule 1: Flagellin



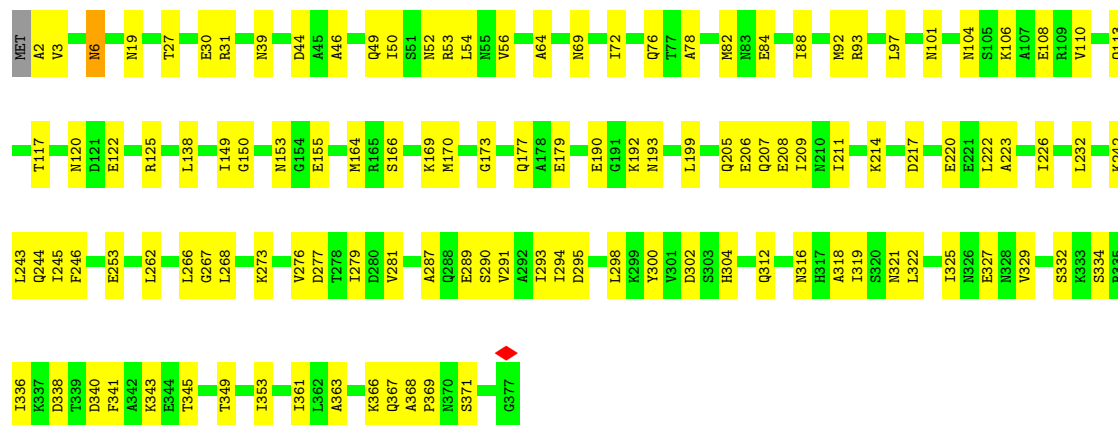
• Molecule 1: Flagellin





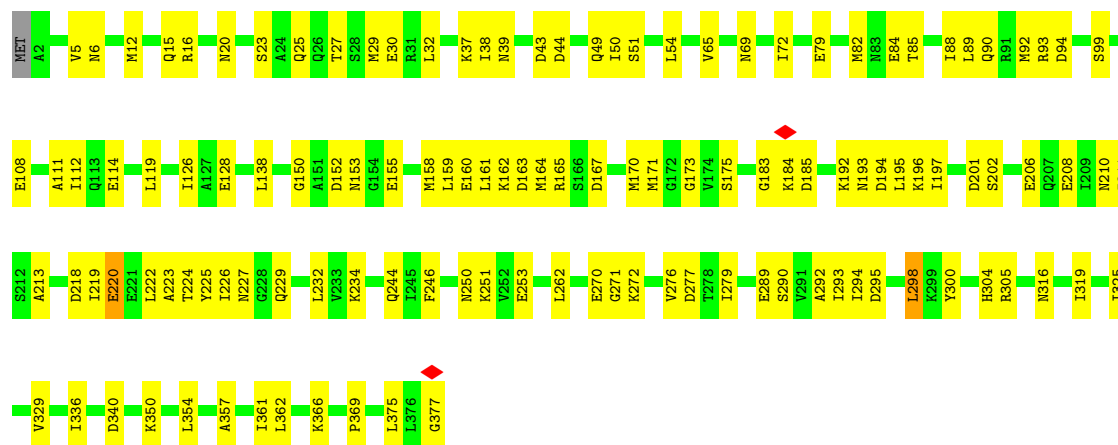
• Molecule 1: Flagellin

Chain C: 68% 31%



• Molecule 1: Flagellin

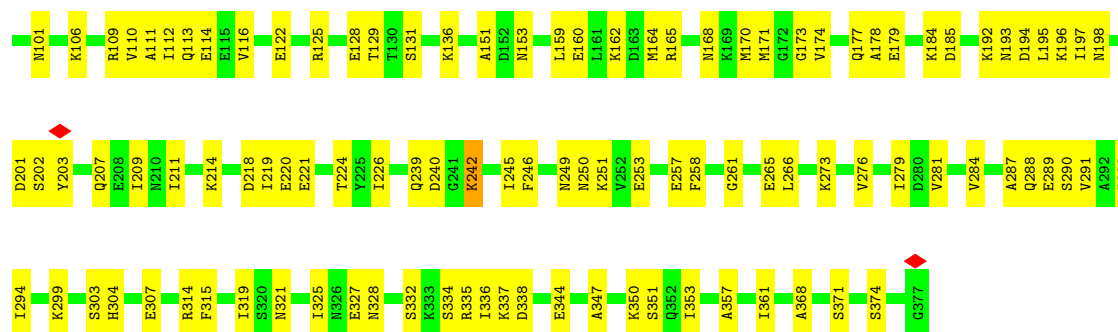
Chain D: 67% 33%



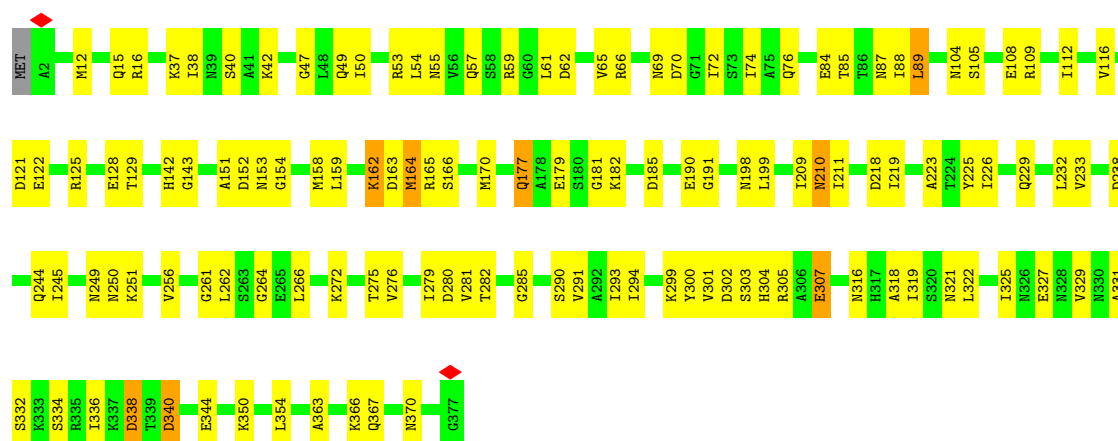
• Molecule 1: Flagellin

Chain E: 63% 36%

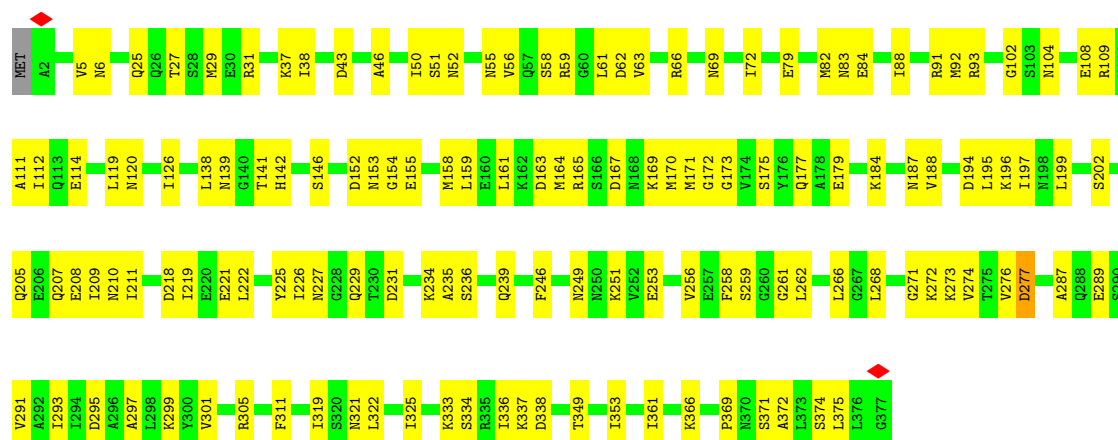




• Molecule 1: Flagellin

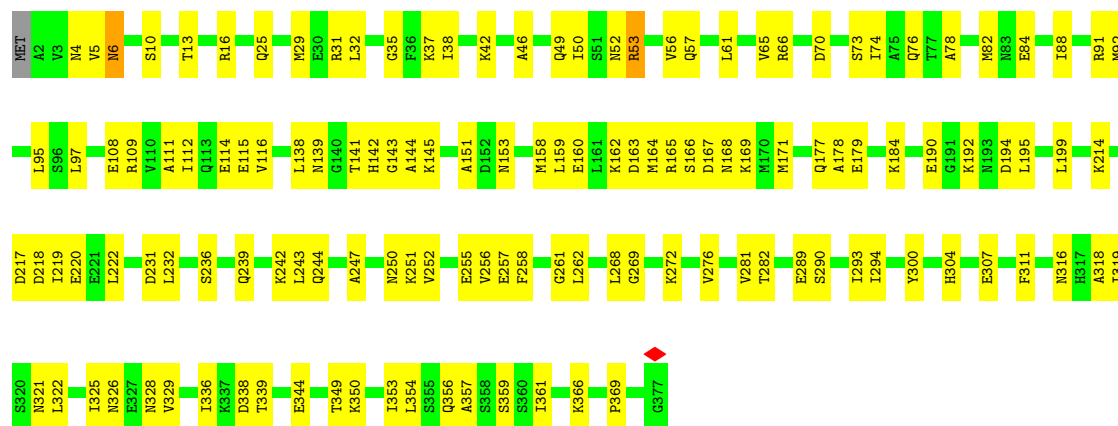


• Molecule 1: Flagellin



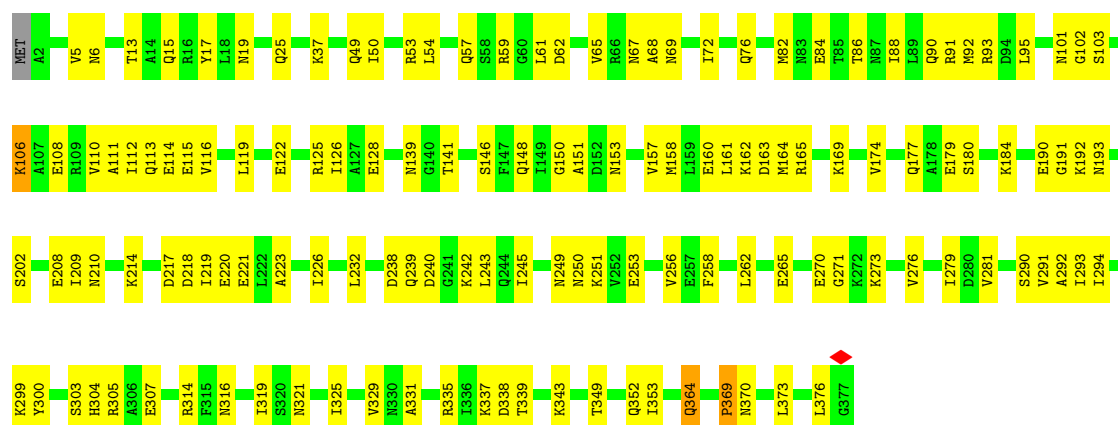
• Molecule 1: Flagellin





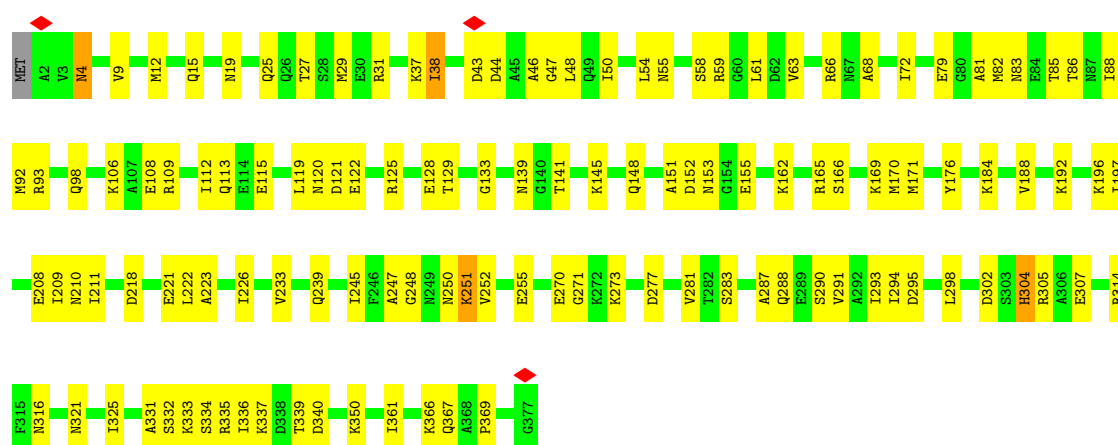
• Molecule 1: Flagellin

Chain I: 63% 36%

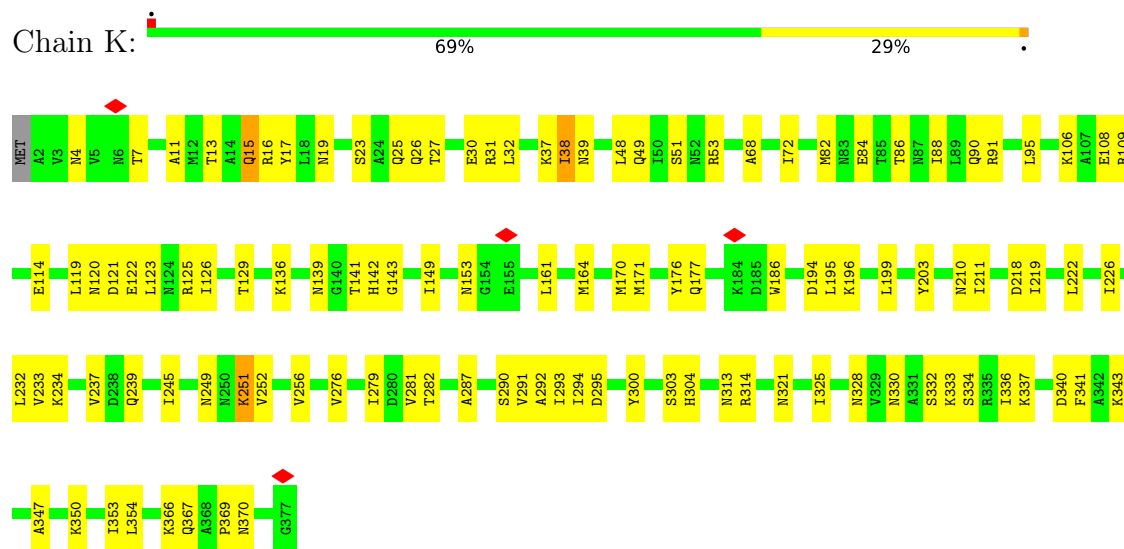


• Molecule 1: Flagellin

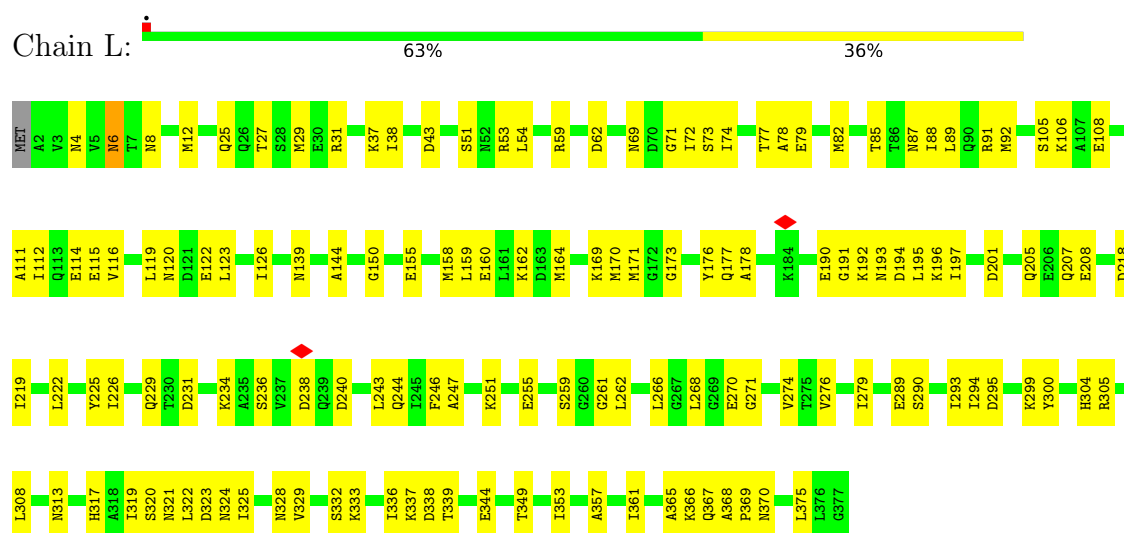
Chain J: 67% 32%



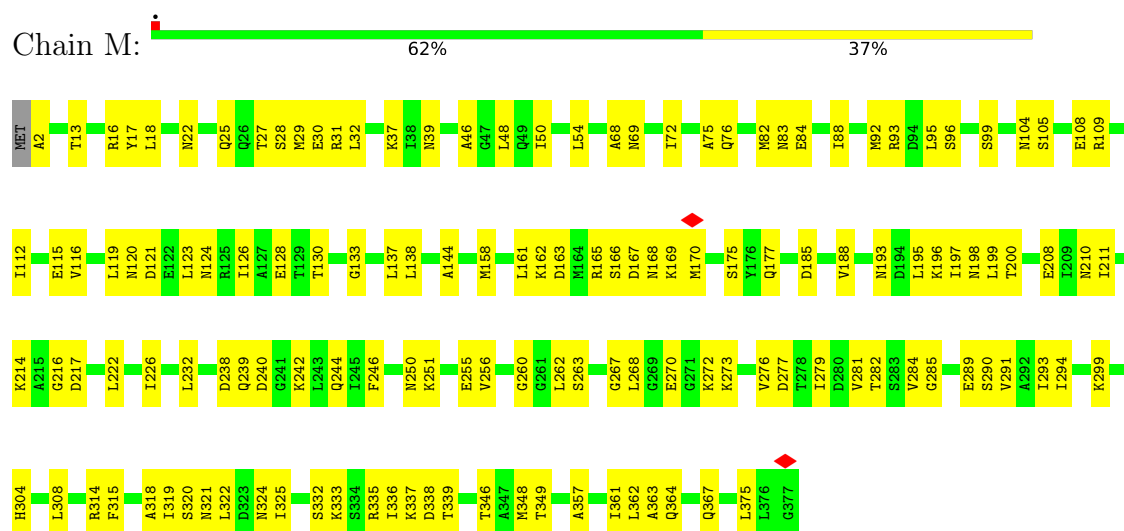
• Molecule 1: Flagellin



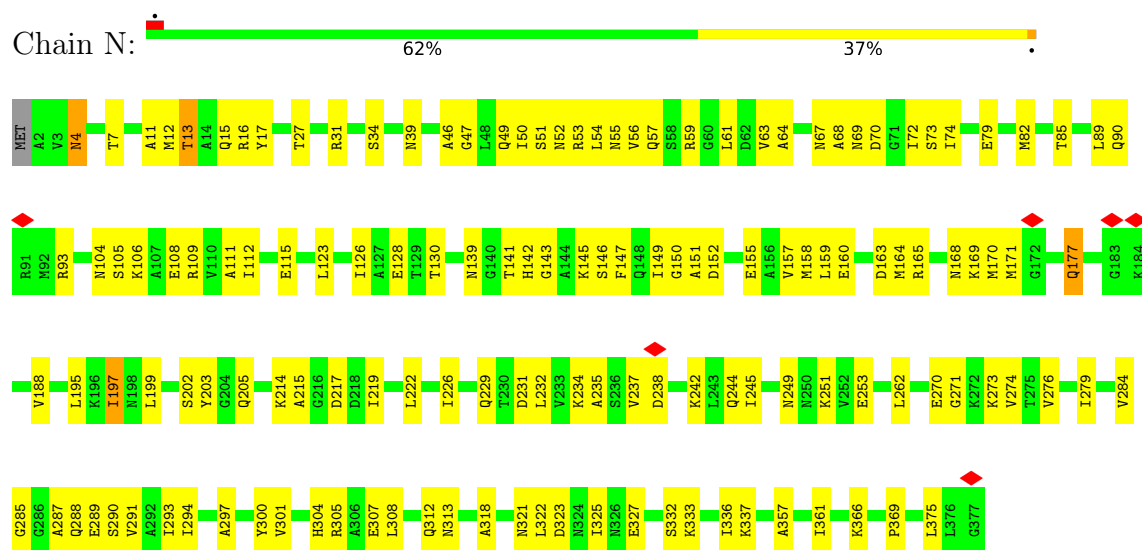
• Molecule 1: Flagellin



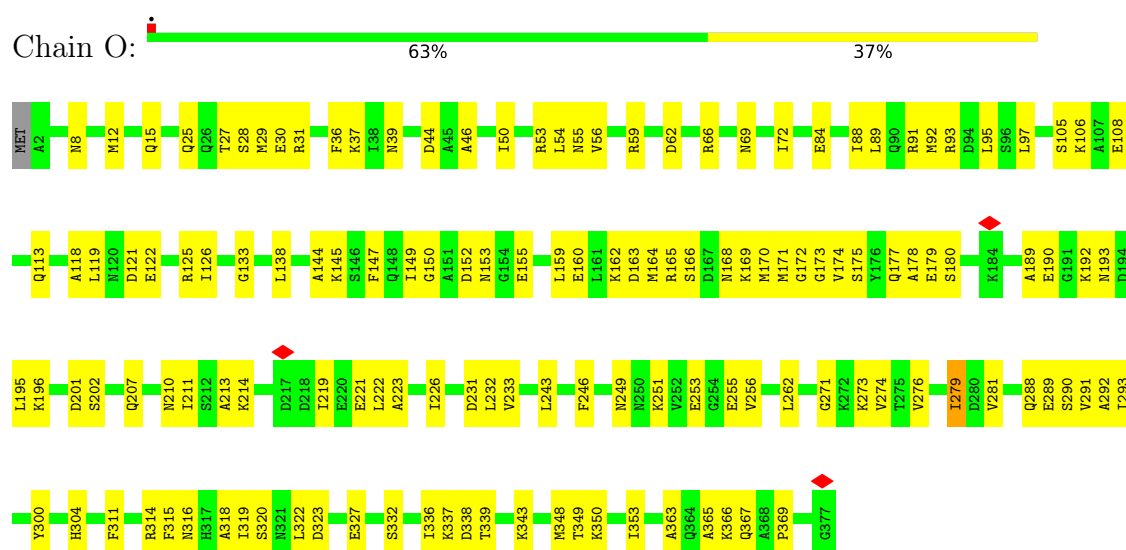
• Molecule 1: Flagellin



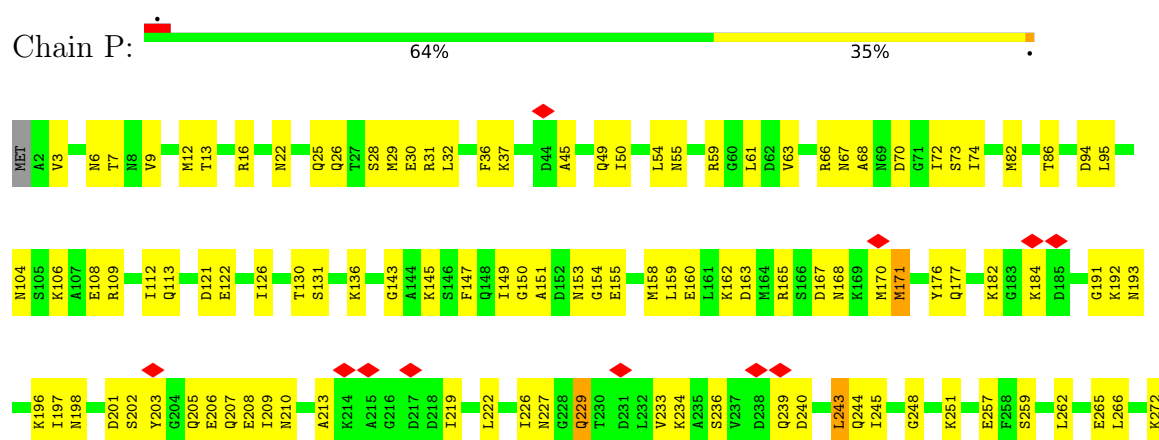
- Molecule 1: Flagellin

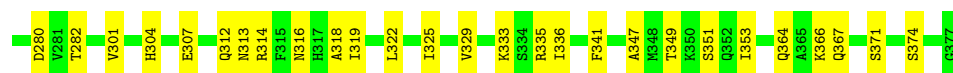


- Molecule 1: Flagellin



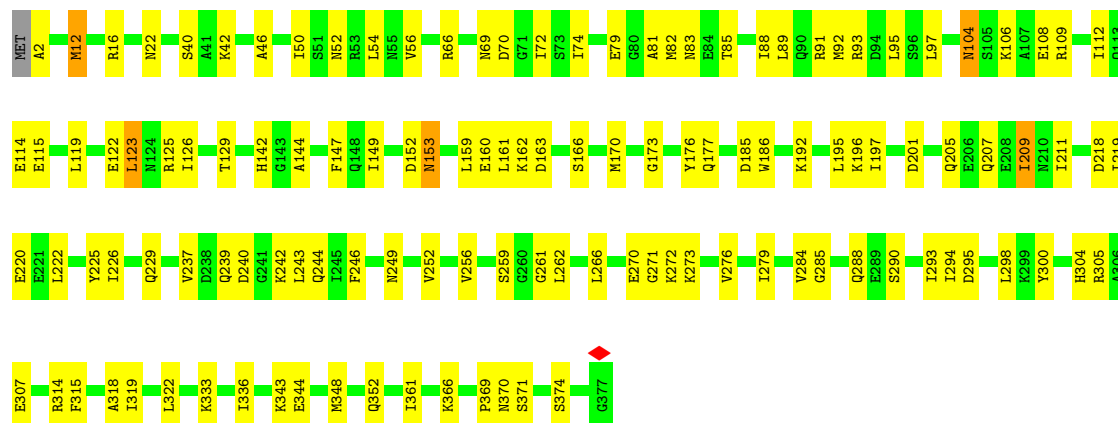
- Molecule 1: Flagellin





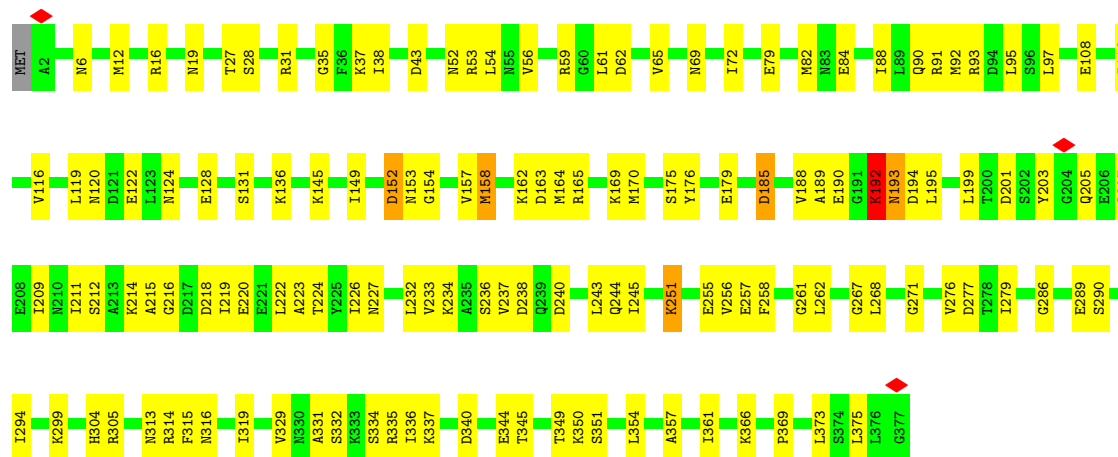
• Molecule 1: Flagellin

Chain Q: 67% 32%



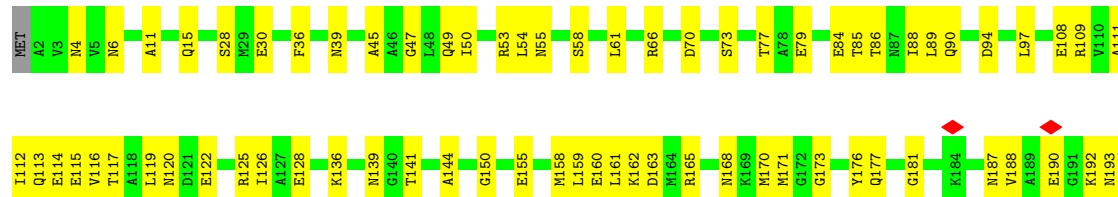
• Molecule 1: Flagellin

Chain R: 63% 35%



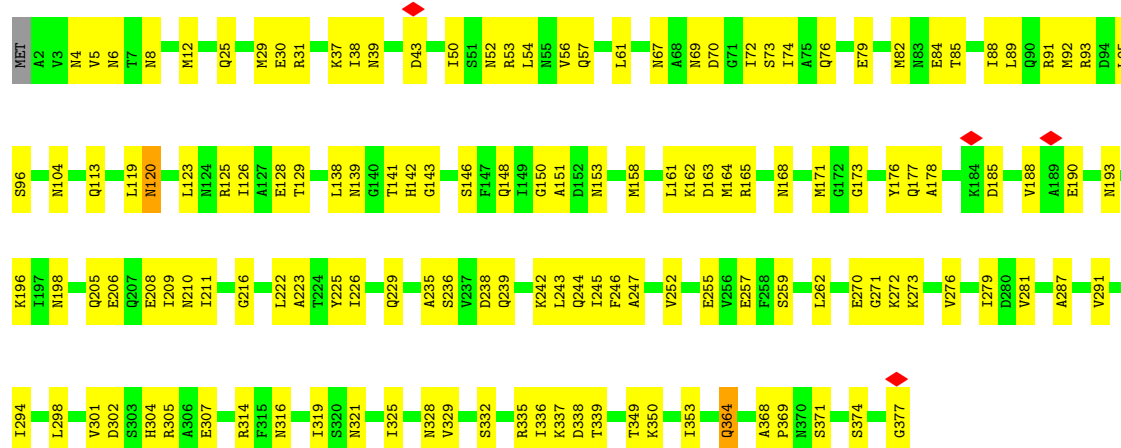
• Molecule 1: Flagellin

Chain S: 62% 38%

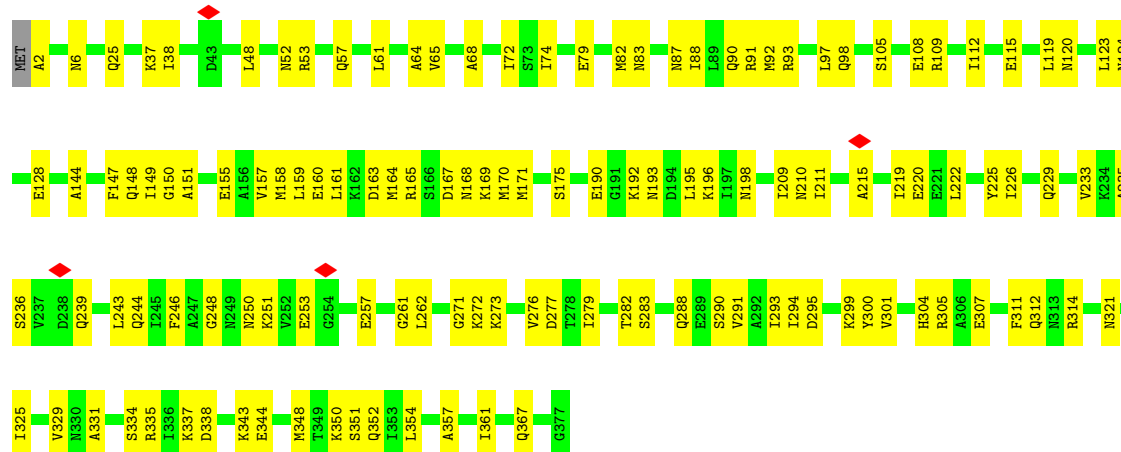




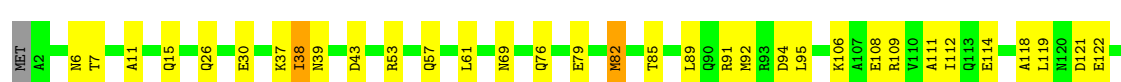
• Molecule 1: Flagellin

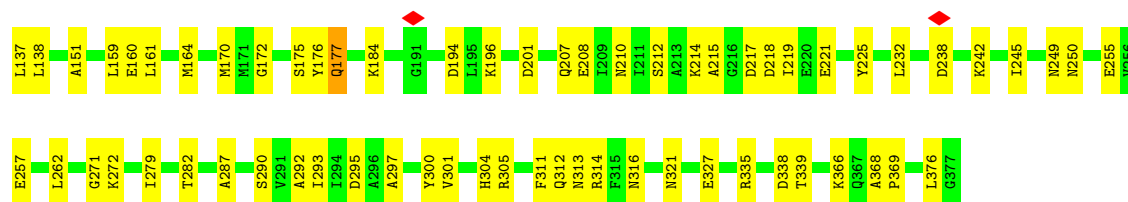


• Molecule 1: Flagellin

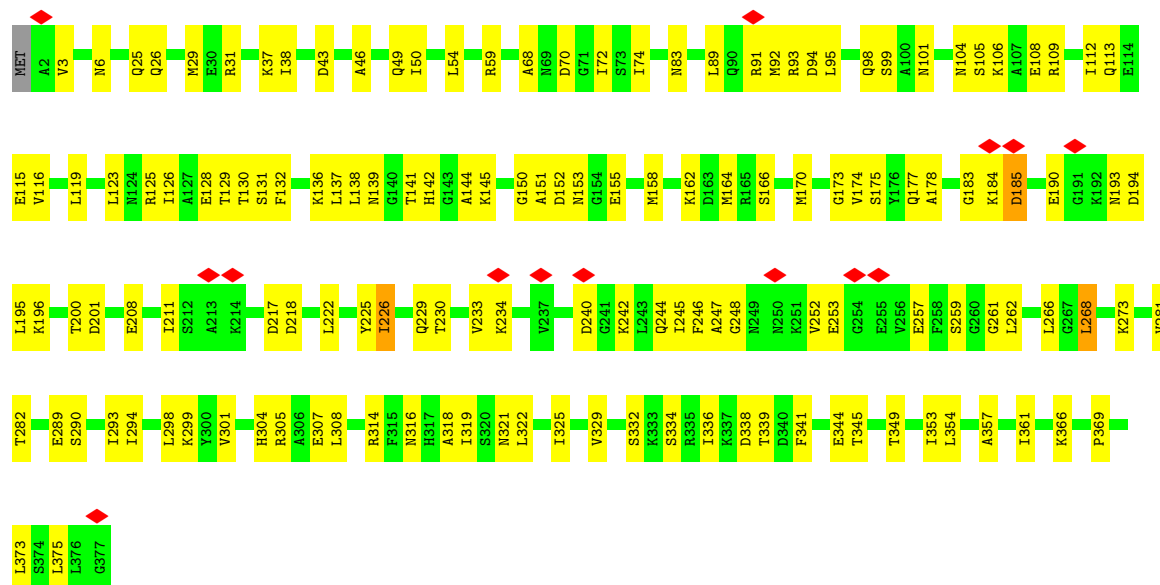


• Molecule 1: Flagellin

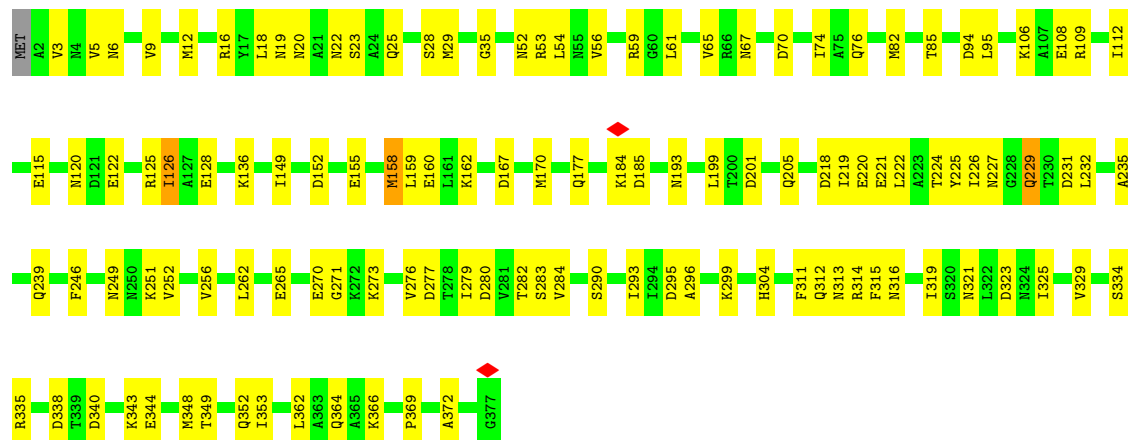




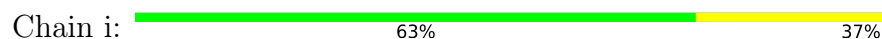
• Molecule 1: Flagellin

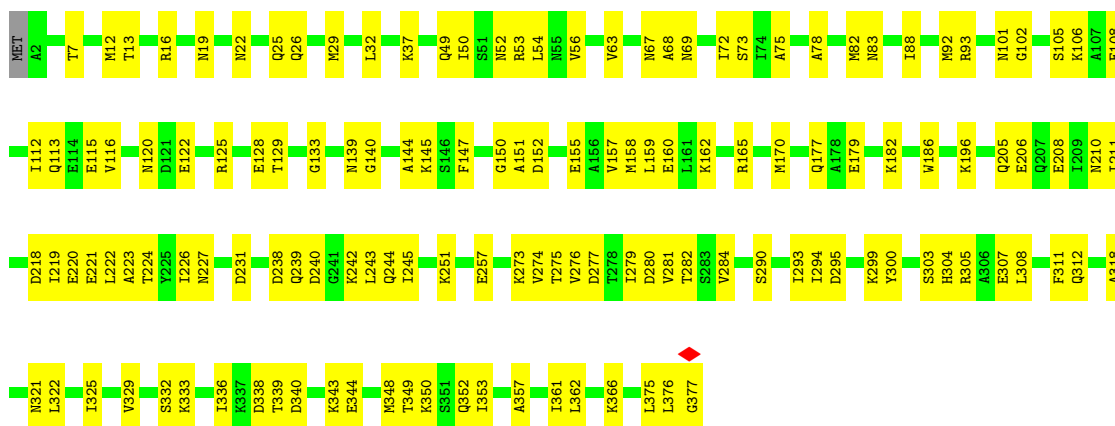


• Molecule 1: Flagellin

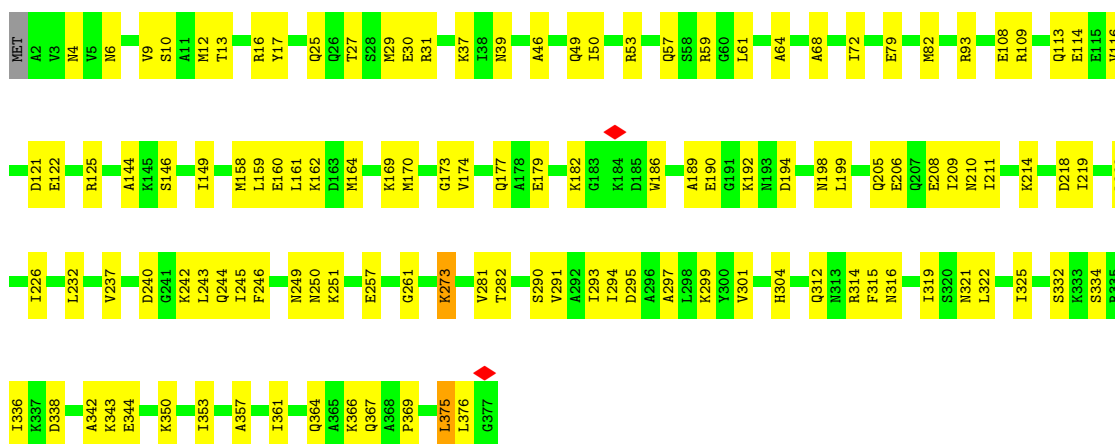


• Molecule 1: Flagellin

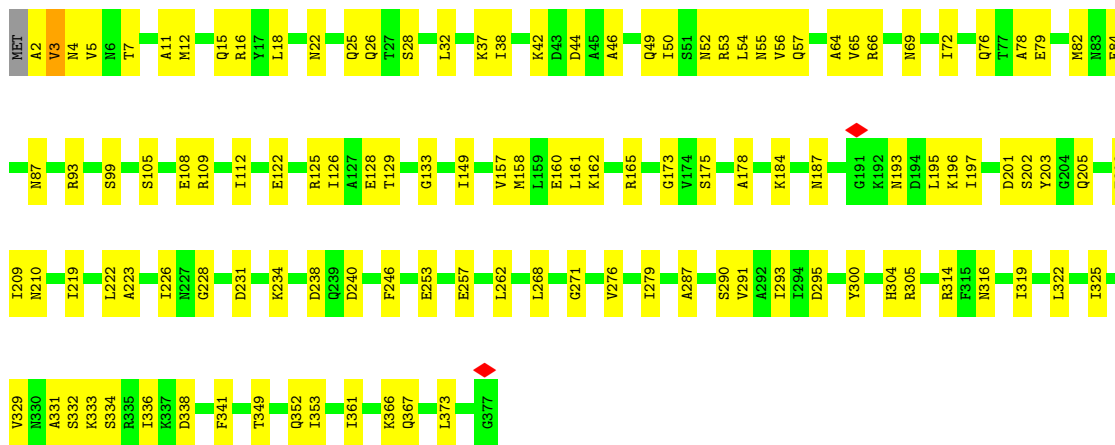




• Molecule 1: Flagellin

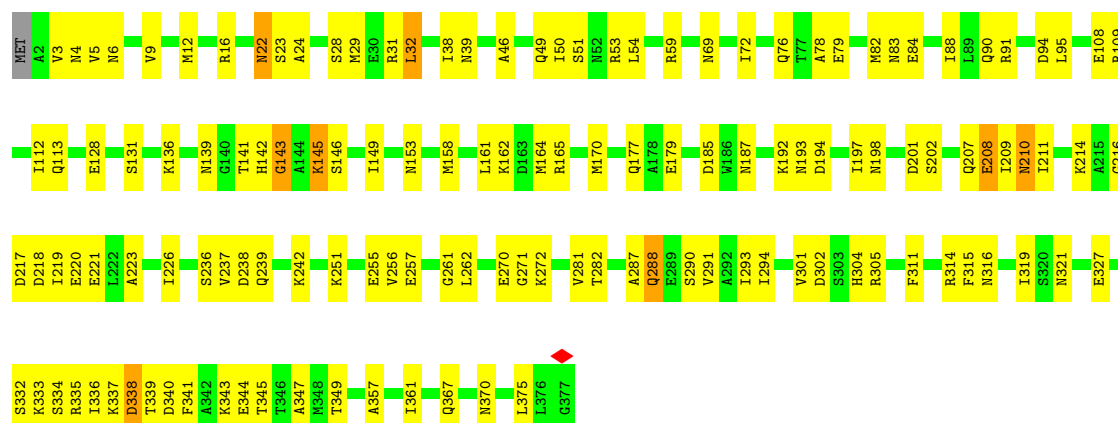


• Molecule 1: Flagellin



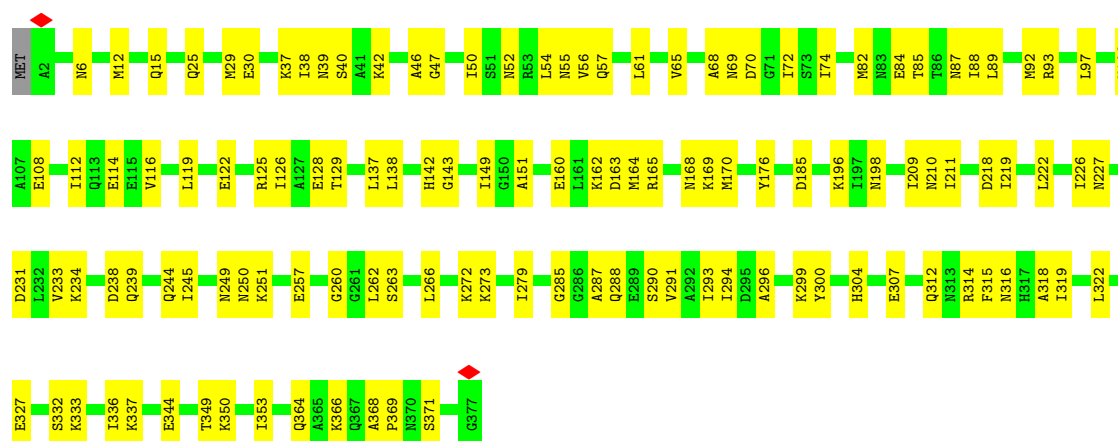
• Molecule 1: Flagellin

Chain l:  64% 34%



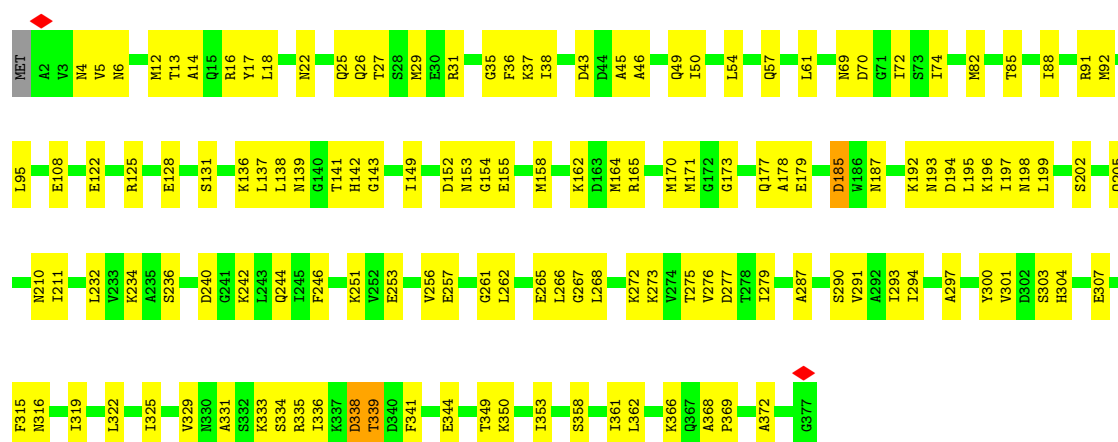
• Molecule 1: Flagellin

Chain m:  67% 33%



• Molecule 1: Flagellin

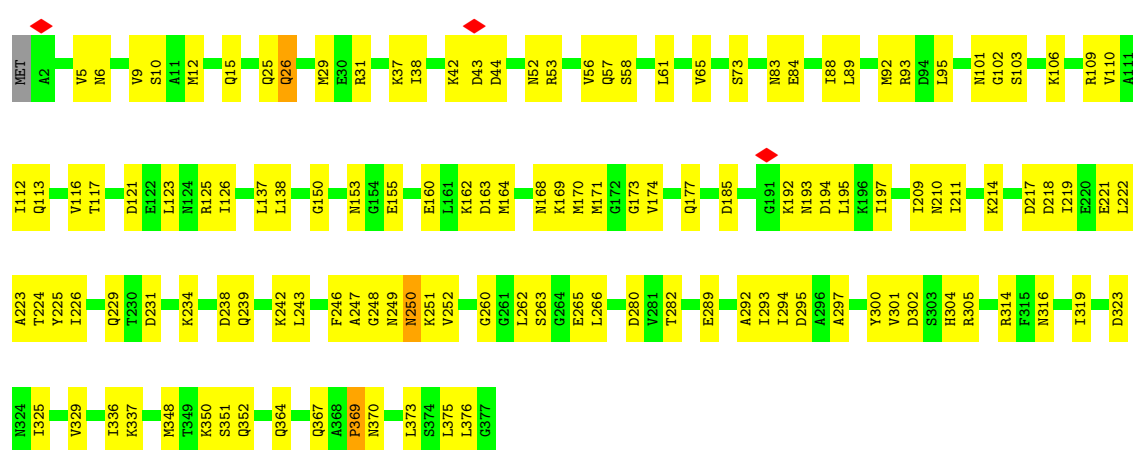
Chain n:  63% 36%



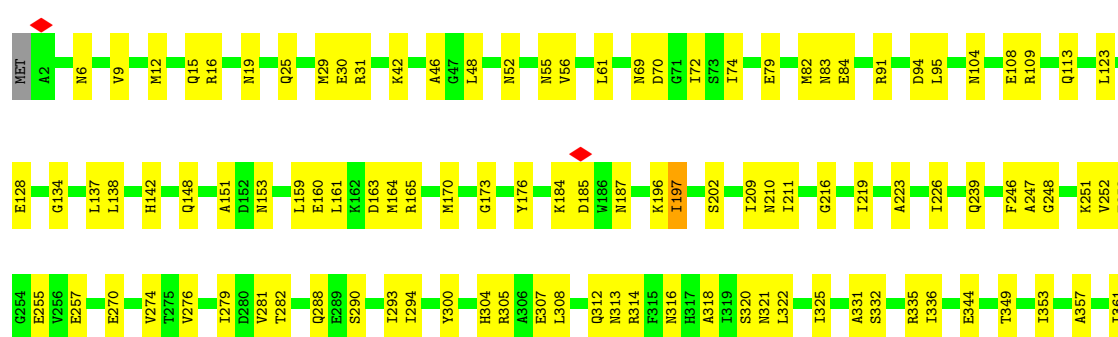
• Molecule 1: Flagellin

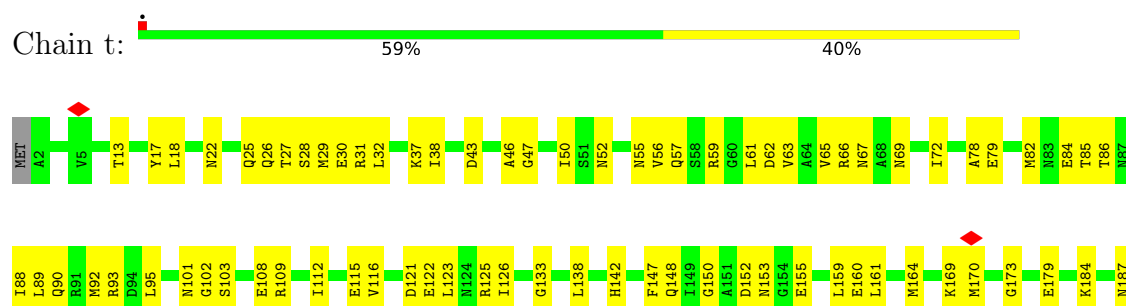
Chain o:  68% 31%

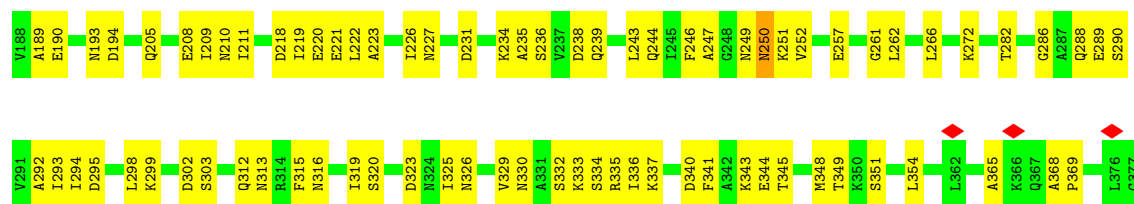
• Molecule 1: Flagellin

Chain p:  65% 34%

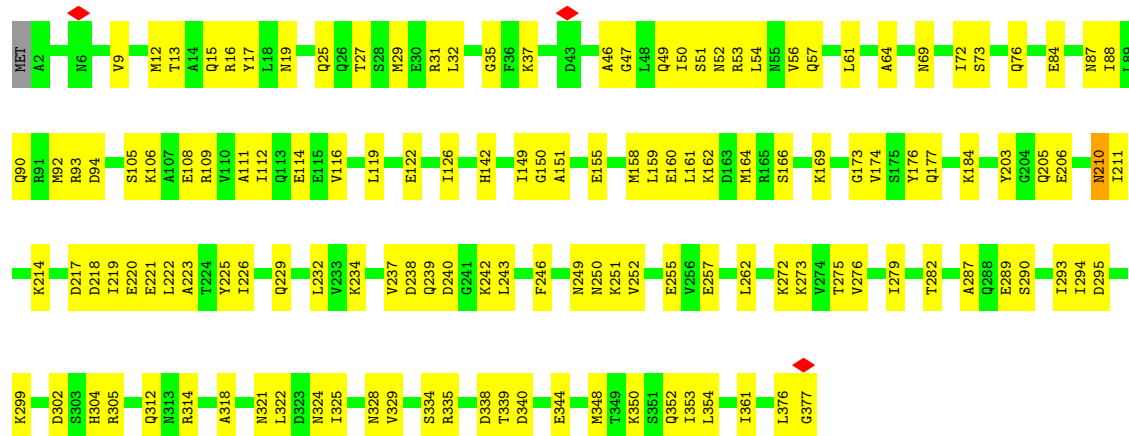
• Molecule 1: Flagellin

Chain q:  71% 28%

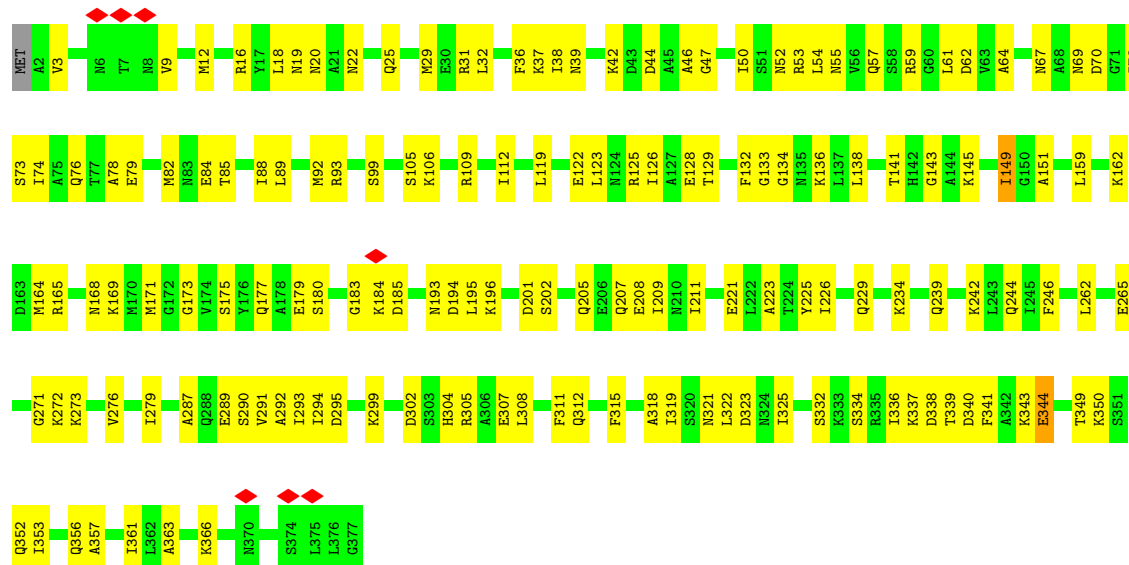




• Molecule 1: Flagellin

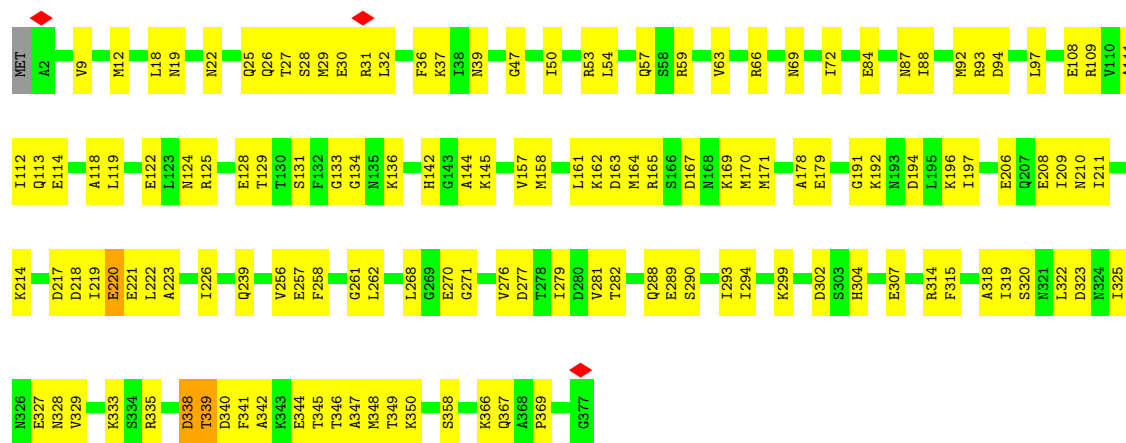


• Molecule 1: Flagellin

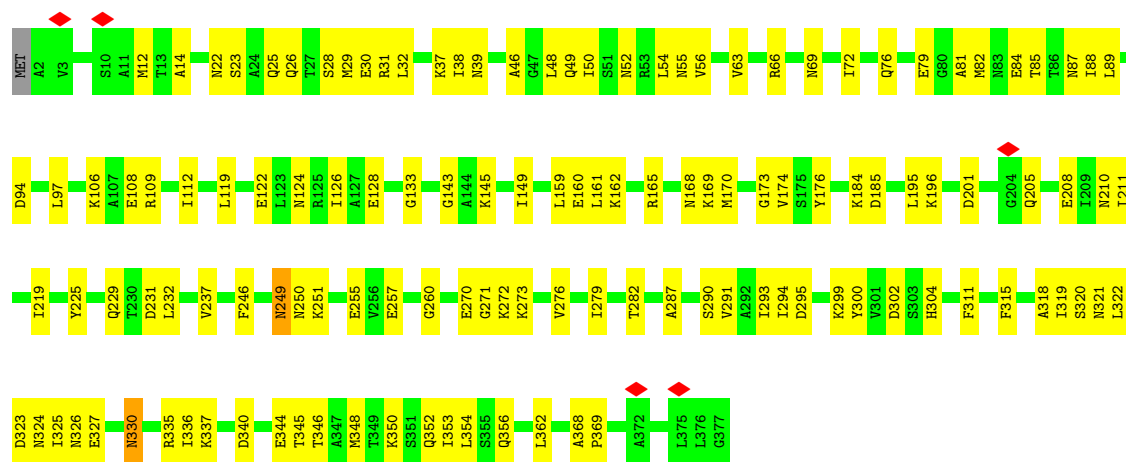


• Molecule 1: Flagellin

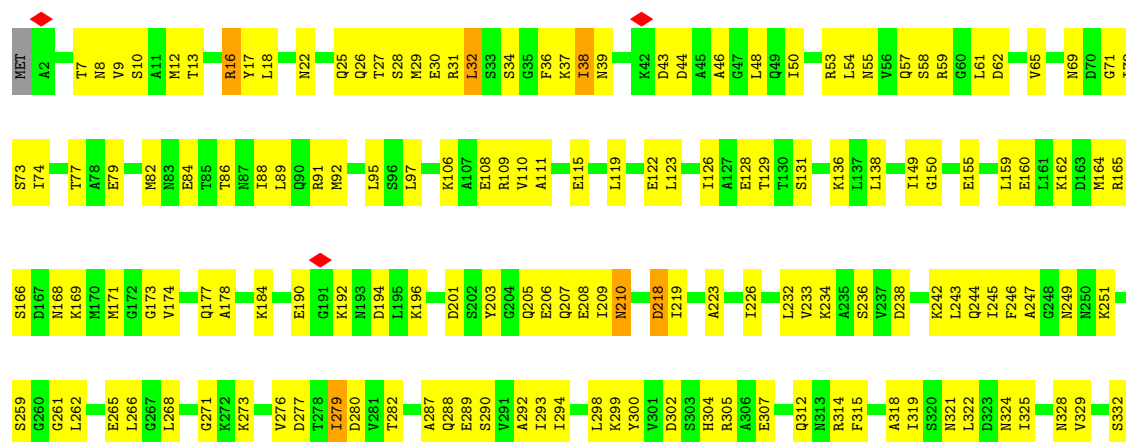




• Molecule 1: Flagellin



• Molecule 1: Flagellin





4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 72779 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 40 | Depositor |
| Minimum defocus (nm) | 900 | Depositor |
| Maximum defocus (nm) | 2700 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.564 | Depositor |
| Minimum map value | -0.392 | Depositor |
| Average map value | 0.006 | Depositor |
| Map value standard deviation | 0.038 | Depositor |
| Recommended contour level | 0.08 | Depositor |
| Map size (\AA) | 550.0, 550.0, 550.0 | wwPDB |
| Map dimensions | 500, 500, 500 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.1, 1.1, 1.1 | 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 | 1 | 0.27 | 0/2816 | 0.64 | 1/3790 (0.0%) |
| 1 | 2 | 0.27 | 0/2816 | 0.58 | 0/3790 |
| 1 | 3 | 0.28 | 0/2816 | 0.64 | 2/3790 (0.1%) |
| 1 | A | 0.30 | 0/2816 | 0.61 | 1/3790 (0.0%) |
| 1 | B | 0.29 | 0/2816 | 0.58 | 0/3790 |
| 1 | C | 0.28 | 0/2816 | 0.60 | 0/3790 |
| 1 | D | 0.27 | 0/2816 | 0.62 | 0/3790 |
| 1 | E | 0.29 | 0/2816 | 0.66 | 0/3790 |
| 1 | F | 0.27 | 0/2816 | 0.59 | 1/3790 (0.0%) |
| 1 | G | 0.28 | 0/2816 | 0.57 | 0/3790 |
| 1 | H | 0.28 | 0/2816 | 0.63 | 0/3790 |
| 1 | I | 0.29 | 0/2816 | 0.62 | 1/3790 (0.0%) |
| 1 | J | 0.26 | 0/2816 | 0.56 | 0/3790 |
| 1 | K | 0.26 | 0/2816 | 0.60 | 1/3790 (0.0%) |
| 1 | L | 0.27 | 0/2816 | 0.61 | 0/3790 |
| 1 | M | 0.30 | 0/2816 | 0.63 | 1/3790 (0.0%) |
| 1 | N | 0.28 | 0/2816 | 0.61 | 0/3790 |
| 1 | O | 0.27 | 0/2816 | 0.63 | 0/3790 |
| 1 | P | 0.28 | 0/2816 | 0.61 | 0/3790 |
| 1 | Q | 0.27 | 0/2816 | 0.59 | 0/3790 |
| 1 | R | 0.32 | 0/2816 | 0.66 | 4/3790 (0.1%) |
| 1 | S | 0.27 | 0/2816 | 0.60 | 0/3790 |
| 1 | T | 0.27 | 0/2816 | 0.60 | 1/3790 (0.0%) |
| 1 | U | 0.26 | 0/2816 | 0.60 | 0/3790 |
| 1 | V | 0.27 | 0/2816 | 0.59 | 0/3790 |
| 1 | c | 0.27 | 0/2816 | 0.66 | 1/3790 (0.0%) |
| 1 | h | 0.25 | 0/2816 | 0.54 | 0/3790 |
| 1 | i | 0.27 | 0/2816 | 0.58 | 0/3790 |
| 1 | j | 0.29 | 0/2816 | 0.59 | 0/3790 |
| 1 | k | 0.27 | 0/2816 | 0.61 | 0/3790 |
| 1 | l | 0.30 | 0/2816 | 0.63 | 1/3790 (0.0%) |
| 1 | m | 0.28 | 0/2816 | 0.60 | 1/3790 (0.0%) |
| 1 | n | 0.28 | 0/2816 | 0.63 | 1/3790 (0.0%) |
| 1 | o | 0.28 | 0/2816 | 0.62 | 0/3790 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | p | 0.29 | 0/2816 | 0.64 | 1/3790 (0.0%) |
| 1 | q | 0.25 | 0/2816 | 0.58 | 1/3790 (0.0%) |
| 1 | r | 0.26 | 0/2816 | 0.61 | 0/3790 |
| 1 | s | 0.25 | 0/2816 | 0.56 | 0/3790 |
| 1 | t | 0.27 | 0/2816 | 0.64 | 0/3790 |
| 1 | u | 0.28 | 0/2816 | 0.59 | 0/3790 |
| 1 | v | 0.26 | 0/2816 | 0.60 | 1/3790 (0.0%) |
| 1 | w | 0.30 | 0/2816 | 0.62 | 1/3790 (0.0%) |
| 1 | x | 0.27 | 0/2816 | 0.61 | 0/3790 |
| 1 | z | 0.32 | 0/2816 | 0.70 | 0/3790 |
| All | All | 0.28 | 0/123904 | 0.61 | 21/166760 (0.0%) |

There are no bond length outliers.

All (21) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1 | R | 185 | ASP | N-CA-C | -10.36 | 101.40 | 114.56 |
| 1 | p | 369 | PRO | CA-N-CD | -8.52 | 100.07 | 112.00 |
| 1 | q | 369 | PRO | CA-N-CD | -7.14 | 102.00 | 112.00 |
| 1 | I | 369 | PRO | CA-N-CD | -7.10 | 102.06 | 112.00 |
| 1 | n | 185 | ASP | N-CA-C | -7.02 | 105.33 | 114.04 |
| 1 | A | 337 | LYS | N-CA-C | 7.00 | 122.11 | 113.50 |
| 1 | 1 | 185 | ASP | N-CA-C | -6.86 | 106.80 | 114.62 |
| 1 | 3 | 185 | ASP | N-CA-C | -6.76 | 105.97 | 114.56 |
| 1 | R | 193 | ASN | N-CA-C | -6.25 | 104.86 | 113.18 |
| 1 | l | 143 | GLY | N-CA-C | 6.16 | 119.50 | 110.38 |
| 1 | c | 185 | ASP | N-CA-C | -5.99 | 107.79 | 114.62 |
| 1 | w | 338 | ASP | N-CA-C | 5.92 | 123.40 | 110.80 |
| 1 | K | 251 | LYS | N-CA-C | -5.86 | 107.94 | 114.62 |
| 1 | M | 281 | VAL | N-CA-C | -5.71 | 107.72 | 113.20 |
| 1 | 3 | 170 | MET | CB-CG-SD | 5.41 | 128.92 | 112.70 |
| 1 | v | 149 | ILE | N-CA-C | -5.29 | 108.13 | 113.47 |
| 1 | R | 192 | LYS | N-CA-C | -5.23 | 99.42 | 108.52 |
| 1 | T | 369 | PRO | CA-N-CD | -5.20 | 104.72 | 112.00 |
| 1 | F | 307 | GLU | CA-CB-CG | 5.15 | 124.39 | 114.10 |
| 1 | R | 251 | LYS | N-CA-C | -5.06 | 106.45 | 113.18 |
| 1 | m | 114 | GLU | CA-CB-CG | 5.05 | 124.21 | 114.10 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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 | 1 | 2798 | 0 | 2745 | 145 | 0 |
| 1 | 2 | 2798 | 0 | 2745 | 126 | 0 |
| 1 | 3 | 2798 | 0 | 2745 | 111 | 0 |
| 1 | A | 2798 | 0 | 2745 | 103 | 0 |
| 1 | B | 2798 | 0 | 2745 | 104 | 0 |
| 1 | C | 2798 | 0 | 2745 | 102 | 0 |
| 1 | D | 2798 | 0 | 2745 | 103 | 0 |
| 1 | E | 2798 | 0 | 2745 | 124 | 0 |
| 1 | F | 2798 | 0 | 2745 | 99 | 0 |
| 1 | G | 2798 | 0 | 2745 | 109 | 0 |
| 1 | H | 2798 | 0 | 2745 | 115 | 0 |
| 1 | I | 2798 | 0 | 2745 | 111 | 0 |
| 1 | J | 2798 | 0 | 2745 | 108 | 0 |
| 1 | K | 2798 | 0 | 2745 | 84 | 0 |
| 1 | L | 2798 | 0 | 2745 | 120 | 0 |
| 1 | M | 2798 | 0 | 2745 | 116 | 0 |
| 1 | N | 2798 | 0 | 2745 | 122 | 0 |
| 1 | O | 2798 | 0 | 2745 | 127 | 0 |
| 1 | P | 2798 | 0 | 2745 | 112 | 0 |
| 1 | Q | 2798 | 0 | 2745 | 110 | 0 |
| 1 | R | 2798 | 0 | 2745 | 125 | 0 |
| 1 | S | 2798 | 0 | 2745 | 117 | 0 |
| 1 | T | 2798 | 0 | 2745 | 112 | 0 |
| 1 | U | 2798 | 0 | 2745 | 99 | 0 |
| 1 | V | 2798 | 0 | 2745 | 79 | 0 |
| 1 | c | 2798 | 0 | 2745 | 119 | 0 |
| 1 | h | 2798 | 0 | 2745 | 95 | 0 |
| 1 | i | 2798 | 0 | 2745 | 116 | 0 |
| 1 | j | 2798 | 0 | 2745 | 98 | 0 |
| 1 | k | 2798 | 0 | 2745 | 100 | 0 |
| 1 | l | 2798 | 0 | 2745 | 107 | 0 |
| 1 | m | 2798 | 0 | 2745 | 105 | 0 |
| 1 | n | 2798 | 0 | 2745 | 118 | 0 |
| 1 | o | 2798 | 0 | 2745 | 98 | 0 |
| 1 | p | 2798 | 0 | 2745 | 115 | 0 |
| 1 | q | 2798 | 0 | 2745 | 85 | 0 |
| 1 | r | 2798 | 0 | 2745 | 107 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 1 | s | 2798 | 0 | 2745 | 106 | 0 |
| 1 | t | 2798 | 0 | 2745 | 134 | 0 |
| 1 | u | 2798 | 0 | 2745 | 111 | 0 |
| 1 | v | 2798 | 0 | 2745 | 124 | 0 |
| 1 | w | 2798 | 0 | 2745 | 131 | 0 |
| 1 | x | 2798 | 0 | 2745 | 117 | 0 |
| 1 | z | 2798 | 0 | 2745 | 163 | 0 |
| All | All | 123112 | 0 | 120780 | 4572 | 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 19.

All (4572) 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:s:10:SER:HB3 | 1:t:29:MET:HE1 | 1.40 | 1.03 |
| 1:P:233:VAL:HB | 1:P:245:ILE:HD11 | 1.37 | 1.01 |
| 1:R:90:GLN:HB3 | 1:c:59:ARG:HH22 | 1.26 | 0.97 |
| 1:k:290:SER:HA | 1:k:293:ILE:HD12 | 1.49 | 0.95 |
| 1:3:302:ASP:HA | 1:3:305:ARG:HG3 | 1.48 | 0.94 |
| 1:P:113:GLN:HE22 | 1:P:280:ASP:HA | 1.31 | 0.93 |
| 1:i:273:LYS:HZ3 | 1:i:275:THR:HG23 | 1.31 | 0.93 |
| 1:J:106:LYS:HA | 1:J:109:ARG:HD3 | 1.51 | 0.92 |
| 1:x:22:ASN:HA | 1:x:25:GLN:HG3 | 1.50 | 0.92 |
| 1:t:62:ASP:O | 1:t:66:ARG:NH1 | 2.04 | 0.91 |
| 1:i:67:ASN:HD22 | 1:t:101:ASN:HB2 | 1.35 | 0.90 |
| 1:T:168:ASN:HB3 | 1:T:171:MET:HG2 | 1.54 | 0.90 |
| 1:I:290:SER:HA | 1:I:293:ILE:HD12 | 1.54 | 0.89 |
| 1:l:69:ASN:HA | 1:l:72:ILE:HD12 | 1.54 | 0.89 |
| 1:n:195:LEU:HB2 | 1:n:262:LEU:HD12 | 1.54 | 0.89 |
| 1:p:6:ASN:HA | 1:z:350:LYS:HZ1 | 1.36 | 0.89 |
| 1:O:12:MET:HA | 1:O:15:GLN:HG3 | 1.56 | 0.88 |
| 1:R:188:VAL:HG21 | 1:R:215:ALA:HA | 1.53 | 0.88 |
| 1:1:223:ALA:HA | 1:1:226:ILE:HD12 | 1.55 | 0.88 |
| 1:3:238:ASP:HB3 | 1:3:244:GLN:HE22 | 1.37 | 0.88 |
| 1:C:279:ILE:HG21 | 1:C:290:SER:HB3 | 1.56 | 0.87 |
| 1:w:314:ARG:NH1 | 1:x:122:GLU:OE1 | 2.07 | 0.87 |
| 1:C:302:ASP:OD2 | 1:N:52:ASN:ND2 | 2.08 | 0.87 |
| 1:u:25:GLN:NE2 | 1:u:29:MET:SD | 2.48 | 0.86 |
| 1:x:88:ILE:HG23 | 1:x:119:LEU:HD12 | 1.57 | 0.86 |
| 1:M:128:GLU:OE2 | 1:M:165:ARG:NH1 | 2.08 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:53:ARG:HH22 | 1:q:134:GLY:H | 1.24 | 0.86 |
| 1:L:226:ILE:HA | 1:L:229:GLN:HE21 | 1.40 | 0.85 |
| 1:w:157:VAL:HG11 | 1:w:314:ARG:HH21 | 1.42 | 0.85 |
| 1:v:61:LEU:HD23 | 1:v:151:ALA:HB2 | 1.58 | 0.85 |
| 1:k:3:VAL:HG22 | 1:v:340:ASP:HA | 1.57 | 0.85 |
| 1:U:193:ASN:HA | 1:U:262:LEU:HD21 | 1.56 | 0.85 |
| 1:C:101:ASN:HB2 | 1:N:67:ASN:HD22 | 1.42 | 0.84 |
| 1:v:290:SER:HA | 1:v:293:ILE:HD12 | 1.59 | 0.84 |
| 1:k:157:VAL:HG21 | 1:k:314:ARG:HH22 | 1.42 | 0.84 |
| 1:T:302:ASP:HA | 1:T:305:ARG:HG3 | 1.57 | 0.83 |
| 1:c:144:ALA:HB1 | 1:c:158:MET:HE2 | 1.59 | 0.83 |
| 1:s:350:LYS:HA | 1:s:353:ILE:HD12 | 1.59 | 0.83 |
| 1:C:49:GLN:OE1 | 1:C:53:ARG:NH1 | 2.12 | 0.83 |
| 1:m:65:VAL:HG13 | 1:m:319:ILE:HD11 | 1.61 | 0.83 |
| 1:w:223:ALA:HA | 1:w:226:ILE:HD12 | 1.60 | 0.83 |
| 1:V:91:ARG:NH1 | 1:V:94:ASP:OD1 | 2.12 | 0.82 |
| 1:B:54:LEU:HD12 | 1:B:329:VAL:HG23 | 1.58 | 0.82 |
| 1:k:49:GLN:NE2 | 1:v:302:ASP:OD1 | 2.12 | 0.82 |
| 1:O:37:LYS:NZ | 1:O:336:ILE:O | 2.12 | 0.82 |
| 1:i:290:SER:HA | 1:i:293:ILE:HD12 | 1.60 | 0.82 |
| 1:i:120:ASN:HD21 | 1:i:277:ASP:HA | 1.41 | 0.82 |
| 1:C:363:ALA:O | 1:C:367:GLN:NE2 | 2.12 | 0.82 |
| 1:k:158:MET:HE1 | 1:k:160:GLU:HB2 | 1.60 | 0.82 |
| 1:o:193:ASN:HA | 1:o:262:LEU:HD21 | 1.62 | 0.81 |
| 1:K:88:ILE:HG23 | 1:K:119:LEU:HD22 | 1.62 | 0.81 |
| 1:N:79:GLU:HG2 | 1:N:308:LEU:HD12 | 1.62 | 0.81 |
| 1:z:169:LYS:H | 1:z:169:LYS:HD2 | 1.46 | 0.81 |
| 1:F:363:ALA:O | 1:F:367:GLN:NE2 | 2.14 | 0.81 |
| 1:2:52:ASN:O | 1:2:55:ASN:ND2 | 2.14 | 0.81 |
| 1:I:88:ILE:HG23 | 1:I:119:LEU:HD12 | 1.62 | 0.81 |
| 1:u:31:ARG:NH2 | 1:u:37:LYS:O | 2.14 | 0.81 |
| 1:J:153:ASN:ND2 | 1:q:288:GLN:O | 2.12 | 0.80 |
| 1:T:173:GLY:HA3 | 1:T:246:PHE:HE1 | 1.46 | 0.80 |
| 1:R:192:LYS:HA | 1:R:261:GLY:HA3 | 1.62 | 0.80 |
| 1:k:193:ASN:HA | 1:k:262:LEU:HD21 | 1.62 | 0.80 |
| 1:c:152:ASP:OD1 | 1:c:153:ASN:N | 2.15 | 0.80 |
| 1:w:196:LYS:NZ | 1:w:208:GLU:OE2 | 2.14 | 0.80 |
| 1:x:170:MET:HE1 | 1:x:250:ASN:HB3 | 1.61 | 0.80 |
| 1:3:205:GLN:NE2 | 1:3:207:GLN:OE1 | 2.14 | 0.80 |
| 1:I:65:VAL:HG13 | 1:I:319:ILE:HD11 | 1.62 | 0.80 |
| 1:c:195:LEU:HD12 | 1:c:262:LEU:HB2 | 1.63 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:v:193:ASN:HA | 1:v:262:LEU:HD21 | 1.63 | 0.80 |
| 1:B:247:ALA:HB1 | 1:B:252:VAL:HG11 | 1.61 | 0.80 |
| 1:l:131:SER:HB3 | 1:l:136:LYS:HD2 | 1.62 | 0.80 |
| 1:w:53:ARG:NH2 | 1:x:133:GLY:O | 2.15 | 0.80 |
| 1:1:26:GLN:HA | 1:1:29:MET:HG2 | 1.63 | 0.80 |
| 1:2:82:MET:HE1 | 1:2:304:HIS:HB2 | 1.64 | 0.79 |
| 1:I:128:GLU:OE2 | 1:I:165:ARG:NH1 | 2.15 | 0.79 |
| 1:k:93:ARG:NH1 | 1:k:295:ASP:OD1 | 2.15 | 0.79 |
| 1:G:152:ASP:OD1 | 1:G:153:ASN:N | 2.15 | 0.79 |
| 1:J:133:GLY:O | 1:T:53:ARG:NH2 | 2.13 | 0.79 |
| 1:h:193:ASN:HA | 1:h:262:LEU:HD21 | 1.64 | 0.79 |
| 1:N:284:VAL:O | 1:N:288:GLN:NE2 | 2.13 | 0.79 |
| 1:Q:162:LYS:HD3 | 1:Q:304:HIS:HB3 | 1.64 | 0.79 |
| 1:v:38:ILE:HD12 | 1:v:337:LYS:HA | 1.65 | 0.79 |
| 1:M:124:ASN:OD1 | 1:M:166:SER:OG | 2.01 | 0.78 |
| 1:h:225:TYR:O | 1:h:229:GLN:NE2 | 2.14 | 0.78 |
| 1:k:3:VAL:HG21 | 1:v:341:PHE:CD1 | 2.19 | 0.78 |
| 1:T:247:ALA:HB1 | 1:T:252:VAL:HG11 | 1.63 | 0.78 |
| 1:l:128:GLU:OE1 | 1:l:165:ARG:NH1 | 2.15 | 0.78 |
| 1:w:18:LEU:HD13 | 1:w:358:SER:HB2 | 1.66 | 0.78 |
| 1:T:162:LYS:HD2 | 1:T:163:ASP:H | 1.48 | 0.78 |
| 1:p:113:GLN:HE22 | 1:p:280:ASP:HA | 1.46 | 0.78 |
| 1:P:45:ALA:O | 1:P:49:GLN:NE2 | 2.12 | 0.78 |
| 1:R:136:LYS:HE2 | 1:R:136:LYS:HA | 1.65 | 0.78 |
| 1:S:113:GLN:HE22 | 1:S:280:ASP:HA | 1.48 | 0.78 |
| 1:k:202:SER:HA | 1:k:253:GLU:HG3 | 1.64 | 0.78 |
| 1:v:37:LYS:NZ | 1:v:336:ILE:O | 2.14 | 0.78 |
| 1:p:9:VAL:HA | 1:p:12:MET:HE1 | 1.66 | 0.78 |
| 1:r:209:ILE:HD11 | 1:r:232:LEU:HD12 | 1.66 | 0.78 |
| 1:t:152:ASP:OD2 | 1:t:153:ASN:N | 2.16 | 0.78 |
| 1:n:152:ASP:OD1 | 1:n:153:ASN:N | 2.17 | 0.78 |
| 1:w:128:GLU:OE1 | 1:w:165:ARG:NH1 | 2.16 | 0.77 |
| 1:2:348:MET:SD | 1:2:352:GLN:NE2 | 2.57 | 0.77 |
| 1:3:51:SER:OG | 1:3:333:LYS:NZ | 2.18 | 0.77 |
| 1:C:193:ASN:HA | 1:C:262:LEU:HD21 | 1.64 | 0.77 |
| 1:n:128:GLU:OE1 | 1:n:165:ARG:NH1 | 2.16 | 0.77 |
| 1:1:320:SER:O | 1:1:324:ASN:ND2 | 2.18 | 0.77 |
| 1:E:192:LYS:NZ | 1:E:265:GLU:OE1 | 2.18 | 0.77 |
| 1:O:232:LEU:HD23 | 1:O:233:VAL:HG13 | 1.65 | 0.77 |
| 1:N:82:MET:HB2 | 1:N:305:ARG:HH11 | 1.49 | 0.77 |
| 1:D:167:ASP:OD2 | 1:j:214:LYS:NZ | 2.17 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:266:LEU:HD13 | 1:L:268:LEU:HD21 | 1.67 | 0.77 |
| 1:j:37:LYS:NZ | 1:j:336:ILE:O | 2.18 | 0.77 |
| 1:r:49:GLN:HB3 | 1:r:53:ARG:HH12 | 1.48 | 0.77 |
| 1:G:38:ILE:HG23 | 1:G:43:ASP:HB2 | 1.67 | 0.77 |
| 1:3:83:ASN:HA | 1:3:305:ARG:HH12 | 1.49 | 0.77 |
| 1:F:238:ASP:HB3 | 1:F:244:GLN:HE21 | 1.49 | 0.77 |
| 1:z:18:LEU:O | 1:z:22:ASN:ND2 | 2.18 | 0.77 |
| 1:x:69:ASN:HA | 1:x:72:ILE:HD12 | 1.65 | 0.77 |
| 1:D:108:GLU:OE2 | 1:D:108:GLU:N | 2.17 | 0.76 |
| 1:O:338:ASP:OD2 | 1:O:339:THR:N | 2.18 | 0.76 |
| 1:m:238:ASP:HB3 | 1:m:244:GLN:HE21 | 1.51 | 0.76 |
| 1:m:37:LYS:NZ | 1:m:336:ILE:O | 2.19 | 0.76 |
| 1:t:250:ASN:O | 1:t:250:ASN:ND2 | 2.18 | 0.76 |
| 1:c:246:PHE:HE1 | 1:c:293:ILE:HD13 | 1.50 | 0.76 |
| 1:U:159:LEU:HD12 | 1:U:160:GLU:H | 1.50 | 0.76 |
| 1:Q:142:HIS:HD2 | 1:Q:161:LEU:HB2 | 1.50 | 0.76 |
| 1:r:363:ALA:O | 1:r:367:GLN:NE2 | 2.19 | 0.76 |
| 1:i:128:GLU:OE2 | 1:i:165:ARG:NH1 | 2.19 | 0.76 |
| 1:x:14:ALA:HB3 | 1:x:362:LEU:HD13 | 1.66 | 0.76 |
| 1:M:276:VAL:HA | 1:M:279:ILE:HD11 | 1.66 | 0.76 |
| 1:c:245:ILE:HD12 | 1:c:268:LEU:HD21 | 1.67 | 0.76 |
| 1:N:301:VAL:HA | 1:N:304:HIS:CD2 | 2.21 | 0.75 |
| 1:T:93:ARG:HG2 | 1:T:294:ILE:HG21 | 1.66 | 0.75 |
| 1:I:184:LYS:NZ | 1:I:218:ASP:OD2 | 2.15 | 0.75 |
| 1:u:53:ARG:NH2 | 1:v:133:GLY:O | 2.19 | 0.75 |
| 1:1:51:SER:HA | 1:1:54:LEU:HG | 1.67 | 0.75 |
| 1:G:58:SER:HA | 1:G:61:LEU:HD12 | 1.68 | 0.75 |
| 1:H:195:LEU:HD12 | 1:H:262:LEU:HD12 | 1.69 | 0.75 |
| 1:1:321:ASN:HA | 1:1:324:ASN:HD21 | 1.52 | 0.75 |
| 1:2:290:SER:HA | 1:2:293:ILE:HD12 | 1.69 | 0.75 |
| 1:H:257:GLU:OE1 | 1:H:257:GLU:N | 2.20 | 0.75 |
| 1:M:199:LEU:HD21 | 1:M:232:LEU:HD13 | 1.66 | 0.75 |
| 1:P:25:GLN:NE2 | 1:P:347:ALA:O | 2.20 | 0.75 |
| 1:v:350:LYS:HA | 1:v:353:ILE:HD12 | 1.69 | 0.75 |
| 1:s:198:ASN:HB2 | 1:s:257:GLU:HB3 | 1.67 | 0.75 |
| 1:m:314:ARG:NE | 1:n:122:GLU:OE2 | 2.20 | 0.75 |
| 1:D:88:ILE:HG23 | 1:D:119:LEU:HD12 | 1.69 | 0.74 |
| 1:E:290:SER:HA | 1:E:293:ILE:HD12 | 1.67 | 0.74 |
| 1:s:314:ARG:HE | 1:t:122:GLU:HB2 | 1.51 | 0.74 |
| 1:F:162:LYS:HD3 | 1:F:162:LYS:N | 2.01 | 0.74 |
| 1:L:193:ASN:HA | 1:L:262:LEU:HD21 | 1.69 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:150:GLY:HA3 | 1:c:155:GLU:HB2 | 1.69 | 0.74 |
| 1:p:218:ASP:OD1 | 1:p:219:ILE:N | 2.19 | 0.74 |
| 1:E:111:ALA:HA | 1:E:114:GLU:OE2 | 1.87 | 0.74 |
| 1:E:162:LYS:HG2 | 1:E:304:HIS:CE1 | 2.21 | 0.74 |
| 1:J:192:LYS:HE2 | 1:J:192:LYS:HA | 1.69 | 0.74 |
| 1:z:219:ILE:HD11 | 1:z:243:LEU:HD12 | 1.70 | 0.74 |
| 1:C:164:MET:HE1 | 1:C:304:HIS:HD2 | 1.52 | 0.74 |
| 1:h:54:LEU:HD12 | 1:h:329:VAL:HG13 | 1.69 | 0.74 |
| 1:n:339:THR:OG1 | 1:n:344:GLU:OE1 | 2.04 | 0.74 |
| 1:1:205:GLN:NE2 | 1:1:206:GLU:O | 2.20 | 0.74 |
| 1:E:38:ILE:HG23 | 1:E:43:ASP:HB2 | 1.70 | 0.74 |
| 1:R:120:ASN:HD21 | 1:R:277:ASP:HA | 1.51 | 0.74 |
| 1:s:162:LYS:HB2 | 1:s:164:MET:HE1 | 1.70 | 0.74 |
| 1:C:205:GLN:HE22 | 1:C:207:GLN:HG2 | 1.51 | 0.74 |
| 1:L:169:LYS:HE2 | 1:L:169:LYS:HA | 1.69 | 0.74 |
| 1:c:208:GLU:N | 1:c:208:GLU:OE2 | 2.21 | 0.74 |
| 1:t:123:LEU:HA | 1:t:126:ILE:HD12 | 1.68 | 0.74 |
| 1:G:202:SER:HA | 1:G:253:GLU:HG2 | 1.69 | 0.74 |
| 1:F:37:LYS:NZ | 1:F:336:ILE:O | 2.21 | 0.74 |
| 1:L:219:ILE:HD12 | 1:L:222:LEU:HD23 | 1.69 | 0.74 |
| 1:c:195:LEU:HB2 | 1:c:262:LEU:HD12 | 1.69 | 0.74 |
| 1:2:133:GLY:HA3 | 1:p:53:ARG:HH12 | 1.53 | 0.73 |
| 1:E:177:GLN:HE22 | 1:E:179:GLU:HA | 1.53 | 0.73 |
| 1:P:196:LYS:NZ | 1:P:208:GLU:OE2 | 2.21 | 0.73 |
| 1:R:124:ASN:OD1 | 1:R:165:ARG:NH2 | 2.20 | 0.73 |
| 1:p:223:ALA:HA | 1:p:226:ILE:HD12 | 1.70 | 0.73 |
| 1:s:174:VAL:HG22 | 1:s:273:LYS:HD2 | 1.70 | 0.73 |
| 1:1:92:MET:HA | 1:1:95:LEU:HD12 | 1.70 | 0.73 |
| 1:V:218:ASP:HB3 | 1:V:221:GLU:HG3 | 1.69 | 0.73 |
| 1:s:234:LYS:NZ | 1:s:295:ASP:OD1 | 2.21 | 0.73 |
| 1:i:223:ALA:HA | 1:i:226:ILE:HD12 | 1.70 | 0.73 |
| 1:x:30:GLU:OE1 | 1:x:39:ASN:ND2 | 2.21 | 0.73 |
| 1:2:159:LEU:HD12 | 1:2:160:GLU:H | 1.53 | 0.73 |
| 1:U:109:ARG:NH2 | 1:U:282:THR:O | 2.21 | 0.73 |
| 1:i:7:THR:HG21 | 1:t:334:SER:HB2 | 1.69 | 0.73 |
| 1:1:288:GLN:O | 1:p:153:ASN:ND2 | 2.22 | 0.73 |
| 1:D:290:SER:HA | 1:D:293:ILE:HD12 | 1.71 | 0.73 |
| 1:N:106:LYS:HA | 1:N:106:LYS:HE3 | 1.70 | 0.73 |
| 1:v:93:ARG:NH1 | 1:v:295:ASP:OD1 | 2.21 | 0.73 |
| 1:w:57:GLN:HE22 | 1:x:133:GLY:HA2 | 1.53 | 0.73 |
| 1:z:138:LEU:HD12 | 1:z:164:MET:HG3 | 1.71 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:25:GLN:NE2 | 1:E:347:ALA:O | 2.21 | 0.73 |
| 1:t:37:LYS:NZ | 1:t:336:ILE:O | 2.19 | 0.73 |
| 1:1:93:ARG:NH1 | 1:1:295:ASP:OD1 | 2.21 | 0.73 |
| 1:I:220:GLU:OE2 | 1:I:220:GLU:N | 2.16 | 0.73 |
| 1:1:321:ASN:O | 1:1:325:ILE:HG12 | 1.89 | 0.73 |
| 1:H:199:LEU:HD21 | 1:H:232:LEU:HD23 | 1.71 | 0.73 |
| 1:J:4:ASN:HD22 | 1:J:4:ASN:C | 1.96 | 0.73 |
| 1:q:314:ARG:NE | 1:r:122:GLU:OE1 | 2.22 | 0.73 |
| 1:t:351:SER:HA | 1:t:354:LEU:HD12 | 1.69 | 0.73 |
| 1:x:352:GLN:O | 1:x:356:GLN:NE2 | 2.21 | 0.73 |
| 1:z:304:HIS:ND1 | 1:z:307:GLU:OE1 | 2.22 | 0.73 |
| 1:V:92:MET:HA | 1:V:95:LEU:HD12 | 1.72 | 0.72 |
| 1:u:69:ASN:HA | 1:u:72:ILE:HD12 | 1.70 | 0.72 |
| 1:v:47:GLY:HA2 | 1:v:50:ILE:HD12 | 1.70 | 0.72 |
| 1:D:232:LEU:HD22 | 1:D:251:LYS:HZ3 | 1.53 | 0.72 |
| 1:L:54:LEU:HD12 | 1:L:329:VAL:HG13 | 1.71 | 0.72 |
| 1:S:128:GLU:O | 1:S:136:LYS:NZ | 2.16 | 0.72 |
| 1:S:144:ALA:HB1 | 1:S:158:MET:HE1 | 1.71 | 0.72 |
| 1:L:38:ILE:HG23 | 1:L:43:ASP:HB2 | 1.71 | 0.72 |
| 1:o:232:LEU:HA | 1:o:251:LYS:HZ1 | 1.55 | 0.72 |
| 1:C:93:ARG:HE | 1:C:291:VAL:HG13 | 1.52 | 0.72 |
| 1:F:250:ASN:OD1 | 1:F:299:LYS:NZ | 2.23 | 0.72 |
| 1:p:247:ALA:HB1 | 1:p:252:VAL:HG11 | 1.70 | 0.72 |
| 1:L:231:ASP:OD2 | 1:L:251:LYS:NZ | 2.21 | 0.72 |
| 1:Q:219:ILE:HD11 | 1:Q:243:LEU:HB2 | 1.72 | 0.72 |
| 1:i:338:ASP:OD1 | 1:i:339:THR:N | 2.22 | 0.72 |
| 1:v:234:LYS:HA | 1:v:234:LYS:HE3 | 1.70 | 0.72 |
| 1:o:31:ARG:NH2 | 1:o:37:LYS:O | 2.22 | 0.72 |
| 1:2:179:GLU:OE1 | 1:2:179:GLU:N | 2.18 | 0.72 |
| 1:E:112:ILE:O | 1:E:116:VAL:HG23 | 1.90 | 0.72 |
| 1:J:290:SER:HA | 1:J:293:ILE:HD12 | 1.72 | 0.72 |
| 1:M:120:ASN:HD21 | 1:M:277:ASP:HA | 1.55 | 0.72 |
| 1:R:128:GLU:O | 1:R:136:LYS:NZ | 2.21 | 0.72 |
| 1:m:260:GLY:O | 1:m:263:SER:OG | 2.06 | 0.72 |
| 1:2:332:SER:HA | 1:2:335:ARG:HD2 | 1.72 | 0.72 |
| 1:3:61:LEU:O | 1:3:65:VAL:HG23 | 1.89 | 0.72 |
| 1:1:289:GLU:HG2 | 1:1:293:ILE:HD11 | 1.72 | 0.71 |
| 1:R:61:LEU:O | 1:R:65:VAL:HG23 | 1.90 | 0.71 |
| 1:c:25:GLN:HG2 | 1:c:29:MET:HE2 | 1.72 | 0.71 |
| 1:A:31:ARG:HH21 | 1:A:37:LYS:HB2 | 1.53 | 0.71 |
| 1:C:290:SER:O | 1:C:294:ILE:HG12 | 1.89 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:65:VAL:HG13 | 1:D:319:ILE:HD11 | 1.71 | 0.71 |
| 1:D:90:GLN:HE22 | 1:O:56:VAL:HB | 1.53 | 0.71 |
| 1:F:65:VAL:O | 1:F:69:ASN:ND2 | 2.23 | 0.71 |
| 1:w:134:GLY:O | 1:w:136:LYS:NZ | 2.23 | 0.71 |
| 1:l:82:MET:HE1 | 1:l:304:HIS:HB2 | 1.70 | 0.71 |
| 1:o:52:ASN:ND2 | 1:z:302:ASP:OD2 | 2.24 | 0.71 |
| 1:u:84:GLU:O | 1:u:88:ILE:HG12 | 1.90 | 0.71 |
| 1:l:171:MET:HE1 | 1:l:300:TYR:CE2 | 2.26 | 0.71 |
| 1:H:258:PHE:HD2 | 1:H:268:LEU:HD13 | 1.54 | 0.71 |
| 1:u:206:GLU:N | 1:u:206:GLU:OE1 | 2.24 | 0.71 |
| 1:2:57:GLN:NE2 | 1:2:152:ASP:OD1 | 2.24 | 0.71 |
| 1:2:314:ARG:NE | 1:3:122:GLU:OE1 | 2.23 | 0.71 |
| 1:h:19:ASN:HA | 1:h:22:ASN:HD21 | 1.55 | 0.71 |
| 1:j:314:ARG:NH1 | 1:k:122:GLU:OE2 | 2.22 | 0.71 |
| 1:v:290:SER:O | 1:v:294:ILE:HG12 | 1.89 | 0.71 |
| 1:A:168:ASN:OD1 | 1:A:170:MET:N | 2.23 | 0.71 |
| 1:M:363:ALA:O | 1:M:367:GLN:NE2 | 2.23 | 0.71 |
| 1:S:335:ARG:NH2 | 1:T:73:SER:OG | 2.24 | 0.71 |
| 1:I:101:ASN:ND2 | 1:T:67:ASN:OD1 | 2.20 | 0.71 |
| 1:K:37:LYS:NZ | 1:K:336:ILE:O | 2.23 | 0.71 |
| 1:V:170:MET:HE1 | 1:V:250:ASN:HD22 | 1.55 | 0.71 |
| 1:n:202:SER:HA | 1:n:253:GLU:HG3 | 1.73 | 0.71 |
| 1:n:350:LYS:HE3 | 1:o:6:ASN:HA | 1.73 | 0.71 |
| 1:3:295:ASP:HA | 1:3:298:LEU:HD12 | 1.73 | 0.71 |
| 1:3:18:LEU:O | 1:3:22:ASN:ND2 | 2.23 | 0.70 |
| 1:c:164:MET:HA | 1:c:164:MET:HE3 | 1.73 | 0.70 |
| 1:q:128:GLU:OE1 | 1:q:165:ARG:NH1 | 2.23 | 0.70 |
| 1:x:272:LYS:HD2 | 1:x:273:LYS:N | 2.06 | 0.70 |
| 1:D:325:ILE:O | 1:D:329:VAL:HG23 | 1.91 | 0.70 |
| 1:P:177:GLN:OE1 | 1:P:244:GLN:NE2 | 2.25 | 0.70 |
| 1:c:101:ASN:O | 1:c:104:ASN:ND2 | 2.24 | 0.70 |
| 1:z:30:GLU:OE2 | 1:z:39:ASN:ND2 | 2.23 | 0.70 |
| 1:h:18:LEU:O | 1:h:22:ASN:ND2 | 2.25 | 0.70 |
| 1:w:206:GLU:OE2 | 1:w:206:GLU:N | 2.22 | 0.70 |
| 1:I:69:ASN:HA | 1:I:72:ILE:HD12 | 1.73 | 0.70 |
| 1:T:123:LEU:O | 1:T:126:ILE:HG22 | 1.92 | 0.70 |
| 1:l:4:ASN:OD1 | 1:l:6:ASN:N | 2.24 | 0.70 |
| 1:w:37:LYS:N | 1:w:339:THR:HG23 | 2.06 | 0.70 |
| 1:l:177:GLN:OE1 | 1:l:177:GLN:N | 2.24 | 0.70 |
| 1:T:138:LEU:HD12 | 1:T:164:MET:HG2 | 1.73 | 0.70 |
| 1:w:84:GLU:HA | 1:w:87:ASN:ND2 | 2.07 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:x:232:LEU:HA | 1:x:251:LYS:HD2 | 1.74 | 0.70 |
| 1:D:38:ILE:HG23 | 1:D:43:ASP:HB2 | 1.74 | 0.70 |
| 1:O:276:VAL:HA | 1:O:279:ILE:HD11 | 1.74 | 0.70 |
| 1:F:65:VAL:HG13 | 1:F:319:ILE:HD11 | 1.73 | 0.70 |
| 1:N:234:LYS:HA | 1:N:234:LYS:HE3 | 1.74 | 0.70 |
| 1:c:349:THR:O | 1:c:353:ILE:HD12 | 1.92 | 0.70 |
| 1:u:290:SER:O | 1:u:294:ILE:HG13 | 1.91 | 0.70 |
| 1:z:27:THR:O | 1:z:31:ARG:HG2 | 1.91 | 0.70 |
| 1:z:79:GLU:HA | 1:z:82:MET:HE3 | 1.73 | 0.70 |
| 1:F:199:LEU:HB3 | 1:F:256:VAL:HG23 | 1.73 | 0.69 |
| 1:I:338:ASP:OD1 | 1:I:339:THR:N | 2.25 | 0.69 |
| 1:p:177:GLN:OE1 | 1:p:177:GLN:N | 2.25 | 0.69 |
| 1:U:331:ALA:O | 1:U:334:SER:OG | 2.08 | 0.69 |
| 1:h:128:GLU:O | 1:h:136:LYS:NZ | 2.20 | 0.69 |
| 1:i:106:LYS:HA | 1:i:106:LYS:HE2 | 1.73 | 0.69 |
| 1:n:162:LYS:HE2 | 1:n:304:HIS:ND1 | 2.08 | 0.69 |
| 1:o:290:SER:HA | 1:o:293:ILE:HD12 | 1.74 | 0.69 |
| 1:w:179:GLU:OE2 | 1:w:179:GLU:N | 2.23 | 0.69 |
| 1:x:326:ASN:O | 1:x:330:ASN:ND2 | 2.25 | 0.69 |
| 1:M:112:ILE:O | 1:M:116:VAL:HG23 | 1.92 | 0.69 |
| 1:h:160:GLU:OE2 | 1:h:162:LYS:NZ | 2.26 | 0.69 |
| 1:2:288:GLN:O | 1:q:153:ASN:ND2 | 2.24 | 0.69 |
| 1:3:122:GLU:O | 1:3:126:ILE:HG13 | 1.93 | 0.69 |
| 1:J:239:GLN:HE22 | 1:J:283:SER:HB2 | 1.58 | 0.69 |
| 1:P:203:TYR:HB3 | 1:P:205:GLN:HE22 | 1.55 | 0.69 |
| 1:A:152:ASP:OD1 | 1:A:153:ASN:N | 2.25 | 0.69 |
| 1:E:332:SER:O | 1:E:336:ILE:HD12 | 1.92 | 0.69 |
| 1:U:290:SER:HA | 1:U:293:ILE:HD12 | 1.75 | 0.69 |
| 1:i:25:GLN:HG2 | 1:i:29:MET:HE2 | 1.74 | 0.69 |
| 1:j:4:ASN:ND2 | 1:u:334:SER:OG | 2.26 | 0.69 |
| 1:v:352:GLN:NE2 | 1:v:356:GLN:OE1 | 2.23 | 0.69 |
| 1:E:159:LEU:HD12 | 1:E:160:GLU:H | 1.58 | 0.69 |
| 1:F:177:GLN:NE2 | 1:F:179:GLU:OE1 | 2.26 | 0.69 |
| 1:S:86:THR:HA | 1:S:89:LEU:HD12 | 1.74 | 0.69 |
| 1:T:338:ASP:OD1 | 1:T:339:THR:N | 2.25 | 0.69 |
| 1:h:177:GLN:OE1 | 1:h:177:GLN:N | 2.26 | 0.69 |
| 1:j:16:ARG:NH1 | 1:u:324:ASN:OD1 | 2.26 | 0.69 |
| 1:m:55:ASN:OD1 | 1:m:333:LYS:NZ | 2.26 | 0.69 |
| 1:p:101:ASN:OD1 | 1:p:102:GLY:N | 2.25 | 0.69 |
| 1:z:177:GLN:OE1 | 1:z:177:GLN:N | 2.26 | 0.69 |
| 1:z:223:ALA:HA | 1:z:226:ILE:HD12 | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:108:GLU:H | 1:G:108:GLU:CD | 2.01 | 0.69 |
| 1:H:219:ILE:HD12 | 1:H:222:LEU:HD23 | 1.74 | 0.69 |
| 1:I:223:ALA:HA | 1:I:226:ILE:HD12 | 1.74 | 0.69 |
| 1:N:57:GLN:O | 1:N:61:LEU:HD22 | 1.93 | 0.69 |
| 1:h:159:LEU:HD12 | 1:h:160:GLU:H | 1.58 | 0.69 |
| 1:l:321:ASN:HA | 1:m:84:GLU:OE1 | 1.92 | 0.69 |
| 1:L:106:LYS:HE3 | 1:L:106:LYS:HA | 1.74 | 0.69 |
| 1:S:276:VAL:HA | 1:S:279:ILE:HD11 | 1.73 | 0.69 |
| 1:A:325:ILE:O | 1:A:329:VAL:HG23 | 1.93 | 0.68 |
| 1:E:201:ASP:OD1 | 1:E:207:GLN:NE2 | 2.26 | 0.68 |
| 1:F:218:ASP:OD2 | 1:F:219:ILE:N | 2.26 | 0.68 |
| 1:N:57:GLN:HE22 | 1:O:133:GLY:HA2 | 1.58 | 0.68 |
| 1:1:184:LYS:HE3 | 1:1:184:LYS:HA | 1.75 | 0.68 |
| 1:j:194:ASP:CG | 1:j:261:GLY:H | 2.01 | 0.68 |
| 1:t:65:VAL:HB | 1:t:66:ARG:HH12 | 1.59 | 0.68 |
| 1:v:134:GLY:O | 1:v:136:LYS:NZ | 2.26 | 0.68 |
| 1:1:192:LYS:HD3 | 1:1:265:GLU:HG2 | 1.73 | 0.68 |
| 1:k:22:ASN:O | 1:k:26:GLN:HG3 | 1.93 | 0.68 |
| 1:s:333:LYS:HA | 1:s:336:ILE:HD12 | 1.73 | 0.68 |
| 1:1:57:GLN:O | 1:1:61:LEU:HG | 1.93 | 0.68 |
| 1:H:184:LYS:HG2 | 1:S:158:MET:HE3 | 1.74 | 0.68 |
| 1:H:325:ILE:O | 1:H:329:VAL:HG23 | 1.93 | 0.68 |
| 1:S:122:GLU:HB2 | 1:c:314:ARG:HD2 | 1.75 | 0.68 |
| 1:c:94:ASP:O | 1:c:98:GLN:NE2 | 2.26 | 0.68 |
| 1:p:302:ASP:HA | 1:p:305:ARG:HG3 | 1.76 | 0.68 |
| 1:q:304:HIS:HA | 1:q:307:GLU:HG2 | 1.74 | 0.68 |
| 1:L:112:ILE:O | 1:L:116:VAL:HG23 | 1.93 | 0.68 |
| 1:P:325:ILE:O | 1:P:329:VAL:HG23 | 1.93 | 0.68 |
| 1:m:122:GLU:OE1 | 1:m:125:ARG:NE | 2.27 | 0.68 |
| 1:J:332:SER:O | 1:J:336:ILE:HD12 | 1.94 | 0.68 |
| 1:o:177:GLN:OE1 | 1:o:177:GLN:N | 2.26 | 0.68 |
| 1:E:84:GLU:HA | 1:E:87:ASN:ND2 | 2.07 | 0.68 |
| 1:U:304:HIS:HA | 1:U:307:GLU:HG2 | 1.74 | 0.68 |
| 1:V:212:SER:O | 1:V:225:TYR:OH | 2.10 | 0.68 |
| 1:i:208:GLU:N | 1:i:208:GLU:OE2 | 2.26 | 0.68 |
| 1:m:84:GLU:HA | 1:m:87:ASN:ND2 | 2.08 | 0.68 |
| 1:u:9:VAL:O | 1:u:12:MET:HG2 | 1.93 | 0.68 |
| 1:v:122:GLU:O | 1:v:126:ILE:HG13 | 1.93 | 0.68 |
| 1:w:161:LEU:C | 1:w:162:LYS:HD3 | 2.19 | 0.68 |
| 1:z:128:GLU:OE2 | 1:z:165:ARG:NH1 | 2.27 | 0.68 |
| 1:I:88:ILE:O | 1:I:92:MET:HG3 | 1.94 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:165:ARG:HB3 | 1:R:165:ARG:HH11 | 1.57 | 0.68 |
| 1:R:234:LYS:NZ | 1:c:152:ASP:OD1 | 2.24 | 0.68 |
| 1:V:79:GLU:HA | 1:V:82:MET:HG3 | 1.76 | 0.68 |
| 1:h:364:GLN:OE1 | 1:h:364:GLN:N | 2.26 | 0.68 |
| 1:D:128:GLU:OE1 | 1:D:165:ARG:NH1 | 2.26 | 0.68 |
| 1:L:89:LEU:HA | 1:L:92:MET:HG3 | 1.76 | 0.68 |
| 1:t:173:GLY:HA3 | 1:t:246:PHE:HE1 | 1.59 | 0.68 |
| 1:2:340:ASP:HB3 | 1:2:343:LYS:HZ2 | 1.59 | 0.67 |
| 1:3:55:ASN:OD1 | 1:3:59:ARG:NH2 | 2.27 | 0.67 |
| 1:p:84:GLU:O | 1:p:88:ILE:HD12 | 1.94 | 0.67 |
| 1:v:332:SER:O | 1:v:336:ILE:HD12 | 1.93 | 0.67 |
| 1:A:27:THR:O | 1:A:31:ARG:HG3 | 1.94 | 0.67 |
| 1:I:101:ASN:OD1 | 1:I:102:GLY:N | 2.27 | 0.67 |
| 1:K:125:ARG:O | 1:K:129:THR:OG1 | 2.12 | 0.67 |
| 1:M:357:ALA:O | 1:M:361:ILE:HG13 | 1.95 | 0.67 |
| 1:N:27:THR:O | 1:N:31:ARG:HG3 | 1.95 | 0.67 |
| 1:N:332:SER:O | 1:N:336:ILE:HD12 | 1.93 | 0.67 |
| 1:R:38:ILE:HG23 | 1:R:43:ASP:HB2 | 1.74 | 0.67 |
| 1:2:83:ASN:O | 1:2:86:THR:OG1 | 2.11 | 0.67 |
| 1:Q:52:ASN:O | 1:Q:56:VAL:HG23 | 1.94 | 0.67 |
| 1:s:296:ALA:HA | 1:s:299:LYS:HD2 | 1.76 | 0.67 |
| 1:B:162:LYS:HE2 | 1:B:304:HIS:NE2 | 2.08 | 0.67 |
| 1:Q:177:GLN:OE1 | 1:Q:177:GLN:N | 2.27 | 0.67 |
| 1:l:59:ARG:HD2 | 1:w:94:ASP:OD2 | 1.95 | 0.67 |
| 1:n:316:ASN:HA | 1:n:319:ILE:HD12 | 1.75 | 0.67 |
| 1:u:219:ILE:HD11 | 1:u:243:LEU:HD12 | 1.75 | 0.67 |
| 1:A:149:ILE:HD12 | 1:A:315:PHE:CE2 | 2.30 | 0.67 |
| 1:C:290:SER:HA | 1:C:293:ILE:HD12 | 1.75 | 0.67 |
| 1:Q:173:GLY:HA3 | 1:Q:246:PHE:HE2 | 1.60 | 0.67 |
| 1:x:52:ASN:O | 1:x:56:VAL:HG23 | 1.94 | 0.67 |
| 1:3:62:ASP:OD2 | 1:3:326:ASN:ND2 | 2.28 | 0.67 |
| 1:3:316:ASN:HA | 1:3:319:ILE:HG22 | 1.74 | 0.67 |
| 1:B:93:ARG:NH1 | 1:B:295:ASP:OD1 | 2.28 | 0.67 |
| 1:H:91:ARG:HH12 | 1:H:95:LEU:HD21 | 1.58 | 0.67 |
| 1:I:304:HIS:HA | 1:I:307:GLU:OE2 | 1.94 | 0.67 |
| 1:h:201:ASP:OD2 | 1:h:205:GLN:NE2 | 2.27 | 0.67 |
| 1:2:122:GLU:O | 1:2:126:ILE:HG13 | 1.95 | 0.67 |
| 1:2:223:ALA:HA | 1:2:226:ILE:HD12 | 1.76 | 0.67 |
| 1:I:190:GLU:CD | 1:I:191:GLY:H | 2.02 | 0.67 |
| 1:R:315:PHE:O | 1:R:319:ILE:HG13 | 1.94 | 0.67 |
| 1:c:38:ILE:HG23 | 1:c:43:ASP:HB2 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:j:290:SER:O | 1:j:294:ILE:HG12 | 1.94 | 0.67 |
| 1:N:150:GLY:HA3 | 1:N:155:GLU:HB2 | 1.76 | 0.67 |
| 1:m:61:LEU:HD23 | 1:m:151:ALA:HB2 | 1.75 | 0.67 |
| 1:t:101:ASN:OD1 | 1:t:103:SER:N | 2.22 | 0.67 |
| 1:J:248:GLY:HA3 | 1:J:251:LYS:HZ3 | 1.59 | 0.67 |
| 1:N:249:ASN:HD21 | 1:N:273:LYS:NZ | 1.92 | 0.67 |
| 1:i:93:ARG:NH1 | 1:i:295:ASP:OD1 | 2.28 | 0.67 |
| 1:o:38:ILE:HG23 | 1:o:43:ASP:HB2 | 1.76 | 0.67 |
| 1:t:173:GLY:HA3 | 1:t:246:PHE:CE1 | 2.30 | 0.67 |
| 1:u:251:LYS:HE3 | 1:u:252:VAL:HG23 | 1.75 | 0.67 |
| 1:1:123:LEU:HA | 1:1:126:ILE:HD12 | 1.77 | 0.67 |
| 1:A:150:GLY:HA3 | 1:A:155:GLU:HB2 | 1.76 | 0.67 |
| 1:Q:2:ALA:N | 1:R:19:ASN:OD1 | 2.28 | 0.67 |
| 1:s:109:ARG:HB3 | 1:s:282:THR:HA | 1.75 | 0.67 |
| 1:l:153:ASN:ND2 | 1:w:288:GLN:O | 2.28 | 0.66 |
| 1:m:273:LYS:HD3 | 1:m:273:LYS:N | 2.10 | 0.66 |
| 1:1:325:ILE:O | 1:1:329:VAL:HG23 | 1.95 | 0.66 |
| 1:p:373:LEU:O | 1:p:376:LEU:HG | 1.94 | 0.66 |
| 1:v:109:ARG:HA | 1:v:112:ILE:HD12 | 1.76 | 0.66 |
| 1:E:276:VAL:O | 1:E:279:ILE:HG12 | 1.94 | 0.66 |
| 1:J:314:ARG:NE | 1:K:122:GLU:OE1 | 2.26 | 0.66 |
| 1:U:335:ARG:HB3 | 1:V:69:ASN:HD21 | 1.59 | 0.66 |
| 1:i:101:ASN:OD1 | 1:i:102:GLY:N | 2.28 | 0.66 |
| 1:j:61:LEU:HD12 | 1:j:322:LEU:HD12 | 1.76 | 0.66 |
| 1:p:194:ASP:OD1 | 1:p:195:LEU:N | 2.28 | 0.66 |
| 1:q:15:GLN:O | 1:q:19:ASN:ND2 | 2.29 | 0.66 |
| 1:u:27:THR:O | 1:u:31:ARG:HG3 | 1.96 | 0.66 |
| 1:2:358:SER:HA | 1:2:361:ILE:HD12 | 1.77 | 0.66 |
| 1:J:25:GLN:NE2 | 1:J:29:MET:HE3 | 2.10 | 0.66 |
| 1:J:247:ALA:HB1 | 1:J:252:VAL:HG11 | 1.77 | 0.66 |
| 1:B:325:ILE:O | 1:B:329:VAL:HG12 | 1.96 | 0.66 |
| 1:J:184:LYS:HD3 | 1:U:158:MET:HE1 | 1.76 | 0.66 |
| 1:n:92:MET:HA | 1:n:95:LEU:HD12 | 1.77 | 0.66 |
| 1:B:179:GLU:N | 1:B:179:GLU:OE2 | 2.26 | 0.66 |
| 1:G:319:ILE:HA | 1:G:322:LEU:HD12 | 1.77 | 0.66 |
| 1:R:54:LEU:HD12 | 1:R:329:VAL:HG13 | 1.76 | 0.66 |
| 1:T:85:THR:HG23 | 1:T:123:LEU:HD11 | 1.76 | 0.66 |
| 1:p:6:ASN:HA | 1:z:350:LYS:NZ | 2.10 | 0.66 |
| 1:w:304:HIS:HA | 1:w:307:GLU:HG2 | 1.78 | 0.66 |
| 1:z:58:SER:HA | 1:z:61:LEU:HD23 | 1.76 | 0.66 |
| 1:P:9:VAL:HA | 1:P:12:MET:HE3 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:t:29:MET:HG2 | 1:t:348:MET:HE1 | 1.77 | 0.66 |
| 1:1:349:THR:O | 1:1:353:ILE:HG13 | 1.95 | 0.66 |
| 1:A:218:ASP:OD1 | 1:A:219:ILE:N | 2.29 | 0.66 |
| 1:B:223:ALA:HA | 1:B:226:ILE:HD12 | 1.77 | 0.66 |
| 1:U:169:LYS:HD3 | 1:U:169:LYS:N | 2.10 | 0.66 |
| 1:U:325:ILE:O | 1:U:329:VAL:HG22 | 1.96 | 0.66 |
| 1:r:162:LYS:N | 1:r:162:LYS:HD3 | 2.11 | 0.66 |
| 1:1:221:GLU:N | 1:1:221:GLU:OE2 | 2.28 | 0.66 |
| 1:2:170:MET:HB3 | 1:2:300:TYR:CE1 | 2.31 | 0.66 |
| 1:I:112:ILE:O | 1:I:116:VAL:HG23 | 1.96 | 0.66 |
| 1:s:295:ASP:OD2 | 1:s:296:ALA:N | 2.28 | 0.66 |
| 1:N:231:ASP:HA | 1:N:234:LYS:HZ3 | 1.61 | 0.65 |
| 1:o:54:LEU:HD12 | 1:o:329:VAL:HG13 | 1.77 | 0.65 |
| 1:w:29:MET:O | 1:w:32:LEU:HG | 1.96 | 0.65 |
| 1:z:289:GLU:O | 1:z:293:ILE:HG13 | 1.96 | 0.65 |
| 1:Q:152:ASP:OD1 | 1:Q:153:ASN:N | 2.25 | 0.65 |
| 1:h:222:LEU:O | 1:h:226:ILE:HG13 | 1.96 | 0.65 |
| 1:o:179:GLU:OE1 | 1:o:179:GLU:N | 2.26 | 0.65 |
| 1:w:315:PHE:O | 1:w:319:ILE:HD12 | 1.95 | 0.65 |
| 1:z:86:THR:HA | 1:z:89:LEU:HD12 | 1.77 | 0.65 |
| 1:z:92:MET:HA | 1:z:95:LEU:HD12 | 1.76 | 0.65 |
| 1:A:162:LYS:HG3 | 1:A:304:HIS:CE1 | 2.31 | 0.65 |
| 1:R:38:ILE:O | 1:R:337:LYS:NZ | 2.29 | 0.65 |
| 1:t:223:ALA:HA | 1:t:226:ILE:HD12 | 1.77 | 0.65 |
| 1:x:315:PHE:O | 1:x:319:ILE:HG13 | 1.95 | 0.65 |
| 1:H:290:SER:O | 1:H:294:ILE:HG13 | 1.96 | 0.65 |
| 1:N:301:VAL:HA | 1:N:304:HIS:HD2 | 1.60 | 0.65 |
| 1:P:335:ARG:HD2 | 1:Q:69:ASN:HB3 | 1.78 | 0.65 |
| 1:V:106:LYS:HA | 1:V:106:LYS:HE2 | 1.78 | 0.65 |
| 1:n:46:ALA:O | 1:n:50:ILE:HG13 | 1.96 | 0.65 |
| 1:1:208:GLU:N | 1:1:208:GLU:OE2 | 2.29 | 0.65 |
| 1:3:82:MET:HE1 | 1:3:308:LEU:HD11 | 1.78 | 0.65 |
| 1:H:158:MET:HE3 | 1:H:159:LEU:H | 1.60 | 0.65 |
| 1:L:4:ASN:OD1 | 1:L:6:ASN:N | 2.29 | 0.65 |
| 1:O:219:ILE:HD11 | 1:O:243:LEU:HD21 | 1.77 | 0.65 |
| 1:S:350:LYS:O | 1:S:354:LEU:HD12 | 1.97 | 0.65 |
| 1:V:111:ALA:HA | 1:V:114:GLU:OE1 | 1.97 | 0.65 |
| 1:3:58:SER:HA | 1:3:61:LEU:HD12 | 1.76 | 0.65 |
| 1:M:244:GLN:HE22 | 1:M:246:PHE:HB2 | 1.61 | 0.65 |
| 1:R:157:VAL:HG21 | 1:R:314:ARG:HH21 | 1.61 | 0.65 |
| 1:i:325:ILE:O | 1:i:329:VAL:HG12 | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:k:65:VAL:HG13 | 1:k:319:ILE:HD11 | 1.77 | 0.65 |
| 1:l:375:LEU:O | 1:m:366:LYS:NZ | 2.29 | 0.65 |
| 1:o:109:ARG:HB3 | 1:o:282:THR:HA | 1.79 | 0.65 |
| 1:o:168:ASN:ND2 | 1:o:300:TYR:OH | 2.29 | 0.65 |
| 1:q:247:ALA:HB1 | 1:q:252:VAL:HG11 | 1.78 | 0.65 |
| 1:r:10:SER:O | 1:r:13:THR:OG1 | 2.13 | 0.65 |
| 1:s:18:LEU:O | 1:s:22:ASN:ND2 | 2.29 | 0.65 |
| 1:w:37:LYS:NZ | 1:w:340:ASP:H | 1.95 | 0.65 |
| 1:x:270:GLU:OE2 | 1:x:271:GLY:N | 2.29 | 0.65 |
| 1:T:325:ILE:O | 1:T:329:VAL:HG23 | 1.95 | 0.65 |
| 1:u:290:SER:HA | 1:u:293:ILE:HD12 | 1.79 | 0.65 |
| 1:z:46:ALA:O | 1:z:50:ILE:HG12 | 1.96 | 0.65 |
| 1:A:220:GLU:O | 1:A:224:THR:HG23 | 1.96 | 0.65 |
| 1:M:108:GLU:N | 1:M:108:GLU:OE1 | 2.30 | 0.65 |
| 1:h:270:GLU:OE2 | 1:h:271:GLY:N | 2.29 | 0.65 |
| 1:p:163:ASP:HB3 | 1:p:168:ASN:HD22 | 1.61 | 0.65 |
| 1:t:231:ASP:OD2 | 1:t:251:LYS:NZ | 2.29 | 0.65 |
| 1:1:312:GLN:NE2 | 1:p:42:LYS:HE2 | 2.12 | 0.65 |
| 1:3:300:TYR:O | 1:3:303:SER:OG | 2.14 | 0.65 |
| 1:H:178:ALA:HB3 | 1:H:242:LYS:HB3 | 1.79 | 0.65 |
| 1:I:202:SER:HA | 1:I:253:GLU:HG3 | 1.79 | 0.65 |
| 1:J:302:ASP:OD2 | 1:U:52:ASN:ND2 | 2.29 | 0.65 |
| 1:h:52:ASN:O | 1:h:56:VAL:HG23 | 1.96 | 0.65 |
| 1:j:219:ILE:HD11 | 1:j:243:LEU:HD13 | 1.78 | 0.65 |
| 1:n:61:LEU:HD21 | 1:n:325:ILE:HG22 | 1.77 | 0.65 |
| 1:s:53:ARG:NH2 | 1:t:133:GLY:O | 2.29 | 0.65 |
| 1:B:105:SER:OG | 1:B:106:LYS:N | 2.30 | 0.65 |
| 1:O:163:ASP:O | 1:O:300:TYR:OH | 2.14 | 0.65 |
| 1:S:223:ALA:HA | 1:S:226:ILE:HD12 | 1.78 | 0.65 |
| 1:T:223:ALA:HA | 1:T:226:ILE:HD12 | 1.79 | 0.65 |
| 1:n:300:TYR:O | 1:n:303:SER:OG | 2.15 | 0.65 |
| 1:w:157:VAL:HG11 | 1:w:314:ARG:NH2 | 2.13 | 0.65 |
| 1:1:337:LYS:HA | 1:1:337:LYS:HE3 | 1.79 | 0.64 |
| 1:I:84:GLU:O | 1:I:88:ILE:HG12 | 1.97 | 0.64 |
| 1:M:25:GLN:O | 1:M:29:MET:HG3 | 1.97 | 0.64 |
| 1:l:9:VAL:HA | 1:l:12:MET:HE3 | 1.78 | 0.64 |
| 1:n:192:LYS:HE2 | 1:n:192:LYS:HA | 1.78 | 0.64 |
| 1:s:198:ASN:ND2 | 1:s:206:GLU:OE2 | 2.29 | 0.64 |
| 1:M:121:ASP:HA | 1:M:124:ASN:ND2 | 2.13 | 0.64 |
| 1:N:203:TYR:HD2 | 1:N:205:GLN:HE21 | 1.44 | 0.64 |
| 1:Q:195:LEU:HB2 | 1:Q:262:LEU:HD23 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:v:349:THR:O | 1:v:353:ILE:HG13 | 1.97 | 0.64 |
| 1:3:30:GLU:OE2 | 1:3:39:ASN:ND2 | 2.31 | 0.64 |
| 1:C:84:GLU:O | 1:C:88:ILE:HG12 | 1.98 | 0.64 |
| 1:O:84:GLU:O | 1:O:88:ILE:HG12 | 1.98 | 0.64 |
| 1:S:139:ASN:OD1 | 1:S:141:THR:HG22 | 1.97 | 0.64 |
| 1:k:173:GLY:HA3 | 1:k:246:PHE:CZ | 2.32 | 0.64 |
| 1:x:149:ILE:HG21 | 1:x:315:PHE:HE2 | 1.61 | 0.64 |
| 1:A:198:ASN:ND2 | 1:A:208:GLU:OE1 | 2.29 | 0.64 |
| 1:C:321:ASN:O | 1:C:325:ILE:HD12 | 1.98 | 0.64 |
| 1:L:92:MET:HE3 | 1:L:119:LEU:HB2 | 1.79 | 0.64 |
| 1:S:58:SER:HA | 1:S:61:LEU:HD12 | 1.78 | 0.64 |
| 1:h:218:ASP:OD1 | 1:h:219:ILE:N | 2.30 | 0.64 |
| 1:h:340:ASP:OD2 | 1:h:343:LYS:NZ | 2.30 | 0.64 |
| 1:q:257:GLU:N | 1:q:257:GLU:OE2 | 2.30 | 0.64 |
| 1:I:6:ASN:HA | 1:o:350:LYS:HE3 | 1.78 | 0.64 |
| 1:K:291:VAL:HA | 1:K:294:ILE:HD12 | 1.79 | 0.64 |
| 1:r:52:ASN:O | 1:r:56:VAL:HG23 | 1.98 | 0.64 |
| 1:s:325:ILE:O | 1:s:329:VAL:HG22 | 1.97 | 0.64 |
| 1:z:173:GLY:HA3 | 1:z:246:PHE:HE1 | 1.62 | 0.64 |
| 1:B:289:GLU:O | 1:B:293:ILE:HG13 | 1.97 | 0.64 |
| 1:D:163:ASP:C | 1:D:164:MET:HE2 | 2.21 | 0.64 |
| 1:G:177:GLN:N | 1:G:177:GLN:OE1 | 2.30 | 0.64 |
| 1:P:226:ILE:HA | 1:P:229:GLN:NE2 | 2.13 | 0.64 |
| 1:S:176:TYR:HB3 | 1:S:268:LEU:HD11 | 1.78 | 0.64 |
| 1:s:246:PHE:CE1 | 1:s:293:ILE:HG13 | 2.33 | 0.64 |
| 1:w:37:LYS:NZ | 1:w:339:THR:HA | 2.13 | 0.64 |
| 1:z:243:LEU:HD13 | 1:z:266:LEU:HD11 | 1.78 | 0.64 |
| 1:z:350:LYS:HA | 1:z:353:ILE:HD12 | 1.79 | 0.64 |
| 1:N:226:ILE:HA | 1:N:229:GLN:HG2 | 1.80 | 0.64 |
| 1:i:108:GLU:O | 1:i:112:ILE:HG13 | 1.96 | 0.64 |
| 1:m:160:GLU:OE2 | 1:m:160:GLU:N | 2.30 | 0.64 |
| 1:p:15:GLN:HE22 | 1:z:343:LYS:NZ | 1.96 | 0.64 |
| 1:s:246:PHE:HE1 | 1:s:293:ILE:HG13 | 1.63 | 0.64 |
| 1:v:169:LYS:HD3 | 1:v:169:LYS:H | 1.62 | 0.64 |
| 1:F:261:GLY:O | 1:F:264:GLY:N | 2.30 | 0.64 |
| 1:M:346:THR:O | 1:M:349:THR:OG1 | 2.16 | 0.64 |
| 1:O:332:SER:O | 1:O:336:ILE:HD12 | 1.98 | 0.64 |
| 1:T:25:GLN:HG2 | 1:T:29:MET:HE2 | 1.78 | 0.64 |
| 1:h:314:ARG:NE | 1:i:122:GLU:OE2 | 2.25 | 0.64 |
| 1:x:290:SER:HA | 1:x:293:ILE:HD12 | 1.80 | 0.64 |
| 1:1:187:ASN:ND2 | 1:1:216:GLY:O | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:6:ASN:HD22 | 1:H:6:ASN:N | 1.95 | 0.64 |
| 1:L:338:ASP:OD2 | 1:L:339:THR:N | 2.31 | 0.64 |
| 1:M:338:ASP:OD1 | 1:M:339:THR:N | 2.30 | 0.64 |
| 1:P:193:ASN:ND2 | 1:P:213:ALA:O | 2.31 | 0.64 |
| 1:c:290:SER:HA | 1:c:293:ILE:HG12 | 1.79 | 0.64 |
| 1:w:69:ASN:O | 1:w:72:ILE:HG22 | 1.97 | 0.64 |
| 1:2:340:ASP:HB3 | 1:2:343:LYS:NZ | 2.12 | 0.64 |
| 1:B:220:GLU:OE1 | 1:B:220:GLU:N | 2.29 | 0.64 |
| 1:C:179:GLU:O | 1:C:242:LYS:NZ | 2.31 | 0.64 |
| 1:C:223:ALA:HA | 1:C:226:ILE:HD12 | 1.80 | 0.64 |
| 1:E:291:VAL:HA | 1:E:294:ILE:HD12 | 1.81 | 0.64 |
| 1:F:290:SER:HA | 1:F:293:ILE:HD12 | 1.80 | 0.64 |
| 1:I:67:ASN:OD1 | 1:p:101:ASN:HB2 | 1.98 | 0.64 |
| 1:J:37:LYS:HE3 | 1:J:339:THR:HA | 1.78 | 0.64 |
| 1:P:55:ASN:O | 1:P:59:ARG:HG2 | 1.98 | 0.64 |
| 1:n:196:LYS:HE3 | 1:n:210:ASN:OD1 | 1.97 | 0.64 |
| 1:q:202:SER:HA | 1:q:253:GLU:HG2 | 1.79 | 0.64 |
| 1:2:57:GLN:O | 1:2:61:LEU:HG | 1.97 | 0.63 |
| 1:2:295:ASP:HA | 1:2:298:LEU:HD12 | 1.79 | 0.63 |
| 1:E:125:ARG:O | 1:E:129:THR:HG23 | 1.98 | 0.63 |
| 1:m:112:ILE:O | 1:m:116:VAL:HG23 | 1.98 | 0.63 |
| 1:n:291:VAL:HA | 1:n:294:ILE:HD12 | 1.80 | 0.63 |
| 1:t:190:GLU:HA | 1:t:193:ASN:HD21 | 1.64 | 0.63 |
| 1:w:342:ALA:O | 1:w:345:THR:HG22 | 1.98 | 0.63 |
| 1:H:25:GLN:HG2 | 1:H:29:MET:HE2 | 1.81 | 0.63 |
| 1:J:350:LYS:HD3 | 1:V:6:ASN:HB2 | 1.80 | 0.63 |
| 1:M:255:GLU:OE2 | 1:M:256:VAL:N | 2.32 | 0.63 |
| 1:q:61:LEU:HD23 | 1:q:151:ALA:HB2 | 1.79 | 0.63 |
| 1:w:163:ASP:C | 1:w:164:MET:HE2 | 2.24 | 0.63 |
| 1:F:276:VAL:O | 1:F:279:ILE:HG12 | 1.99 | 0.63 |
| 1:J:273:LYS:HD3 | 1:J:273:LYS:N | 2.13 | 0.63 |
| 1:U:222:LEU:O | 1:U:226:ILE:HG12 | 1.98 | 0.63 |
| 1:c:299:LYS:HA | 1:c:299:LYS:HE3 | 1.79 | 0.63 |
| 1:z:345:THR:O | 1:z:349:THR:HG23 | 1.97 | 0.63 |
| 1:F:154:GLY:HA3 | 1:m:227:ASN:ND2 | 2.13 | 0.63 |
| 1:K:30:GLU:OE2 | 1:K:39:ASN:ND2 | 2.32 | 0.63 |
| 1:O:221:GLU:OE1 | 1:P:121:ASP:HB2 | 1.99 | 0.63 |
| 1:k:332:SER:O | 1:k:336:ILE:HD12 | 1.98 | 0.63 |
| 1:p:173:GLY:HA3 | 1:p:246:PHE:CE2 | 2.34 | 0.63 |
| 1:v:195:LEU:HB2 | 1:v:262:LEU:HD12 | 1.79 | 0.63 |
| 1:l:26:GLN:HG3 | 1:z:10:SER:HB3 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:3:19:ASN:HA | 1:3:22:ASN:HD21 | 1.63 | 0.63 |
| 1:I:177:GLN:OE1 | 1:I:177:GLN:N | 2.31 | 0.63 |
| 1:J:83:ASN:O | 1:J:86:THR:OG1 | 2.16 | 0.63 |
| 1:K:332:SER:O | 1:K:336:ILE:HD12 | 1.99 | 0.63 |
| 1:R:190:GLU:HA | 1:R:193:ASN:ND2 | 2.14 | 0.63 |
| 1:U:314:ARG:NE | 1:V:122:GLU:OE1 | 2.30 | 0.63 |
| 1:j:27:THR:O | 1:j:31:ARG:HG2 | 1.98 | 0.63 |
| 1:k:373:LEU:HB2 | 1:u:353:ILE:HG23 | 1.81 | 0.63 |
| 1:m:290:SER:HA | 1:m:293:ILE:HD12 | 1.80 | 0.63 |
| 1:o:148:GLN:NE2 | 1:o:150:GLY:O | 2.32 | 0.63 |
| 1:t:290:SER:HA | 1:t:293:ILE:HD12 | 1.81 | 0.63 |
| 1:v:25:GLN:O | 1:v:29:MET:HG3 | 1.97 | 0.63 |
| 1:2:138:LEU:HD13 | 1:2:164:MET:HG3 | 1.80 | 0.63 |
| 1:O:159:LEU:HD12 | 1:O:160:GLU:H | 1.63 | 0.63 |
| 1:c:46:ALA:O | 1:c:50:ILE:HG13 | 1.98 | 0.63 |
| 1:E:288:GLN:NE2 | 1:P:154:GLY:H | 1.96 | 0.63 |
| 1:E:315:PHE:O | 1:E:319:ILE:HG13 | 1.99 | 0.63 |
| 1:U:248:GLY:H | 1:U:251:LYS:HE2 | 1.64 | 0.63 |
| 1:U:321:ASN:O | 1:U:325:ILE:HG12 | 1.98 | 0.63 |
| 1:l:218:ASP:OD2 | 1:l:219:ILE:N | 2.32 | 0.63 |
| 1:x:318:ALA:O | 1:x:322:LEU:HG | 1.98 | 0.63 |
| 1:K:222:LEU:O | 1:K:226:ILE:HG12 | 1.99 | 0.63 |
| 1:O:105:SER:OG | 1:O:108:GLU:OE1 | 2.12 | 0.63 |
| 1:p:5:VAL:HG12 | 1:p:6:ASN:H | 1.64 | 0.63 |
| 1:p:109:ARG:HA | 1:p:112:ILE:HD12 | 1.79 | 0.63 |
| 1:t:257:GLU:OE2 | 1:t:257:GLU:N | 2.32 | 0.63 |
| 1:z:166:SER:HB2 | 1:z:276:VAL:HB | 1.80 | 0.63 |
| 1:C:52:ASN:O | 1:C:56:VAL:HG23 | 1.99 | 0.63 |
| 1:U:198:ASN:HB3 | 1:U:257:GLU:HB3 | 1.80 | 0.63 |
| 1:h:53:ARG:NH1 | 1:i:133:GLY:O | 2.32 | 0.63 |
| 1:i:273:LYS:NZ | 1:i:275:THR:HG23 | 2.11 | 0.63 |
| 1:k:46:ALA:O | 1:k:50:ILE:HG12 | 1.99 | 0.63 |
| 1:o:73:SER:O | 1:o:77:THR:HG23 | 1.99 | 0.63 |
| 1:u:302:ASP:HA | 1:u:305:ARG:HG3 | 1.80 | 0.63 |
| 1:v:12:MET:SD | 1:v:16:ARG:NE | 2.71 | 0.63 |
| 1:w:178:ALA:HB2 | 1:w:268:LEU:HD23 | 1.80 | 0.63 |
| 1:M:158:MET:HA | 1:M:158:MET:HE2 | 1.81 | 0.62 |
| 1:N:307:GLU:OE2 | 1:N:308:LEU:HD23 | 1.98 | 0.62 |
| 1:c:108:GLU:OE2 | 1:c:108:GLU:N | 2.31 | 0.62 |
| 1:p:93:ARG:HG3 | 1:p:294:ILE:HG21 | 1.80 | 0.62 |
| 1:q:9:VAL:HA | 1:q:12:MET:HE3 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:u:109:ARG:HA | 1:u:112:ILE:HD12 | 1.80 | 0.62 |
| 1:2:169:LYS:HB3 | 1:2:170:MET:HE2 | 1.81 | 0.62 |
| 1:B:159:LEU:HD12 | 1:B:160:GLU:H | 1.64 | 0.62 |
| 1:G:93:ARG:NH2 | 1:R:152:ASP:OD1 | 2.32 | 0.62 |
| 1:M:289:GLU:O | 1:M:293:ILE:HG13 | 2.00 | 0.62 |
| 1:N:231:ASP:HA | 1:N:234:LYS:NZ | 2.14 | 0.62 |
| 1:Q:142:HIS:CD2 | 1:Q:161:LEU:HB2 | 2.34 | 0.62 |
| 1:w:162:LYS:HD3 | 1:w:162:LYS:N | 2.14 | 0.62 |
| 1:D:6:ASN:O | 1:j:350:LYS:NZ | 2.30 | 0.62 |
| 1:F:152:ASP:OD1 | 1:m:93:ARG:NH2 | 2.28 | 0.62 |
| 1:H:115:GLU:OE2 | 1:R:313:ASN:ND2 | 2.29 | 0.62 |
| 1:J:128:GLU:OE1 | 1:J:165:ARG:NH1 | 2.33 | 0.62 |
| 1:t:29:MET:CG | 1:t:348:MET:HE1 | 2.28 | 0.62 |
| 1:t:184:LYS:NZ | 1:t:218:ASP:OD2 | 2.23 | 0.62 |
| 1:z:332:SER:HA | 1:z:335:ARG:NH1 | 2.14 | 0.62 |
| 1:z:343:LYS:HA | 1:z:343:LYS:HE3 | 1.81 | 0.62 |
| 1:3:219:ILE:HG23 | 1:3:237:VAL:HG21 | 1.82 | 0.62 |
| 1:C:349:THR:O | 1:C:353:ILE:HG12 | 2.00 | 0.62 |
| 1:P:143:GLY:HA3 | 1:P:145:LYS:HE3 | 1.81 | 0.62 |
| 1:V:159:LEU:HD11 | 1:V:161:LEU:HD21 | 1.80 | 0.62 |
| 1:l:357:ALA:O | 1:l:361:ILE:HG12 | 1.99 | 0.62 |
| 1:t:343:LYS:HA | 1:t:343:LYS:HE3 | 1.81 | 0.62 |
| 1:u:46:ALA:O | 1:u:50:ILE:HG13 | 1.98 | 0.62 |
| 1:u:361:ILE:HD12 | 1:v:29:MET:HB3 | 1.81 | 0.62 |
| 1:C:69:ASN:O | 1:C:72:ILE:HG22 | 1.99 | 0.62 |
| 1:N:4:ASN:C | 1:N:4:ASN:HD22 | 2.07 | 0.62 |
| 1:V:137:LEU:HD11 | 1:V:161:LEU:HD12 | 1.82 | 0.62 |
| 1:c:25:GLN:HG2 | 1:c:29:MET:CE | 2.29 | 0.62 |
| 1:q:368:ALA:O | 1:q:371:SER:OG | 2.17 | 0.62 |
| 1:z:8:ASN:OD1 | 1:z:10:SER:OG | 2.13 | 0.62 |
| 1:1:304:HIS:HA | 1:1:307:GLU:HG2 | 1.81 | 0.62 |
| 1:B:276:VAL:O | 1:B:279:ILE:HG12 | 2.00 | 0.62 |
| 1:G:222:LEU:O | 1:G:226:ILE:HD12 | 1.99 | 0.62 |
| 1:G:289:GLU:O | 1:G:293:ILE:HG13 | 2.00 | 0.62 |
| 1:U:88:ILE:O | 1:U:92:MET:HG3 | 2.00 | 0.62 |
| 1:3:142:HIS:CG | 1:3:143:GLY:H | 2.17 | 0.62 |
| 1:F:54:LEU:HD12 | 1:F:329:VAL:HG13 | 1.82 | 0.62 |
| 1:J:176:TYR:OH | 1:J:255:GLU:OE1 | 2.12 | 0.62 |
| 1:K:194:ASP:HB2 | 1:K:196:LYS:NZ | 2.14 | 0.62 |
| 1:M:195:LEU:HB2 | 1:M:262:LEU:HD12 | 1.82 | 0.62 |
| 1:R:93:ARG:NH2 | 1:c:151:ALA:O | 2.33 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:239:GLN:OE1 | 1:h:284:VAL:HB | 1.98 | 0.62 |
| 1:v:262:LEU:HA | 1:v:265:GLU:HB2 | 1.82 | 0.62 |
| 1:1:30:GLU:OE2 | 1:1:39:ASN:ND2 | 2.30 | 0.62 |
| 1:E:128:GLU:OE2 | 1:E:165:ARG:NH1 | 2.32 | 0.62 |
| 1:R:179:GLU:OE1 | 1:R:179:GLU:N | 2.33 | 0.62 |
| 1:R:222:LEU:O | 1:R:226:ILE:HG13 | 1.99 | 0.62 |
| 1:c:54:LEU:HD12 | 1:c:329:VAL:HG13 | 1.82 | 0.62 |
| 1:k:55:ASN:OD1 | 1:k:56:VAL:N | 2.33 | 0.62 |
| 1:m:30:GLU:OE1 | 1:m:39:ASN:ND2 | 2.32 | 0.62 |
| 1:t:47:GLY:HA2 | 1:t:50:ILE:HD12 | 1.82 | 0.62 |
| 1:u:318:ALA:O | 1:u:322:LEU:HD22 | 1.99 | 0.62 |
| 1:x:196:LYS:HZ3 | 1:x:260:GLY:HA3 | 1.65 | 0.62 |
| 1:C:316:ASN:HA | 1:C:319:ILE:HD12 | 1.81 | 0.62 |
| 1:K:350:LYS:O | 1:K:354:LEU:HG | 2.00 | 0.62 |
| 1:U:235:ALA:HB1 | 1:U:243:LEU:HD11 | 1.81 | 0.62 |
| 1:c:162:LYS:HG3 | 1:c:304:HIS:CE1 | 2.34 | 0.62 |
| 1:m:170:MET:HB3 | 1:m:300:TYR:CE1 | 2.35 | 0.62 |
| 1:B:190:GLU:OE1 | 1:B:193:ASN:ND2 | 2.33 | 0.62 |
| 1:F:280:ASP:OD2 | 1:F:281:VAL:N | 2.33 | 0.62 |
| 1:M:50:ILE:O | 1:M:54:LEU:HG | 2.00 | 0.62 |
| 1:T:120:ASN:C | 1:T:120:ASN:HD22 | 2.08 | 0.62 |
| 1:i:177:GLN:OE1 | 1:i:177:GLN:N | 2.33 | 0.62 |
| 1:q:331:ALA:HB1 | 1:q:335:ARG:HH12 | 1.64 | 0.62 |
| 1:u:88:ILE:O | 1:u:92:MET:HG3 | 2.00 | 0.62 |
| 1:2:162:LYS:HZ3 | 1:2:304:HIS:HB3 | 1.65 | 0.61 |
| 1:K:38:ILE:HD11 | 1:K:48:LEU:HB2 | 1.82 | 0.61 |
| 1:R:169:LYS:HA | 1:R:169:LYS:HE3 | 1.82 | 0.61 |
| 1:S:113:GLN:NE2 | 1:S:280:ASP:HA | 2.15 | 0.61 |
| 1:j:375:LEU:O | 1:k:366:LYS:NZ | 2.33 | 0.61 |
| 1:l:170:MET:HE2 | 1:l:170:MET:HA | 1.81 | 0.61 |
| 1:q:148:GLN:NE2 | 1:q:153:ASN:OD1 | 2.33 | 0.61 |
| 1:w:335:ARG:HD2 | 1:x:69:ASN:HB3 | 1.81 | 0.61 |
| 1:x:29:MET:HE1 | 1:x:348:MET:HG3 | 1.82 | 0.61 |
| 1:H:168:ASN:O | 1:H:171:MET:HB2 | 2.00 | 0.61 |
| 1:M:315:PHE:O | 1:M:319:ILE:HG13 | 1.99 | 0.61 |
| 1:Q:273:LYS:HD3 | 1:Q:273:LYS:N | 2.14 | 0.61 |
| 1:w:219:ILE:HG23 | 1:w:220:GLU:OE2 | 1.99 | 0.61 |
| 1:x:208:GLU:N | 1:x:208:GLU:OE2 | 2.34 | 0.61 |
| 1:1:290:SER:HA | 1:1:293:ILE:HD12 | 1.81 | 0.61 |
| 1:D:201:ASP:OD2 | 1:D:202:SER:N | 2.33 | 0.61 |
| 1:J:120:ASN:HD21 | 1:J:277:ASP:HA | 1.66 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:177:GLN:OE1 | 1:L:178:ALA:N | 2.34 | 0.61 |
| 1:T:84:GLU:O | 1:T:88:ILE:HG13 | 2.00 | 0.61 |
| 1:p:325:ILE:O | 1:p:329:VAL:HG23 | 2.00 | 0.61 |
| 1:r:170:MET:SD | 1:r:250:ASN:HB3 | 2.39 | 0.61 |
| 1:B:108:GLU:O | 1:B:112:ILE:HG13 | 2.00 | 0.61 |
| 1:J:61:LEU:HD23 | 1:J:151:ALA:HB2 | 1.81 | 0.61 |
| 1:m:279:ILE:HB | 1:m:290:SER:OG | 2.00 | 0.61 |
| 1:v:69:ASN:O | 1:v:72:ILE:HG22 | 2.01 | 0.61 |
| 1:2:276:VAL:O | 1:2:279:ILE:HG12 | 1.99 | 0.61 |
| 1:H:46:ALA:O | 1:H:50:ILE:HG13 | 2.00 | 0.61 |
| 1:L:162:LYS:HG2 | 1:L:304:HIS:CE1 | 2.34 | 0.61 |
| 1:U:276:VAL:O | 1:U:279:ILE:HG12 | 2.00 | 0.61 |
| 1:i:122:GLU:OE1 | 1:i:125:ARG:NE | 2.27 | 0.61 |
| 1:n:277:ASP:OD1 | 1:n:277:ASP:N | 2.31 | 0.61 |
| 1:s:222:LEU:O | 1:s:226:ILE:HG13 | 2.01 | 0.61 |
| 1:u:52:ASN:O | 1:u:56:VAL:HG23 | 2.01 | 0.61 |
| 1:z:55:ASN:O | 1:z:59:ARG:HG3 | 2.01 | 0.61 |
| 1:z:201:ASP:OD1 | 1:z:207:GLN:NE2 | 2.33 | 0.61 |
| 1:3:318:ALA:O | 1:3:322:LEU:HG | 2.00 | 0.61 |
| 1:J:169:LYS:HD3 | 1:J:169:LYS:H | 1.65 | 0.61 |
| 1:L:31:ARG:NH2 | 1:L:37:LYS:O | 2.33 | 0.61 |
| 1:M:321:ASN:O | 1:M:325:ILE:HG12 | 2.01 | 0.61 |
| 1:P:149:ILE:HD11 | 1:Q:125:ARG:HH12 | 1.64 | 0.61 |
| 1:q:82:MET:HE3 | 1:q:305:ARG:HG2 | 1.81 | 0.61 |
| 1:s:122:GLU:OE1 | 1:s:125:ARG:NE | 2.34 | 0.61 |
| 1:C:325:ILE:O | 1:C:329:VAL:HG23 | 2.01 | 0.61 |
| 1:D:272:LYS:N | 1:D:272:LYS:HD3 | 2.15 | 0.61 |
| 1:E:218:ASP:OD1 | 1:E:219:ILE:N | 2.33 | 0.61 |
| 1:G:231:ASP:N | 1:G:231:ASP:OD2 | 2.32 | 0.61 |
| 1:Q:170:MET:HA | 1:Q:170:MET:HE3 | 1.82 | 0.61 |
| 1:R:256:VAL:HG12 | 1:R:258:PHE:CE1 | 2.35 | 0.61 |
| 1:i:158:MET:HE1 | 1:i:160:GLU:HB2 | 1.81 | 0.61 |
| 1:j:162:LYS:HE2 | 1:j:304:HIS:CE1 | 2.36 | 0.61 |
| 1:3:83:ASN:CA | 1:3:305:ARG:HH12 | 2.13 | 0.61 |
| 1:E:344:GLU:OE2 | 1:E:344:GLU:N | 2.24 | 0.61 |
| 1:F:84:GLU:O | 1:F:88:ILE:HG12 | 2.01 | 0.61 |
| 1:M:165:ARG:NE | 1:M:167:ASP:OD1 | 2.33 | 0.61 |
| 1:S:108:GLU:O | 1:S:112:ILE:HG13 | 2.01 | 0.61 |
| 1:s:148:GLN:NE2 | 1:s:150:GLY:O | 2.28 | 0.61 |
| 1:1:159:LEU:HD12 | 1:1:311:PHE:CZ | 2.36 | 0.61 |
| 1:A:222:LEU:O | 1:A:226:ILE:HG13 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:171:MET:HA | 1:E:171:MET:HE3 | 1.83 | 0.61 |
| 1:H:349:THR:O | 1:H:353:ILE:HG12 | 2.00 | 0.61 |
| 1:I:325:ILE:O | 1:I:329:VAL:HG23 | 2.00 | 0.61 |
| 1:V:312:GLN:O | 1:V:316:ASN:ND2 | 2.33 | 0.61 |
| 1:s:92:MET:HG2 | 1:s:119:LEU:HD12 | 1.83 | 0.61 |
| 1:1:68:ALA:O | 1:1:72:ILE:HG12 | 2.01 | 0.61 |
| 1:2:17:TYR:OH | 1:3:30:GLU:OE1 | 2.17 | 0.61 |
| 1:2:52:ASN:O | 1:2:56:VAL:HG23 | 2.00 | 0.61 |
| 1:A:158:MET:HG3 | 1:h:184:LYS:HE3 | 1.83 | 0.61 |
| 1:G:277:ASP:N | 1:G:277:ASP:OD1 | 2.31 | 0.61 |
| 1:P:86:THR:HG22 | 1:P:301:VAL:HG11 | 1.83 | 0.61 |
| 1:U:168:ASN:OD1 | 1:U:171:MET:N | 2.25 | 0.61 |
| 1:l:5:VAL:HB | 1:w:341:PHE:CE1 | 2.36 | 0.61 |
| 1:1:86:THR:OG1 | 1:1:305:ARG:NH2 | 2.34 | 0.60 |
| 1:J:196:LYS:O | 1:J:197:ILE:HD13 | 2.01 | 0.60 |
| 1:N:108:GLU:O | 1:N:112:ILE:HG12 | 2.00 | 0.60 |
| 1:O:159:LEU:HD12 | 1:O:160:GLU:N | 2.15 | 0.60 |
| 1:c:246:PHE:CE1 | 1:c:293:ILE:HD13 | 2.35 | 0.60 |
| 1:2:46:ALA:O | 1:2:50:ILE:HG13 | 2.01 | 0.60 |
| 1:2:221:GLU:N | 1:2:221:GLU:OE2 | 2.34 | 0.60 |
| 1:3:170:MET:HG3 | 1:3:249:ASN:ND2 | 2.16 | 0.60 |
| 1:A:5:VAL:HG13 | 1:K:353:ILE:HD11 | 1.83 | 0.60 |
| 1:D:162:LYS:HD3 | 1:D:162:LYS:N | 2.16 | 0.60 |
| 1:L:324:ASN:ND2 | 1:M:84:GLU:OE2 | 2.34 | 0.60 |
| 1:Q:106:LYS:HA | 1:Q:106:LYS:HE3 | 1.83 | 0.60 |
| 1:k:331:ALA:O | 1:k:334:SER:OG | 2.17 | 0.60 |
| 1:v:138:LEU:HD12 | 1:v:164:MET:HG3 | 1.81 | 0.60 |
| 1:A:149:ILE:O | 1:A:149:ILE:HG12 | 2.02 | 0.60 |
| 1:C:243:LEU:HD12 | 1:C:244:GLN:H | 1.65 | 0.60 |
| 1:H:338:ASP:OD2 | 1:H:339:THR:N | 2.34 | 0.60 |
| 1:V:196:LYS:HB3 | 1:V:208:GLU:OE2 | 2.02 | 0.60 |
| 1:q:25:GLN:O | 1:q:29:MET:HG3 | 2.01 | 0.60 |
| 1:t:108:GLU:H | 1:t:108:GLU:CD | 2.08 | 0.60 |
| 1:w:197:ILE:HG22 | 1:w:209:ILE:HB | 1.83 | 0.60 |
| 1:2:313:ASN:HA | 1:2:316:ASN:ND2 | 2.16 | 0.60 |
| 1:N:104:ASN:O | 1:N:109:ARG:NH2 | 2.34 | 0.60 |
| 1:S:50:ILE:O | 1:S:54:LEU:HG | 2.01 | 0.60 |
| 1:i:93:ARG:HG2 | 1:i:294:ILE:HG21 | 1.83 | 0.60 |
| 1:n:164:MET:HE2 | 1:n:164:MET:HA | 1.83 | 0.60 |
| 1:u:314:ARG:NE | 1:v:122:GLU:OE1 | 2.34 | 0.60 |
| 1:x:29:MET:HA | 1:x:29:MET:HE3 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:218:ASP:OD1 | 1:2:219:ILE:N | 2.34 | 0.60 |
| 1:A:279:ILE:H | 1:A:279:ILE:HD12 | 1.66 | 0.60 |
| 1:p:231:ASP:OD2 | 1:p:251:LYS:NZ | 2.34 | 0.60 |
| 1:u:72:ILE:HG23 | 1:u:312:GLN:HG2 | 1.84 | 0.60 |
| 1:w:63:VAL:O | 1:w:66:ARG:HG2 | 2.01 | 0.60 |
| 1:z:332:SER:O | 1:z:336:ILE:HG12 | 2.02 | 0.60 |
| 1:T:163:ASP:C | 1:T:164:MET:HE2 | 2.26 | 0.60 |
| 1:T:349:THR:O | 1:T:353:ILE:HG12 | 2.02 | 0.60 |
| 1:l:146:SER:HA | 1:l:158:MET:HA | 1.83 | 0.60 |
| 1:n:18:LEU:O | 1:n:22:ASN:ND2 | 2.34 | 0.60 |
| 1:o:86:THR:O | 1:o:90:GLN:HG2 | 2.02 | 0.60 |
| 1:z:53:ARG:O | 1:z:57:GLN:HG3 | 2.01 | 0.60 |
| 1:3:159:LEU:HD12 | 1:3:160:GLU:N | 2.17 | 0.60 |
| 1:c:99:SER:HB2 | 1:c:112:ILE:HG21 | 1.83 | 0.60 |
| 1:3:111:ALA:HA | 1:3:114:GLU:OE2 | 2.02 | 0.60 |
| 1:C:88:ILE:O | 1:C:92:MET:HG3 | 2.02 | 0.60 |
| 1:I:57:GLN:O | 1:I:61:LEU:HD23 | 2.02 | 0.60 |
| 1:O:201:ASP:OD1 | 1:O:202:SER:N | 2.35 | 0.60 |
| 1:P:63:VAL:HG13 | 1:P:66:ARG:HH12 | 1.66 | 0.60 |
| 1:i:125:ARG:NH1 | 1:i:129:THR:HG21 | 2.16 | 0.60 |
| 1:i:300:TYR:HE1 | 1:i:304:HIS:CE1 | 2.20 | 0.60 |
| 1:k:223:ALA:HA | 1:k:226:ILE:HD12 | 1.83 | 0.60 |
| 1:t:159:LEU:HD12 | 1:t:160:GLU:H | 1.67 | 0.60 |
| 1:A:108:GLU:H | 1:A:108:GLU:CD | 2.10 | 0.60 |
| 1:A:143:GLY:HA3 | 1:A:145:LYS:HE2 | 1.84 | 0.60 |
| 1:D:276:VAL:O | 1:D:279:ILE:HG12 | 2.01 | 0.60 |
| 1:L:73:SER:O | 1:L:77:THR:HG23 | 2.02 | 0.60 |
| 1:P:171:MET:N | 1:P:171:MET:SD | 2.75 | 0.60 |
| 1:R:120:ASN:ND2 | 1:R:277:ASP:HA | 2.17 | 0.60 |
| 1:t:315:PHE:O | 1:t:319:ILE:HG13 | 2.02 | 0.60 |
| 1:t:343:LYS:NZ | 1:u:15:GLN:HE22 | 2.00 | 0.60 |
| 1:w:84:GLU:O | 1:w:88:ILE:HD12 | 2.00 | 0.60 |
| 1:w:290:SER:HA | 1:w:293:ILE:HD12 | 1.83 | 0.60 |
| 1:D:170:MET:HE3 | 1:D:250:ASN:HB2 | 1.84 | 0.60 |
| 1:l:46:ALA:O | 1:l:50:ILE:HG13 | 2.02 | 0.60 |
| 1:l:270:GLU:CD | 1:l:271:GLY:H | 2.10 | 0.60 |
| 1:m:68:ALA:O | 1:m:72:ILE:HG13 | 2.02 | 0.60 |
| 1:n:361:ILE:HD11 | 1:z:29:MET:HG3 | 1.84 | 0.60 |
| 1:t:236:SER:HB2 | 1:t:244:GLN:HG3 | 1.84 | 0.60 |
| 1:l:79:GLU:OE1 | 1:p:42:LYS:NZ | 2.35 | 0.59 |
| 1:D:290:SER:O | 1:D:294:ILE:HG13 | 2.01 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:53:ARG:NH2 | 1:m:108:GLU:OE1 | 2.35 | 0.59 |
| 1:E:299:LYS:HD2 | 1:E:299:LYS:O | 2.01 | 0.59 |
| 1:L:122:GLU:O | 1:L:126:ILE:HG13 | 2.02 | 0.59 |
| 1:N:203:TYR:O | 1:N:205:GLN:NE2 | 2.34 | 0.59 |
| 1:r:210:ASN:C | 1:r:211:ILE:HD13 | 2.27 | 0.59 |
| 1:u:112:ILE:O | 1:u:116:VAL:HG23 | 2.02 | 0.59 |
| 1:2:88:ILE:HG22 | 1:2:92:MET:HE2 | 1.84 | 0.59 |
| 1:H:108:GLU:O | 1:H:112:ILE:HG13 | 2.03 | 0.59 |
| 1:K:210:ASN:C | 1:K:211:ILE:HD13 | 2.27 | 0.59 |
| 1:S:209:ILE:HD11 | 1:S:232:LEU:HD23 | 1.83 | 0.59 |
| 1:U:170:MET:HA | 1:U:170:MET:HE3 | 1.82 | 0.59 |
| 1:q:290:SER:O | 1:q:294:ILE:HG12 | 2.02 | 0.59 |
| 1:F:185:ASP:N | 1:F:185:ASP:OD1 | 2.35 | 0.59 |
| 1:M:318:ALA:O | 1:M:322:LEU:HG | 2.03 | 0.59 |
| 1:Q:46:ALA:O | 1:Q:50:ILE:HG12 | 2.03 | 0.59 |
| 1:R:165:ARG:HB3 | 1:R:165:ARG:NH1 | 2.16 | 0.59 |
| 1:p:26:GLN:NE2 | 1:p:26:GLN:O | 2.35 | 0.59 |
| 1:B:38:ILE:HD11 | 1:B:44:ASP:HB3 | 1.84 | 0.59 |
| 1:G:46:ALA:O | 1:G:50:ILE:HG13 | 2.03 | 0.59 |
| 1:N:104:ASN:OD1 | 1:N:108:GLU:HB2 | 2.02 | 0.59 |
| 1:O:30:GLU:OE2 | 1:O:39:ASN:ND2 | 2.32 | 0.59 |
| 1:T:177:GLN:HG2 | 1:T:244:GLN:HG2 | 1.84 | 0.59 |
| 1:l:198:ASN:HB2 | 1:l:257:GLU:HB2 | 1.83 | 0.59 |
| 1:m:163:ASP:OD2 | 1:m:168:ASN:ND2 | 2.35 | 0.59 |
| 1:w:276:VAL:O | 1:w:279:ILE:HG12 | 2.02 | 0.59 |
| 1:1:289:GLU:O | 1:1:293:ILE:HG13 | 2.01 | 0.59 |
| 1:C:117:THR:HA | 1:C:120:ASN:ND2 | 2.18 | 0.59 |
| 1:F:327:GLU:OE1 | 1:Q:16:ARG:NE | 2.33 | 0.59 |
| 1:Q:125:ARG:O | 1:Q:129:THR:HG22 | 2.02 | 0.59 |
| 1:Q:244:GLN:HE22 | 1:Q:285:GLY:HA3 | 1.67 | 0.59 |
| 1:S:162:LYS:HD3 | 1:S:162:LYS:N | 2.18 | 0.59 |
| 1:S:323:ASP:O | 1:S:327:GLU:HG3 | 2.01 | 0.59 |
| 1:n:69:ASN:O | 1:n:72:ILE:HG22 | 2.02 | 0.59 |
| 1:t:345:THR:O | 1:t:349:THR:HG23 | 2.01 | 0.59 |
| 1:z:349:THR:O | 1:z:353:ILE:HG13 | 2.03 | 0.59 |
| 1:D:316:ASN:O | 1:D:319:ILE:HG22 | 2.03 | 0.59 |
| 1:J:125:ARG:O | 1:J:129:THR:HG23 | 2.03 | 0.59 |
| 1:J:239:GLN:NE2 | 1:J:283:SER:HB2 | 2.17 | 0.59 |
| 1:Q:300:TYR:CD1 | 1:Q:304:HIS:HE1 | 2.20 | 0.59 |
| 1:j:232:LEU:HA | 1:j:251:LYS:NZ | 2.17 | 0.59 |
| 1:k:82:MET:HE3 | 1:k:305:ARG:HG2 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:m:272:LYS:HD2 | 1:m:273:LYS:H | 1.66 | 0.59 |
| 1:p:173:GLY:HA3 | 1:p:246:PHE:HE2 | 1.67 | 0.59 |
| 1:B:113:GLN:OE1 | 1:B:117:THR:OG1 | 2.19 | 0.59 |
| 1:C:93:ARG:NH1 | 1:C:295:ASP:OD2 | 2.36 | 0.59 |
| 1:N:285:GLY:O | 1:N:289:GLU:HG2 | 2.01 | 0.59 |
| 1:s:18:LEU:HD13 | 1:s:362:LEU:HD11 | 1.85 | 0.59 |
| 1:u:210:ASN:C | 1:u:211:ILE:HD13 | 2.28 | 0.59 |
| 1:3:192:LYS:HE3 | 1:3:192:LYS:HA | 1.85 | 0.59 |
| 1:A:194:ASP:CG | 1:A:261:GLY:H | 2.10 | 0.59 |
| 1:J:121:ASP:OD1 | 1:J:122:GLU:N | 2.36 | 0.59 |
| 1:h:70:ASP:O | 1:h:74:ILE:HD12 | 2.02 | 0.59 |
| 1:h:155:GLU:OE1 | 1:i:129:THR:HG22 | 2.02 | 0.59 |
| 1:i:349:THR:O | 1:i:353:ILE:HG12 | 2.03 | 0.59 |
| 1:n:267:GLY:O | 1:n:268:LEU:HD23 | 2.03 | 0.59 |
| 1:p:369:PRO:HD2 | 1:p:370:ASN:H | 1.68 | 0.59 |
| 1:w:162:LYS:HE2 | 1:w:304:HIS:CE1 | 2.38 | 0.59 |
| 1:z:325:ILE:O | 1:z:329:VAL:HG12 | 2.03 | 0.59 |
| 1:3:159:LEU:HD12 | 1:3:160:GLU:H | 1.67 | 0.59 |
| 1:E:46:ALA:O | 1:E:50:ILE:HG13 | 2.03 | 0.59 |
| 1:G:111:ALA:HA | 1:G:114:GLU:OE2 | 2.03 | 0.59 |
| 1:H:321:ASN:O | 1:H:325:ILE:HG13 | 2.03 | 0.59 |
| 1:J:290:SER:O | 1:J:294:ILE:HG13 | 2.03 | 0.59 |
| 1:j:290:SER:HA | 1:j:293:ILE:HD12 | 1.85 | 0.59 |
| 1:m:25:GLN:HG2 | 1:m:29:MET:HE2 | 1.84 | 0.59 |
| 1:m:368:ALA:O | 1:m:371:SER:OG | 2.21 | 0.59 |
| 1:p:168:ASN:OD1 | 1:p:170:MET:N | 2.33 | 0.59 |
| 1:B:327:GLU:OE1 | 1:M:16:ARG:NE | 2.34 | 0.59 |
| 1:F:69:ASN:O | 1:F:72:ILE:HG22 | 2.02 | 0.59 |
| 1:H:61:LEU:O | 1:H:65:VAL:HG23 | 2.02 | 0.59 |
| 1:L:349:THR:O | 1:L:353:ILE:HG12 | 2.03 | 0.59 |
| 1:O:290:SER:O | 1:O:293:ILE:HG22 | 2.02 | 0.59 |
| 1:w:289:GLU:O | 1:w:293:ILE:HG13 | 2.02 | 0.59 |
| 1:B:85:THR:HA | 1:B:88:ILE:HD12 | 1.84 | 0.58 |
| 1:F:280:ASP:OD2 | 1:F:282:THR:N | 2.22 | 0.58 |
| 1:N:219:ILE:HG23 | 1:N:237:VAL:HG21 | 1.85 | 0.58 |
| 1:o:25:GLN:HG2 | 1:o:29:MET:HE3 | 1.85 | 0.58 |
| 1:v:363:ALA:HA | 1:v:366:LYS:HD2 | 1.84 | 0.58 |
| 1:A:122:GLU:OE2 | 1:V:314:ARG:NE | 2.36 | 0.58 |
| 1:A:149:ILE:HD13 | 1:B:125:ARG:HH12 | 1.69 | 0.58 |
| 1:D:292:ALA:HA | 1:D:295:ASP:OD1 | 2.03 | 0.58 |
| 1:I:101:ASN:OD1 | 1:I:103:SER:N | 2.34 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:157:VAL:HG21 | 1:I:314:ARG:HH12 | 1.68 | 0.58 |
| 1:c:101:ASN:HB3 | 1:c:104:ASN:HD21 | 1.68 | 0.58 |
| 1:c:301:VAL:O | 1:c:305:ARG:HG3 | 2.03 | 0.58 |
| 1:c:332:SER:O | 1:c:336:ILE:HG13 | 2.02 | 0.58 |
| 1:i:179:GLU:OE2 | 1:i:179:GLU:N | 2.28 | 0.58 |
| 1:n:57:GLN:O | 1:n:61:LEU:HD12 | 2.03 | 0.58 |
| 1:t:246:PHE:HD2 | 1:t:292:ALA:HB1 | 1.67 | 0.58 |
| 1:v:89:LEU:HA | 1:v:92:MET:HE3 | 1.84 | 0.58 |
| 1:x:195:LEU:C | 1:x:196:LYS:HD3 | 2.27 | 0.58 |
| 1:K:108:GLU:OE2 | 1:U:53:ARG:NH2 | 2.33 | 0.58 |
| 1:M:68:ALA:O | 1:M:72:ILE:HG13 | 2.03 | 0.58 |
| 1:O:125:ARG:HE | 1:O:126:ILE:HD13 | 1.68 | 0.58 |
| 1:h:290:SER:O | 1:h:293:ILE:HG22 | 2.04 | 0.58 |
| 1:j:57:GLN:O | 1:j:61:LEU:HD22 | 2.03 | 0.58 |
| 1:j:205:GLN:HG2 | 1:j:206:GLU:N | 2.17 | 0.58 |
| 1:u:218:ASP:HB3 | 1:u:221:GLU:HG3 | 1.84 | 0.58 |
| 1:N:170:MET:SD | 1:N:170:MET:N | 2.76 | 0.58 |
| 1:x:106:LYS:HE2 | 1:x:106:LYS:HA | 1.85 | 0.58 |
| 1:A:226:ILE:O | 1:A:230:THR:HG22 | 2.04 | 0.58 |
| 1:B:31:ARG:HD3 | 1:B:37:LYS:HA | 1.84 | 0.58 |
| 1:D:195:LEU:HD21 | 1:D:262:LEU:HB2 | 1.84 | 0.58 |
| 1:G:83:ASN:OD1 | 1:G:305:ARG:NH2 | 2.36 | 0.58 |
| 1:G:142:HIS:CD2 | 1:G:161:LEU:HD12 | 2.38 | 0.58 |
| 1:K:194:ASP:HB2 | 1:K:196:LYS:HZ3 | 1.68 | 0.58 |
| 1:S:50:ILE:HA | 1:S:53:ARG:NH1 | 2.19 | 0.58 |
| 1:S:240:ASP:HB2 | 1:S:242:LYS:HG3 | 1.84 | 0.58 |
| 1:i:113:GLN:HE22 | 1:i:280:ASP:HA | 1.68 | 0.58 |
| 1:m:231:ASP:OD2 | 1:m:251:LYS:NZ | 2.35 | 0.58 |
| 1:x:323:ASP:O | 1:x:327:GLU:HG2 | 2.03 | 0.58 |
| 1:D:30:GLU:OE1 | 1:D:39:ASN:ND2 | 2.34 | 0.58 |
| 1:E:159:LEU:HD12 | 1:E:160:GLU:N | 2.19 | 0.58 |
| 1:H:57:GLN:O | 1:H:61:LEU:HD23 | 2.03 | 0.58 |
| 1:O:318:ALA:O | 1:O:322:LEU:HG | 2.03 | 0.58 |
| 1:h:246:PHE:HZ | 1:h:293:ILE:HD13 | 1.68 | 0.58 |
| 1:A:177:GLN:OE1 | 1:A:178:ALA:N | 2.36 | 0.58 |
| 1:C:166:SER:HB2 | 1:C:276:VAL:HB | 1.85 | 0.58 |
| 1:F:47:GLY:HA2 | 1:F:50:ILE:HD12 | 1.86 | 0.58 |
| 1:L:25:GLN:HG2 | 1:L:29:MET:CE | 2.33 | 0.58 |
| 1:R:332:SER:O | 1:R:336:ILE:HG13 | 2.04 | 0.58 |
| 1:S:173:GLY:HA3 | 1:S:246:PHE:HE2 | 1.68 | 0.58 |
| 1:T:371:SER:O | 1:T:374:SER:OG | 2.21 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:p:160:GLU:OE1 | 1:p:162:LYS:NZ | 2.33 | 0.58 |
| 1:H:247:ALA:HB1 | 1:H:252:VAL:HG21 | 1.86 | 0.58 |
| 1:I:364:GLN:OE1 | 1:I:364:GLN:N | 2.36 | 0.58 |
| 1:J:340:ASP:HB2 | 1:U:2:ALA:HB1 | 1.83 | 0.58 |
| 1:V:76:GLN:HA | 1:V:76:GLN:NE2 | 2.18 | 0.58 |
| 1:p:83:ASN:HA | 1:p:305:ARG:HH12 | 1.69 | 0.58 |
| 1:r:68:ALA:O | 1:r:72:ILE:HG13 | 2.04 | 0.58 |
| 1:s:84:GLU:O | 1:s:88:ILE:HG13 | 2.03 | 0.58 |
| 1:t:208:GLU:C | 1:t:209:ILE:HD13 | 2.29 | 0.58 |
| 1:u:25:GLN:O | 1:u:29:MET:HG3 | 2.04 | 0.58 |
| 1:w:29:MET:HG3 | 1:w:348:MET:HB2 | 1.85 | 0.58 |
| 1:A:133:GLY:O | 1:V:53:ARG:NH2 | 2.29 | 0.58 |
| 1:H:4:ASN:HB2 | 1:o:338:ASP:CG | 2.27 | 0.58 |
| 1:I:139:ASN:OD1 | 1:I:141:THR:HG22 | 2.03 | 0.58 |
| 1:I:218:ASP:HB3 | 1:I:221:GLU:HG3 | 1.86 | 0.58 |
| 1:L:279:ILE:HG21 | 1:L:290:SER:HA | 1.86 | 0.58 |
| 1:S:73:SER:O | 1:S:77:THR:HG23 | 2.04 | 0.58 |
| 1:j:190:GLU:CD | 1:j:190:GLU:H | 2.12 | 0.58 |
| 1:p:162:LYS:HE2 | 1:p:304:HIS:CE1 | 2.39 | 0.58 |
| 1:p:210:ASN:C | 1:p:211:ILE:HD13 | 2.29 | 0.58 |
| 1:t:341:PHE:O | 1:t:345:THR:HG22 | 2.04 | 0.58 |
| 1:w:9:VAL:HA | 1:w:12:MET:HE1 | 1.86 | 0.58 |
| 1:x:174:VAL:HG23 | 1:x:249:ASN:HD21 | 1.68 | 0.58 |
| 1:J:68:ALA:O | 1:J:72:ILE:HG13 | 2.04 | 0.58 |
| 1:K:170:MET:HE3 | 1:K:300:TYR:HB2 | 1.86 | 0.58 |
| 1:L:234:LYS:HA | 1:L:234:LYS:HE3 | 1.86 | 0.58 |
| 1:R:331:ALA:O | 1:R:334:SER:OG | 2.20 | 0.58 |
| 1:U:88:ILE:HG21 | 1:U:123:LEU:HD21 | 1.86 | 0.58 |
| 1:i:19:ASN:HA | 1:i:22:ASN:HD21 | 1.69 | 0.58 |
| 1:j:179:GLU:OE1 | 1:j:179:GLU:N | 2.34 | 0.58 |
| 1:k:162:LYS:HD3 | 1:k:162:LYS:N | 2.19 | 0.58 |
| 1:u:109:ARG:HB3 | 1:u:282:THR:HA | 1.86 | 0.58 |
| 1:C:173:GLY:HA3 | 1:C:246:PHE:CZ | 2.39 | 0.57 |
| 1:E:63:VAL:HG22 | 1:E:66:ARG:HH22 | 1.68 | 0.57 |
| 1:G:236:SER:OG | 1:R:153:ASN:ND2 | 2.36 | 0.57 |
| 1:O:210:ASN:C | 1:O:211:ILE:HD13 | 2.29 | 0.57 |
| 1:R:108:GLU:O | 1:R:112:ILE:HG13 | 2.04 | 0.57 |
| 1:U:112:ILE:O | 1:U:115:GLU:HG3 | 2.04 | 0.57 |
| 1:k:37:LYS:NZ | 1:k:336:ILE:O | 2.37 | 0.57 |
| 1:m:6:ASN:HA | 1:w:350:LYS:HE3 | 1.86 | 0.57 |
| 1:o:349:THR:O | 1:o:353:ILE:HG12 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:t:79:GLU:HA | 1:t:82:MET:SD | 2.44 | 0.57 |
| 1:v:169:LYS:HD3 | 1:v:169:LYS:N | 2.18 | 0.57 |
| 1:1:27:THR:HG22 | 1:1:31:ARG:HD2 | 1.86 | 0.57 |
| 1:A:173:GLY:HA3 | 1:A:246:PHE:CZ | 2.39 | 0.57 |
| 1:J:48:LEU:HD11 | 1:q:305:ARG:HH21 | 1.70 | 0.57 |
| 1:L:150:GLY:HA3 | 1:L:155:GLU:HB2 | 1.85 | 0.57 |
| 1:n:205:GLN:OE1 | 1:n:205:GLN:N | 2.38 | 0.57 |
| 1:1:98:GLN:HE21 | 1:1:98:GLN:C | 2.12 | 0.57 |
| 1:3:112:ILE:HD11 | 1:q:46:ALA:HB2 | 1.86 | 0.57 |
| 1:D:88:ILE:HG22 | 1:D:92:MET:HE2 | 1.86 | 0.57 |
| 1:H:78:ALA:O | 1:H:82:MET:HG3 | 2.04 | 0.57 |
| 1:P:182:LYS:NZ | 1:P:265:GLU:OE2 | 2.37 | 0.57 |
| 1:l:79:GLU:OE1 | 1:l:305:ARG:HG2 | 2.04 | 0.57 |
| 1:n:185:ASP:OD1 | 1:n:185:ASP:N | 2.38 | 0.57 |
| 1:q:270:GLU:N | 1:q:270:GLU:OE2 | 2.36 | 0.57 |
| 1:x:170:MET:HG3 | 1:x:300:TYR:CE1 | 2.40 | 0.57 |
| 1:3:68:ALA:O | 1:3:72:ILE:HG13 | 2.04 | 0.57 |
| 1:V:159:LEU:HD13 | 1:V:311:PHE:CE2 | 2.39 | 0.57 |
| 1:c:174:VAL:HG22 | 1:c:273:LYS:HD3 | 1.86 | 0.57 |
| 1:c:174:VAL:N | 1:c:247:ALA:O | 2.24 | 0.57 |
| 1:i:321:ASN:O | 1:i:325:ILE:HG12 | 2.05 | 0.57 |
| 1:M:108:GLU:O | 1:M:112:ILE:HG13 | 2.05 | 0.57 |
| 1:O:201:ASP:HB2 | 1:O:207:GLN:OE1 | 2.04 | 0.57 |
| 1:O:213:ALA:C | 1:O:214:LYS:HD3 | 2.29 | 0.57 |
| 1:S:109:ARG:HB3 | 1:S:282:THR:HA | 1.85 | 0.57 |
| 1:S:170:MET:SD | 1:S:170:MET:N | 2.78 | 0.57 |
| 1:m:366:LYS:O | 1:m:369:PRO:HD2 | 2.05 | 0.57 |
| 1:r:315:PHE:O | 1:r:319:ILE:HD12 | 2.04 | 0.57 |
| 1:t:227:ASN:ND2 | 1:t:235:ALA:H | 2.02 | 0.57 |
| 1:w:162:LYS:HG3 | 1:w:304:HIS:CE1 | 2.39 | 0.57 |
| 1:x:46:ALA:O | 1:x:50:ILE:HG12 | 2.04 | 0.57 |
| 1:C:321:ASN:ND2 | 1:D:126:ILE:HG12 | 2.18 | 0.57 |
| 1:C:341:PHE:O | 1:C:345:THR:HG23 | 2.05 | 0.57 |
| 1:D:210:ASN:C | 1:D:211:ILE:HD13 | 2.29 | 0.57 |
| 1:M:18:LEU:O | 1:M:22:ASN:ND2 | 2.38 | 0.57 |
| 1:O:46:ALA:O | 1:O:50:ILE:HG12 | 2.04 | 0.57 |
| 1:Q:144:ALA:HB2 | 1:Q:160:GLU:HG2 | 1.86 | 0.57 |
| 1:j:10:SER:HA | 1:j:13:THR:HG22 | 1.85 | 0.57 |
| 1:l:255:GLU:HG3 | 1:l:256:VAL:H | 1.70 | 0.57 |
| 1:p:37:LYS:NZ | 1:p:336:ILE:O | 2.36 | 0.57 |
| 1:r:144:ALA:C | 1:r:145:LYS:HD3 | 2.29 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:t:189:ALA:O | 1:t:193:ASN:ND2 | 2.37 | 0.57 |
| 1:z:192:LYS:NZ | 1:z:261:GLY:O | 2.32 | 0.57 |
| 1:1:272:LYS:HE2 | 1:1:272:LYS:HA | 1.86 | 0.57 |
| 1:E:50:ILE:O | 1:E:54:LEU:HG | 2.04 | 0.57 |
| 1:L:222:LEU:HD12 | 1:L:226:ILE:HD11 | 1.85 | 0.57 |
| 1:M:137:LEU:HB2 | 1:M:138:LEU:HD22 | 1.86 | 0.57 |
| 1:U:159:LEU:HD12 | 1:U:160:GLU:N | 2.19 | 0.57 |
| 1:o:61:LEU:O | 1:o:65:VAL:HG23 | 2.04 | 0.57 |
| 1:o:69:ASN:O | 1:o:72:ILE:HG22 | 2.03 | 0.57 |
| 1:r:49:GLN:HB3 | 1:r:53:ARG:NH1 | 2.19 | 0.57 |
| 1:w:161:LEU:HA | 1:w:162:LYS:NZ | 2.19 | 0.57 |
| 1:z:290:SER:O | 1:z:294:ILE:HG13 | 2.04 | 0.57 |
| 1:J:4:ASN:O | 1:J:4:ASN:ND2 | 2.26 | 0.57 |
| 1:Q:88:ILE:O | 1:Q:92:MET:HE2 | 2.04 | 0.57 |
| 1:S:193:ASN:HA | 1:S:262:LEU:HD21 | 1.86 | 0.57 |
| 1:U:108:GLU:O | 1:U:112:ILE:HG12 | 2.03 | 0.57 |
| 1:V:170:MET:HE2 | 1:V:300:TYR:HD1 | 1.69 | 0.57 |
| 1:h:5:VAL:HG13 | 1:r:353:ILE:HD11 | 1.86 | 0.57 |
| 1:h:349:THR:O | 1:h:353:ILE:HG12 | 2.05 | 0.57 |
| 1:j:6:ASN:ND2 | 1:u:35:GLY:O | 2.33 | 0.57 |
| 1:k:3:VAL:H | 1:v:340:ASP:HB2 | 1.70 | 0.57 |
| 1:q:163:ASP:C | 1:q:164:MET:HE2 | 2.30 | 0.57 |
| 1:r:166:SER:HA | 1:r:171:MET:HE3 | 1.84 | 0.57 |
| 1:r:225:TYR:CE2 | 1:r:229:GLN:NE2 | 2.73 | 0.57 |
| 1:B:32:LEU:HG | 1:B:344:GLU:HG3 | 1.87 | 0.57 |
| 1:L:178:ALA:HB2 | 1:L:266:LEU:HD22 | 1.87 | 0.57 |
| 1:P:236:SER:HB2 | 1:P:244:GLN:HB2 | 1.87 | 0.57 |
| 1:c:83:ASN:HA | 1:c:305:ARG:HH12 | 1.69 | 0.57 |
| 1:c:345:THR:O | 1:c:349:THR:HG23 | 2.05 | 0.57 |
| 1:i:68:ALA:O | 1:i:72:ILE:HG13 | 2.05 | 0.57 |
| 1:m:125:ARG:NH1 | 1:m:129:THR:HG21 | 2.19 | 0.57 |
| 1:s:49:GLN:O | 1:s:53:ARG:HG3 | 2.05 | 0.57 |
| 1:v:184:LYS:HD2 | 1:v:184:LYS:O | 2.04 | 0.57 |
| 1:v:201:ASP:OD1 | 1:v:202:SER:N | 2.37 | 0.57 |
| 1:v:318:ALA:O | 1:v:322:LEU:HG | 2.04 | 0.57 |
| 1:2:357:ALA:O | 1:2:361:ILE:HG13 | 2.05 | 0.57 |
| 1:A:250:ASN:ND2 | 1:A:296:ALA:HB1 | 2.20 | 0.57 |
| 1:J:248:GLY:HA3 | 1:J:251:LYS:NZ | 2.20 | 0.57 |
| 1:L:8:ASN:ND2 | 1:L:365:ALA:O | 2.36 | 0.57 |
| 1:N:93:ARG:HB2 | 1:N:294:ILE:HG21 | 1.87 | 0.57 |
| 1:O:189:ALA:HB1 | 1:O:192:LYS:HE2 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:63:VAL:HG22 | 1:P:66:ARG:HH22 | 1.69 | 0.57 |
| 1:i:219:ILE:HD11 | 1:i:243:LEU:HD13 | 1.87 | 0.57 |
| 1:k:201:ASP:N | 1:k:205:GLN:O | 2.32 | 0.57 |
| 1:m:318:ALA:O | 1:m:322:LEU:HD22 | 2.05 | 0.57 |
| 1:o:84:GLU:O | 1:o:88:ILE:HG12 | 2.05 | 0.57 |
| 1:p:101:ASN:ND2 | 1:p:103:SER:OG | 2.37 | 0.57 |
| 1:r:25:GLN:HE22 | 1:r:29:MET:HE2 | 1.69 | 0.57 |
| 1:t:65:VAL:HB | 1:t:66:ARG:NH1 | 2.19 | 0.57 |
| 1:z:50:ILE:O | 1:z:54:LEU:HD22 | 2.05 | 0.57 |
| 1:z:122:GLU:O | 1:z:126:ILE:HG13 | 2.04 | 0.57 |
| 1:M:82:MET:HE1 | 1:M:304:HIS:HB3 | 1.86 | 0.56 |
| 1:O:246:PHE:CD2 | 1:O:292:ALA:HB1 | 2.40 | 0.56 |
| 1:P:318:ALA:O | 1:P:322:LEU:HG | 2.05 | 0.56 |
| 1:Q:290:SER:O | 1:Q:293:ILE:HG22 | 2.04 | 0.56 |
| 1:S:45:ALA:O | 1:S:49:GLN:HG3 | 2.05 | 0.56 |
| 1:i:19:ASN:HA | 1:i:22:ASN:ND2 | 2.20 | 0.56 |
| 1:m:89:LEU:HA | 1:m:92:MET:HG3 | 1.87 | 0.56 |
| 1:q:184:LYS:HD2 | 1:q:184:LYS:O | 2.05 | 0.56 |
| 1:u:169:LYS:C | 1:u:169:LYS:HD3 | 2.30 | 0.56 |
| 1:w:325:ILE:O | 1:w:329:VAL:HG22 | 2.04 | 0.56 |
| 1:x:196:LYS:NZ | 1:x:260:GLY:HA3 | 2.20 | 0.56 |
| 1:z:69:ASN:HA | 1:z:72:ILE:HD12 | 1.86 | 0.56 |
| 1:z:168:ASN:HB3 | 1:z:171:MET:HG2 | 1.85 | 0.56 |
| 1:2:164:MET:HE1 | 1:2:304:HIS:CD2 | 2.40 | 0.56 |
| 1:D:153:ASN:HD22 | 1:k:234:LYS:HD2 | 1.68 | 0.56 |
| 1:E:196:LYS:C | 1:E:197:ILE:HD13 | 2.30 | 0.56 |
| 1:E:368:ALA:O | 1:E:371:SER:OG | 2.23 | 0.56 |
| 1:J:46:ALA:O | 1:J:50:ILE:HG13 | 2.04 | 0.56 |
| 1:L:226:ILE:HA | 1:L:229:GLN:NE2 | 2.17 | 0.56 |
| 1:Q:196:LYS:N | 1:Q:259:SER:O | 2.34 | 0.56 |
| 1:U:299:LYS:HD2 | 1:U:299:LYS:C | 2.30 | 0.56 |
| 1:n:85:THR:HA | 1:n:88:ILE:HD12 | 1.86 | 0.56 |
| 1:w:270:GLU:CD | 1:w:271:GLY:H | 2.13 | 0.56 |
| 1:1:249:ASN:HA | 1:1:252:VAL:O | 2.06 | 0.56 |
| 1:2:162:LYS:HD3 | 1:2:162:LYS:N | 2.19 | 0.56 |
| 1:C:46:ALA:O | 1:C:50:ILE:HG12 | 2.05 | 0.56 |
| 1:C:50:ILE:HD11 | 1:k:108:GLU:HG2 | 1.87 | 0.56 |
| 1:C:279:ILE:CG2 | 1:C:290:SER:HB3 | 2.32 | 0.56 |
| 1:E:214:LYS:HD3 | 1:E:214:LYS:N | 2.20 | 0.56 |
| 1:E:327:GLU:OE1 | 1:P:16:ARG:NH1 | 2.33 | 0.56 |
| 1:F:153:ASN:HD21 | 1:m:288:GLN:HB3 | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:162:LYS:HE3 | 1:F:304:HIS:ND1 | 2.20 | 0.56 |
| 1:F:190:GLU:OE2 | 1:F:191:GLY:N | 2.30 | 0.56 |
| 1:F:291:VAL:HA | 1:F:294:ILE:HD12 | 1.86 | 0.56 |
| 1:G:104:ASN:O | 1:G:109:ARG:NH2 | 2.35 | 0.56 |
| 1:J:152:ASP:N | 1:J:155:GLU:OE2 | 2.38 | 0.56 |
| 1:O:69:ASN:O | 1:O:72:ILE:HG22 | 2.05 | 0.56 |
| 1:Q:88:ILE:HG23 | 1:Q:119:LEU:HD23 | 1.86 | 0.56 |
| 1:T:168:ASN:O | 1:T:171:MET:HB2 | 2.05 | 0.56 |
| 1:U:148:GLN:OE1 | 1:U:150:GLY:N | 2.36 | 0.56 |
| 1:U:225:TYR:HD2 | 1:U:226:ILE:HD13 | 1.70 | 0.56 |
| 1:V:38:ILE:HD13 | 1:V:43:ASP:HB2 | 1.88 | 0.56 |
| 1:c:200:THR:OG1 | 1:c:253:GLU:O | 2.24 | 0.56 |
| 1:l:177:GLN:HE22 | 1:l:272:LYS:HB2 | 1.71 | 0.56 |
| 1:q:187:ASN:ND2 | 1:q:216:GLY:O | 2.38 | 0.56 |
| 1:r:82:MET:O | 1:r:85:THR:OG1 | 2.23 | 0.56 |
| 1:s:321:ASN:ND2 | 1:t:126:ILE:HG23 | 2.19 | 0.56 |
| 1:t:92:MET:HA | 1:t:95:LEU:HD12 | 1.87 | 0.56 |
| 1:w:366:LYS:HG3 | 1:w:367:GLN:NE2 | 2.20 | 0.56 |
| 1:z:25:GLN:O | 1:z:28:SER:OG | 2.16 | 0.56 |
| 1:1:61:LEU:O | 1:1:65:VAL:HG23 | 2.05 | 0.56 |
| 1:2:315:PHE:O | 1:2:319:ILE:HG13 | 2.04 | 0.56 |
| 1:G:79:GLU:OE2 | 1:G:305:ARG:NE | 2.38 | 0.56 |
| 1:I:82:MET:HE2 | 1:I:305:ARG:HG2 | 1.88 | 0.56 |
| 1:L:313:ASN:ND2 | 1:M:115:GLU:OE2 | 2.39 | 0.56 |
| 1:N:57:GLN:NE2 | 1:O:133:GLY:HA2 | 2.20 | 0.56 |
| 1:P:333:LYS:HA | 1:P:336:ILE:HD12 | 1.85 | 0.56 |
| 1:m:364:GLN:OE1 | 1:m:364:GLN:N | 2.39 | 0.56 |
| 1:p:348:MET:HE3 | 1:p:352:GLN:OE1 | 2.05 | 0.56 |
| 1:2:312:GLN:HE21 | 1:q:42:LYS:HD3 | 1.71 | 0.56 |
| 1:2:324:ASN:O | 1:2:328:ASN:ND2 | 2.38 | 0.56 |
| 1:L:25:GLN:HG2 | 1:L:29:MET:HE2 | 1.87 | 0.56 |
| 1:M:290:SER:O | 1:M:294:ILE:HG13 | 2.05 | 0.56 |
| 1:U:273:LYS:HD3 | 1:U:273:LYS:N | 2.20 | 0.56 |
| 1:w:299:LYS:HD2 | 1:w:299:LYS:O | 2.06 | 0.56 |
| 1:2:109:ARG:HB3 | 1:2:282:THR:HA | 1.87 | 0.56 |
| 1:A:246:PHE:HZ | 1:A:293:ILE:HD13 | 1.70 | 0.56 |
| 1:A:321:ASN:HD22 | 1:B:126:ILE:HD12 | 1.70 | 0.56 |
| 1:M:196:LYS:NZ | 1:M:198:ASN:OD1 | 2.39 | 0.56 |
| 1:N:195:LEU:HD21 | 1:N:197:ILE:HG12 | 1.87 | 0.56 |
| 1:P:201:ASP:OD1 | 1:P:202:SER:N | 2.39 | 0.56 |
| 1:Q:162:LYS:HZ1 | 1:Q:307:GLU:HB2 | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:v:88:ILE:HG22 | 1:v:92:MET:HE2 | 1.88 | 0.56 |
| 1:w:214:LYS:HD3 | 1:w:214:LYS:N | 2.20 | 0.56 |
| 1:3:79:GLU:OE2 | 1:r:40:SER:HB2 | 2.06 | 0.56 |
| 1:D:222:LEU:HG | 1:D:226:ILE:HD11 | 1.87 | 0.56 |
| 1:E:29:MET:HA | 1:E:29:MET:HE3 | 1.87 | 0.56 |
| 1:G:256:VAL:HG12 | 1:G:258:PHE:CE1 | 2.41 | 0.56 |
| 1:H:179:GLU:OE2 | 1:H:269:GLY:N | 2.39 | 0.56 |
| 1:N:146:SER:HA | 1:N:158:MET:HA | 1.88 | 0.56 |
| 1:O:196:LYS:N | 1:O:196:LYS:HD3 | 2.20 | 0.56 |
| 1:S:162:LYS:HE2 | 1:S:304:HIS:ND1 | 2.21 | 0.56 |
| 1:T:210:ASN:C | 1:T:211:ILE:HD13 | 2.30 | 0.56 |
| 1:V:176:TYR:HB2 | 1:V:245:ILE:HG22 | 1.88 | 0.56 |
| 1:c:319:ILE:HA | 1:c:322:LEU:HD12 | 1.87 | 0.56 |
| 1:m:128:GLU:OE2 | 1:m:165:ARG:NH1 | 2.39 | 0.56 |
| 1:s:310:ALA:HB2 | 1:t:115:GLU:HG2 | 1.88 | 0.56 |
| 1:E:37:LYS:O | 1:E:37:LYS:HD3 | 2.06 | 0.56 |
| 1:L:71:GLY:HA2 | 1:L:74:ILE:HD12 | 1.87 | 0.56 |
| 1:S:171:MET:HB3 | 1:S:276:VAL:HG23 | 1.86 | 0.56 |
| 1:j:210:ASN:C | 1:j:211:ILE:HD13 | 2.30 | 0.56 |
| 1:n:171:MET:O | 1:n:293:ILE:HD11 | 2.05 | 0.56 |
| 1:v:272:LYS:NZ | 1:v:273:LYS:O | 2.39 | 0.56 |
| 1:z:173:GLY:HA3 | 1:z:246:PHE:CE1 | 2.39 | 0.56 |
| 1:z:280:ASP:OD1 | 1:z:282:THR:HG23 | 2.06 | 0.56 |
| 1:B:29:MET:HG3 | 1:B:348:MET:HE3 | 1.87 | 0.56 |
| 1:D:150:GLY:HA3 | 1:D:155:GLU:HB2 | 1.88 | 0.56 |
| 1:F:209:ILE:HG22 | 1:F:211:ILE:HD11 | 1.86 | 0.56 |
| 1:H:190:GLU:N | 1:H:190:GLU:OE2 | 2.39 | 0.56 |
| 1:K:170:MET:SD | 1:K:249:ASN:ND2 | 2.78 | 0.56 |
| 1:K:328:ASN:OD1 | 1:h:76:GLN:NE2 | 2.35 | 0.56 |
| 1:L:31:ARG:HH21 | 1:L:37:LYS:HB2 | 1.70 | 0.56 |
| 1:M:175:SER:HB2 | 1:M:244:GLN:HE21 | 1.70 | 0.56 |
| 1:N:47:GLY:O | 1:N:51:SER:OG | 2.23 | 0.56 |
| 1:S:122:GLU:O | 1:S:126:ILE:HG13 | 2.05 | 0.56 |
| 1:S:270:GLU:OE1 | 1:S:271:GLY:N | 2.39 | 0.56 |
| 1:j:49:GLN:NE2 | 1:j:53:ARG:HE | 2.04 | 0.56 |
| 1:m:142:HIS:CG | 1:m:143:GLY:H | 2.23 | 0.56 |
| 1:n:4:ASN:OD1 | 1:n:6:ASN:N | 2.38 | 0.56 |
| 1:r:50:ILE:HD13 | 1:r:53:ARG:NH2 | 2.21 | 0.56 |
| 1:v:50:ILE:O | 1:v:54:LEU:HG | 2.06 | 0.56 |
| 1:3:89:LEU:HA | 1:3:92:MET:CE | 2.36 | 0.56 |
| 1:M:177:GLN:OE1 | 1:M:242:LYS:HB3 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:249:ASN:HD21 | 1:N:273:LYS:HZ1 | 1.54 | 0.56 |
| 1:P:131:SER:HB3 | 1:P:136:LYS:HD3 | 1.88 | 0.56 |
| 1:P:206:GLU:O | 1:P:207:GLN:NE2 | 2.39 | 0.56 |
| 1:S:272:LYS:HD3 | 1:S:273:LYS:N | 2.21 | 0.56 |
| 1:V:82:MET:O | 1:V:85:THR:OG1 | 2.24 | 0.56 |
| 1:v:304:HIS:HA | 1:v:307:GLU:OE2 | 2.06 | 0.56 |
| 1:l:95:LEU:HB3 | 1:l:112:ILE:HD11 | 1.88 | 0.55 |
| 1:G:218:ASP:HB3 | 1:G:221:GLU:HG3 | 1.88 | 0.55 |
| 1:H:111:ALA:HA | 1:H:114:GLU:OE2 | 2.05 | 0.55 |
| 1:L:218:ASP:OD1 | 1:L:219:ILE:N | 2.40 | 0.55 |
| 1:O:138:LEU:HD23 | 1:O:164:MET:HG3 | 1.87 | 0.55 |
| 1:T:162:LYS:CD | 1:T:163:ASP:H | 2.18 | 0.55 |
| 1:c:37:LYS:NZ | 1:c:336:ILE:O | 2.38 | 0.55 |
| 1:i:108:GLU:H | 1:i:108:GLU:CD | 2.14 | 0.55 |
| 1:j:109:ARG:HB3 | 1:j:282:THR:HA | 1.88 | 0.55 |
| 1:j:199:LEU:HD21 | 1:j:232:LEU:HD23 | 1.88 | 0.55 |
| 1:k:157:VAL:HG21 | 1:k:314:ARG:NH2 | 2.17 | 0.55 |
| 1:l:49:GLN:O | 1:l:53:ARG:HG3 | 2.06 | 0.55 |
| 1:q:223:ALA:HA | 1:q:226:ILE:HD12 | 1.88 | 0.55 |
| 1:z:61:LEU:O | 1:z:65:VAL:HG23 | 2.07 | 0.55 |
| 1:z:159:LEU:HD12 | 1:z:160:GLU:N | 2.21 | 0.55 |
| 1:l:219:ILE:HD11 | 1:l:243:LEU:HD12 | 1.87 | 0.55 |
| 1:A:246:PHE:CZ | 1:A:293:ILE:HD13 | 2.42 | 0.55 |
| 1:D:90:GLN:NE2 | 1:O:56:VAL:HB | 2.20 | 0.55 |
| 1:E:164:MET:HA | 1:E:164:MET:HE3 | 1.87 | 0.55 |
| 1:M:121:ASP:HA | 1:M:124:ASN:HD22 | 1.71 | 0.55 |
| 1:O:350:LYS:NZ | 1:P:6:ASN:OD1 | 2.35 | 0.55 |
| 1:S:161:LEU:C | 1:S:162:LYS:HD3 | 2.31 | 0.55 |
| 1:V:91:ARG:HH22 | 1:V:95:LEU:HD21 | 1.70 | 0.55 |
| 1:c:357:ALA:O | 1:c:361:ILE:HG12 | 2.06 | 0.55 |
| 1:i:160:GLU:OE1 | 1:i:162:LYS:NZ | 2.27 | 0.55 |
| 1:k:361:ILE:HD11 | 1:w:30:GLU:OE1 | 2.06 | 0.55 |
| 1:l:210:ASN:C | 1:l:211:ILE:HD13 | 2.30 | 0.55 |
| 1:n:193:ASN:HA | 1:n:262:LEU:HD21 | 1.87 | 0.55 |
| 1:q:210:ASN:C | 1:q:211:ILE:HD12 | 2.31 | 0.55 |
| 1:A:316:ASN:O | 1:A:319:ILE:HG22 | 2.07 | 0.55 |
| 1:G:69:ASN:HA | 1:G:72:ILE:HG22 | 1.88 | 0.55 |
| 1:J:25:GLN:HE22 | 1:J:29:MET:HE3 | 1.72 | 0.55 |
| 1:N:168:ASN:HB3 | 1:N:171:MET:HE2 | 1.87 | 0.55 |
| 1:R:188:VAL:HG11 | 1:R:216:GLY:H | 1.71 | 0.55 |
| 1:i:75:ALA:HB1 | 1:i:312:GLN:HE21 | 1.70 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:k:69:ASN:O | 1:k:72:ILE:HG22 | 2.06 | 0.55 |
| 1:n:173:GLY:HA3 | 1:n:246:PHE:CZ | 2.42 | 0.55 |
| 1:o:316:ASN:HA | 1:o:319:ILE:HD12 | 1.88 | 0.55 |
| 1:s:162:LYS:HE2 | 1:s:304:HIS:ND1 | 2.21 | 0.55 |
| 1:t:93:ARG:HG2 | 1:t:294:ILE:HG21 | 1.89 | 0.55 |
| 1:u:325:ILE:O | 1:u:329:VAL:HG12 | 2.07 | 0.55 |
| 1:w:346:THR:O | 1:w:349:THR:N | 2.39 | 0.55 |
| 1:x:128:GLU:OE2 | 1:x:165:ARG:NH1 | 2.39 | 0.55 |
| 1:z:201:ASP:OD2 | 1:z:203:TYR:N | 2.39 | 0.55 |
| 1:2:61:LEU:HD23 | 1:2:151:ALA:HB2 | 1.88 | 0.55 |
| 1:2:68:ALA:O | 1:2:72:ILE:HG13 | 2.05 | 0.55 |
| 1:B:69:ASN:O | 1:B:72:ILE:HG22 | 2.06 | 0.55 |
| 1:D:161:LEU:C | 1:D:162:LYS:HD3 | 2.31 | 0.55 |
| 1:E:314:ARG:NH2 | 1:F:121:ASP:OD2 | 2.39 | 0.55 |
| 1:G:146:SER:HA | 1:G:158:MET:HA | 1.86 | 0.55 |
| 1:G:199:LEU:HB3 | 1:G:256:VAL:HG22 | 1.89 | 0.55 |
| 1:J:197:ILE:HG22 | 1:J:209:ILE:HD13 | 1.87 | 0.55 |
| 1:K:170:MET:HA | 1:K:249:ASN:HD21 | 1.71 | 0.55 |
| 1:L:222:LEU:O | 1:L:226:ILE:HG12 | 2.07 | 0.55 |
| 1:Q:284:VAL:O | 1:Q:288:GLN:NE2 | 2.22 | 0.55 |
| 1:Q:300:TYR:CG | 1:Q:304:HIS:HE1 | 2.23 | 0.55 |
| 1:S:171:MET:N | 1:S:171:MET:HE2 | 2.21 | 0.55 |
| 1:S:176:TYR:O | 1:S:245:ILE:N | 2.34 | 0.55 |
| 1:T:364:GLN:N | 1:T:364:GLN:OE1 | 2.40 | 0.55 |
| 1:m:46:ALA:O | 1:m:50:ILE:HG13 | 2.06 | 0.55 |
| 1:n:38:ILE:HG23 | 1:n:43:ASP:HB2 | 1.87 | 0.55 |
| 1:p:373:LEU:HD11 | 1:z:353:ILE:HG23 | 1.88 | 0.55 |
| 1:s:358:SER:O | 1:s:362:LEU:HG | 2.06 | 0.55 |
| 1:v:78:ALA:O | 1:v:82:MET:HG3 | 2.06 | 0.55 |
| 1:w:37:LYS:HZ1 | 1:w:339:THR:HA | 1.72 | 0.55 |
| 1:x:55:ASN:OD1 | 1:x:56:VAL:N | 2.40 | 0.55 |
| 1:z:108:GLU:H | 1:z:108:GLU:CD | 2.14 | 0.55 |
| 1:2:305:ARG:HH12 | 1:q:48:LEU:HD11 | 1.72 | 0.55 |
| 1:C:138:LEU:HD12 | 1:C:164:MET:HG3 | 1.88 | 0.55 |
| 1:D:220:GLU:O | 1:D:224:THR:HG23 | 2.06 | 0.55 |
| 1:F:331:ALA:O | 1:F:334:SER:OG | 2.25 | 0.55 |
| 1:G:208:GLU:C | 1:G:209:ILE:HD13 | 2.32 | 0.55 |
| 1:M:232:LEU:HD23 | 1:M:251:LYS:HE3 | 1.88 | 0.55 |
| 1:P:349:THR:O | 1:P:353:ILE:HG12 | 2.07 | 0.55 |
| 1:R:65:VAL:HG13 | 1:R:319:ILE:HG23 | 1.86 | 0.55 |
| 1:S:272:LYS:HD3 | 1:S:273:LYS:H | 1.71 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:n:366:LYS:HE2 | 1:x:346:THR:HA | 1.88 | 0.55 |
| 1:o:350:LYS:O | 1:o:354:LEU:HD22 | 2.07 | 0.55 |
| 1:s:359:SER:HA | 1:s:362:LEU:HD12 | 1.88 | 0.55 |
| 1:z:72:ILE:HG23 | 1:z:312:GLN:HG2 | 1.88 | 0.55 |
| 1:1:73:SER:OG | 1:z:335:ARG:NH1 | 2.40 | 0.55 |
| 1:2:353:ILE:HD13 | 1:r:373:LEU:HB2 | 1.88 | 0.55 |
| 1:3:88:ILE:O | 1:3:92:MET:HE2 | 2.06 | 0.55 |
| 1:B:119:LEU:O | 1:B:123:LEU:HD12 | 2.07 | 0.55 |
| 1:H:91:ARG:HH12 | 1:H:95:LEU:CD2 | 2.18 | 0.55 |
| 1:H:214:LYS:HD3 | 1:T:165:ARG:NH2 | 2.21 | 0.55 |
| 1:K:31:ARG:HE | 1:K:37:LYS:HA | 1.70 | 0.55 |
| 1:P:196:LYS:NZ | 1:P:210:ASN:OD1 | 2.32 | 0.55 |
| 1:P:196:LYS:C | 1:P:197:ILE:HD13 | 2.31 | 0.55 |
| 1:Q:40:SER:OG | 1:Q:42:LYS:NZ | 2.39 | 0.55 |
| 1:R:220:GLU:OE1 | 1:c:158:MET:HB2 | 2.06 | 0.55 |
| 1:c:321:ASN:O | 1:c:325:ILE:HG13 | 2.06 | 0.55 |
| 1:n:198:ASN:HB2 | 1:n:257:GLU:OE2 | 2.07 | 0.55 |
| 1:r:50:ILE:HD13 | 1:r:53:ARG:HH21 | 1.71 | 0.55 |
| 1:s:339:THR:HG23 | 1:s:344:GLU:OE1 | 2.06 | 0.55 |
| 1:u:150:GLY:HA3 | 1:u:155:GLU:HB2 | 1.89 | 0.55 |
| 1:v:315:PHE:O | 1:v:319:ILE:HG13 | 2.06 | 0.55 |
| 1:v:321:ASN:O | 1:v:325:ILE:HG12 | 2.06 | 0.55 |
| 1:I:50:ILE:O | 1:I:54:LEU:HG | 2.05 | 0.55 |
| 1:J:108:GLU:O | 1:J:112:ILE:HG13 | 2.07 | 0.55 |
| 1:M:88:ILE:O | 1:M:92:MET:HG3 | 2.05 | 0.55 |
| 1:O:350:LYS:NZ | 1:P:6:ASN:O | 2.36 | 0.55 |
| 1:V:214:LYS:HE3 | 1:V:217:ASP:OD1 | 2.07 | 0.55 |
| 1:c:123:LEU:HA | 1:c:126:ILE:HG12 | 1.89 | 0.55 |
| 1:k:160:GLU:HG3 | 1:v:184:LYS:HE2 | 1.87 | 0.55 |
| 1:o:203:TYR:HB2 | 1:o:205:GLN:OE1 | 2.07 | 0.55 |
| 1:p:150:GLY:HA3 | 1:p:155:GLU:HB2 | 1.89 | 0.55 |
| 1:z:31:ARG:HB2 | 1:z:344:GLU:OE2 | 2.07 | 0.55 |
| 1:z:321:ASN:OD1 | 1:z:325:ILE:HD11 | 2.07 | 0.55 |
| 1:3:206:GLU:N | 1:3:206:GLU:OE2 | 2.40 | 0.55 |
| 1:C:179:GLU:CD | 1:C:179:GLU:H | 2.15 | 0.55 |
| 1:C:199:LEU:HD21 | 1:C:232:LEU:HD23 | 1.89 | 0.55 |
| 1:C:243:LEU:HD23 | 1:C:266:LEU:HD11 | 1.87 | 0.55 |
| 1:G:84:GLU:O | 1:G:88:ILE:HG13 | 2.06 | 0.55 |
| 1:H:194:ASP:OD1 | 1:H:195:LEU:N | 2.40 | 0.55 |
| 1:H:258:PHE:CD2 | 1:H:268:LEU:HD13 | 2.37 | 0.55 |
| 1:I:373:LEU:HA | 1:I:376:LEU:HD23 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:195:LEU:C | 1:K:196:LYS:HD3 | 2.32 | 0.55 |
| 1:N:159:LEU:HD12 | 1:N:160:GLU:H | 1.70 | 0.55 |
| 1:P:208:GLU:C | 1:P:209:ILE:HD13 | 2.32 | 0.55 |
| 1:h:82:MET:O | 1:h:85:THR:OG1 | 2.22 | 0.55 |
| 1:n:162:LYS:HG3 | 1:n:304:HIS:CE1 | 2.42 | 0.55 |
| 1:q:313:ASN:HA | 1:q:316:ASN:ND2 | 2.22 | 0.55 |
| 1:v:201:ASP:HB2 | 1:v:207:GLN:OE1 | 2.07 | 0.55 |
| 1:3:231:ASP:OD1 | 1:3:232:LEU:N | 2.40 | 0.55 |
| 1:B:93:ARG:HG2 | 1:B:294:ILE:HG21 | 1.88 | 0.55 |
| 1:C:52:ASN:OD1 | 1:C:53:ARG:N | 2.40 | 0.55 |
| 1:E:61:LEU:HD23 | 1:E:151:ALA:HB2 | 1.89 | 0.55 |
| 1:M:169:LYS:HD3 | 1:M:169:LYS:N | 2.21 | 0.55 |
| 1:R:199:LEU:HB3 | 1:R:256:VAL:HG22 | 1.88 | 0.55 |
| 1:S:47:GLY:HA2 | 1:S:50:ILE:HD12 | 1.89 | 0.55 |
| 1:h:25:GLN:HG2 | 1:h:29:MET:HE3 | 1.89 | 0.55 |
| 1:p:350:LYS:HE3 | 1:q:6:ASN:HA | 1.88 | 0.55 |
| 1:u:162:LYS:N | 1:u:162:LYS:HD3 | 2.22 | 0.55 |
| 1:w:29:MET:N | 1:w:29:MET:SD | 2.80 | 0.55 |
| 1:w:210:ASN:C | 1:w:211:ILE:HD13 | 2.32 | 0.55 |
| 1:2:93:ARG:HE | 1:2:291:VAL:HG13 | 1.72 | 0.55 |
| 1:3:71:GLY:HA2 | 1:3:74:ILE:HD12 | 1.89 | 0.55 |
| 1:A:91:ARG:HH22 | 1:A:95:LEU:HD21 | 1.70 | 0.55 |
| 1:G:196:LYS:C | 1:G:197:ILE:HD13 | 2.31 | 0.55 |
| 1:H:139:ASN:O | 1:H:165:ARG:NH1 | 2.40 | 0.55 |
| 1:H:169:LYS:H | 1:H:169:LYS:HD2 | 1.72 | 0.55 |
| 1:S:300:TYR:CE1 | 1:S:304:HIS:CD2 | 2.95 | 0.55 |
| 1:U:115:GLU:O | 1:U:119:LEU:HD13 | 2.07 | 0.55 |
| 1:i:67:ASN:HB3 | 1:t:101:ASN:HD22 | 1.71 | 0.55 |
| 1:i:159:LEU:HD13 | 1:i:311:PHE:CD2 | 2.41 | 0.55 |
| 1:k:109:ARG:HA | 1:k:112:ILE:HD12 | 1.88 | 0.55 |
| 1:k:165:ARG:HH21 | 1:u:214:LYS:HE3 | 1.72 | 0.55 |
| 1:l:16:ARG:NH2 | 1:w:327:GLU:OE2 | 2.28 | 0.55 |
| 1:m:162:LYS:N | 1:m:162:LYS:HD3 | 2.22 | 0.55 |
| 1:q:170:MET:HE3 | 1:q:170:MET:HA | 1.88 | 0.55 |
| 1:r:46:ALA:O | 1:r:50:ILE:HG12 | 2.07 | 0.55 |
| 1:s:182:LYS:NZ | 1:s:265:GLU:OE2 | 2.35 | 0.55 |
| 1:u:287:ALA:O | 1:u:290:SER:OG | 2.20 | 0.55 |
| 1:v:149:ILE:HG21 | 1:v:315:PHE:HE2 | 1.72 | 0.55 |
| 1:1:339:THR:OG1 | 1:1:344:GLU:OE1 | 2.22 | 0.54 |
| 1:3:147:PHE:CE1 | 1:3:159:LEU:HD23 | 2.42 | 0.54 |
| 1:O:195:LEU:C | 1:O:196:LYS:HD3 | 2.32 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:348:MET:HE3 | 1:Q:352:GLN:HE22 | 1.72 | 0.54 |
| 1:T:222:LEU:O | 1:T:226:ILE:HG13 | 2.08 | 0.54 |
| 1:T:257:GLU:N | 1:T:257:GLU:OE2 | 2.41 | 0.54 |
| 1:V:61:LEU:HD23 | 1:V:151:ALA:HB2 | 1.89 | 0.54 |
| 1:V:172:GLY:O | 1:V:249:ASN:ND2 | 2.29 | 0.54 |
| 1:j:222:LEU:O | 1:j:226:ILE:HG12 | 2.07 | 0.54 |
| 1:j:315:PHE:O | 1:j:319:ILE:HG13 | 2.08 | 0.54 |
| 1:t:69:ASN:HA | 1:t:72:ILE:HD12 | 1.88 | 0.54 |
| 1:u:93:ARG:NE | 1:u:295:ASP:OD1 | 2.34 | 0.54 |
| 1:v:64:ALA:HB1 | 1:v:149:ILE:O | 2.07 | 0.54 |
| 1:v:173:GLY:HA3 | 1:v:246:PHE:CZ | 2.41 | 0.54 |
| 1:w:122:GLU:OE2 | 1:w:125:ARG:NH2 | 2.40 | 0.54 |
| 1:1:78:ALA:O | 1:1:82:MET:HG3 | 2.07 | 0.54 |
| 1:1:210:ASN:C | 1:1:211:ILE:HD13 | 2.32 | 0.54 |
| 1:2:47:GLY:HA2 | 1:2:50:ILE:HD12 | 1.89 | 0.54 |
| 1:3:37:LYS:NZ | 1:3:336:ILE:O | 2.41 | 0.54 |
| 1:3:59:ARG:CZ | 1:3:59:ARG:HB2 | 2.38 | 0.54 |
| 1:J:331:ALA:O | 1:J:334:SER:OG | 2.18 | 0.54 |
| 1:O:149:ILE:HG21 | 1:O:315:PHE:HE2 | 1.72 | 0.54 |
| 1:P:61:LEU:HD22 | 1:P:151:ALA:HB2 | 1.90 | 0.54 |
| 1:V:290:SER:O | 1:V:293:ILE:HG22 | 2.07 | 0.54 |
| 1:j:357:ALA:O | 1:j:361:ILE:HG13 | 2.07 | 0.54 |
| 1:k:105:SER:OG | 1:k:108:GLU:OE1 | 2.20 | 0.54 |
| 1:r:319:ILE:HA | 1:r:322:LEU:HD12 | 1.89 | 0.54 |
| 1:r:350:LYS:O | 1:r:354:LEU:HD22 | 2.08 | 0.54 |
| 1:t:218:ASP:HB3 | 1:t:221:GLU:HG3 | 1.88 | 0.54 |
| 1:3:88:ILE:HG23 | 1:3:119:LEU:HD22 | 1.90 | 0.54 |
| 1:B:314:ARG:HH21 | 1:j:121:ASP:C | 2.15 | 0.54 |
| 1:E:299:LYS:HD2 | 1:E:299:LYS:C | 2.32 | 0.54 |
| 1:L:85:THR:O | 1:L:89:LEU:HG | 2.07 | 0.54 |
| 1:P:198:ASN:HD22 | 1:P:257:GLU:HB2 | 1.72 | 0.54 |
| 1:i:210:ASN:C | 1:i:211:ILE:HD12 | 2.32 | 0.54 |
| 1:l:291:VAL:HA | 1:l:294:ILE:HD12 | 1.89 | 0.54 |
| 1:m:12:MET:HA | 1:m:15:GLN:NE2 | 2.22 | 0.54 |
| 1:p:163:ASP:C | 1:p:164:MET:HE2 | 2.32 | 0.54 |
| 1:p:367:GLN:OE1 | 1:p:370:ASN:ND2 | 2.26 | 0.54 |
| 1:q:197:ILE:HB | 1:q:209:ILE:HB | 1.88 | 0.54 |
| 1:x:84:GLU:HA | 1:x:87:ASN:OD1 | 2.08 | 0.54 |
| 1:B:159:LEU:HD22 | 1:B:311:PHE:CZ | 2.42 | 0.54 |
| 1:C:332:SER:O | 1:C:336:ILE:HD12 | 2.06 | 0.54 |
| 1:F:316:ASN:O | 1:F:319:ILE:HG22 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:371:SER:O | 1:G:374:SER:OG | 2.25 | 0.54 |
| 1:H:328:ASN:OD1 | 1:I:76:GLN:NE2 | 2.32 | 0.54 |
| 1:I:193:ASN:HA | 1:I:262:LEU:HD21 | 1.90 | 0.54 |
| 1:S:274:VAL:HG21 | 1:S:289:GLU:OE2 | 2.06 | 0.54 |
| 1:V:30:GLU:OE1 | 1:V:39:ASN:ND2 | 2.41 | 0.54 |
| 1:t:326:ASN:O | 1:t:330:ASN:ND2 | 2.40 | 0.54 |
| 1:x:50:ILE:O | 1:x:54:LEU:HG | 2.08 | 0.54 |
| 1:z:71:GLY:HA2 | 1:z:74:ILE:HD12 | 1.89 | 0.54 |
| 1:z:150:GLY:HA3 | 1:z:155:GLU:HB2 | 1.87 | 0.54 |
| 1:1:162:LYS:HD2 | 1:1:304:HIS:CE1 | 2.41 | 0.54 |
| 1:2:70:ASP:O | 1:2:73:SER:OG | 2.24 | 0.54 |
| 1:3:276:VAL:O | 1:3:279:ILE:HG12 | 2.08 | 0.54 |
| 1:D:195:LEU:CD2 | 1:D:262:LEU:HB2 | 2.37 | 0.54 |
| 1:D:218:ASP:OD2 | 1:D:219:ILE:N | 2.40 | 0.54 |
| 1:E:211:ILE:HG21 | 1:E:226:ILE:HD13 | 1.89 | 0.54 |
| 1:G:79:GLU:O | 1:G:83:ASN:ND2 | 2.39 | 0.54 |
| 1:I:238:ASP:OD1 | 1:I:242:LYS:HB2 | 2.08 | 0.54 |
| 1:M:210:ASN:C | 1:M:211:ILE:HD13 | 2.33 | 0.54 |
| 1:P:113:GLN:OE1 | 1:P:282:THR:HG23 | 2.08 | 0.54 |
| 1:P:150:GLY:HA3 | 1:P:155:GLU:HB2 | 1.89 | 0.54 |
| 1:U:93:ARG:NH1 | 1:U:295:ASP:OD1 | 2.41 | 0.54 |
| 1:U:357:ALA:O | 1:U:361:ILE:HG12 | 2.07 | 0.54 |
| 1:c:91:ARG:NH1 | 1:c:94:ASP:OD1 | 2.36 | 0.54 |
| 1:c:137:LEU:O | 1:c:142:HIS:HB2 | 2.07 | 0.54 |
| 1:i:32:LEU:HD21 | 1:i:344:GLU:HB3 | 1.89 | 0.54 |
| 1:m:316:ASN:O | 1:m:319:ILE:HG22 | 2.07 | 0.54 |
| 1:n:14:ALA:HB3 | 1:n:362:LEU:HD13 | 1.90 | 0.54 |
| 1:t:170:MET:HE2 | 1:t:170:MET:HA | 1.89 | 0.54 |
| 1:x:143:GLY:HA3 | 1:x:145:LYS:HE3 | 1.90 | 0.54 |
| 1:3:290:SER:O | 1:3:293:ILE:HG22 | 2.08 | 0.54 |
| 1:C:243:LEU:HD12 | 1:C:244:GLN:N | 2.23 | 0.54 |
| 1:D:50:ILE:O | 1:D:54:LEU:HG | 2.08 | 0.54 |
| 1:H:184:LYS:HD2 | 1:S:158:MET:HG2 | 1.90 | 0.54 |
| 1:I:49:GLN:NE2 | 1:p:302:ASP:HB2 | 2.23 | 0.54 |
| 1:J:210:ASN:C | 1:J:211:ILE:HD13 | 2.33 | 0.54 |
| 1:K:233:VAL:HG23 | 1:K:245:ILE:HD11 | 1.89 | 0.54 |
| 1:M:272:LYS:NZ | 1:M:273:LYS:H | 2.06 | 0.54 |
| 1:P:262:LEU:O | 1:P:266:LEU:HG | 2.08 | 0.54 |
| 1:V:214:LYS:HD2 | 1:V:215:ALA:N | 2.21 | 0.54 |
| 1:j:68:ALA:O | 1:j:72:ILE:HG13 | 2.07 | 0.54 |
| 1:j:198:ASN:ND2 | 1:j:208:GLU:OE2 | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:k:160:GLU:OE2 | 1:k:161:LEU:N | 2.40 | 0.54 |
| 1:k:228:GLY:HA2 | 1:l:136:LYS:HZ2 | 1.72 | 0.54 |
| 1:l:3:VAL:CG1 | 1:w:342:ALA:HB2 | 2.37 | 0.54 |
| 1:m:52:ASN:O | 1:m:56:VAL:HG23 | 2.08 | 0.54 |
| 1:m:218:ASP:OD2 | 1:m:219:ILE:N | 2.40 | 0.54 |
| 1:o:276:VAL:O | 1:o:279:ILE:HG12 | 2.07 | 0.54 |
| 1:q:69:ASN:O | 1:q:72:ILE:HG22 | 2.08 | 0.54 |
| 1:t:46:ALA:O | 1:t:50:ILE:HG13 | 2.06 | 0.54 |
| 1:t:243:LEU:HD13 | 1:t:266:LEU:HD11 | 1.90 | 0.54 |
| 1:2:148:GLN:NE2 | 1:2:150:GLY:O | 2.38 | 0.54 |
| 1:F:66:ARG:HA | 1:F:69:ASN:HD22 | 1.72 | 0.54 |
| 1:F:350:LYS:NZ | 1:R:6:ASN:O | 2.40 | 0.54 |
| 1:G:153:ASN:OD1 | 1:G:154:GLY:N | 2.41 | 0.54 |
| 1:G:349:THR:O | 1:G:353:ILE:HG23 | 2.07 | 0.54 |
| 1:J:125:ARG:HD3 | 1:T:314:ARG:HH21 | 1.73 | 0.54 |
| 1:M:166:SER:HB2 | 1:M:276:VAL:HG23 | 1.89 | 0.54 |
| 1:O:316:ASN:O | 1:O:319:ILE:HG22 | 2.08 | 0.54 |
| 1:R:54:LEU:CD1 | 1:R:329:VAL:HG13 | 2.37 | 0.54 |
| 1:k:3:VAL:HG11 | 1:v:341:PHE:HB2 | 1.90 | 0.54 |
| 1:n:272:LYS:HB2 | 1:n:272:LYS:NZ | 2.22 | 0.54 |
| 1:o:290:SER:O | 1:o:294:ILE:HD12 | 2.08 | 0.54 |
| 1:q:336:ILE:HD12 | 1:q:336:ILE:H | 1.71 | 0.54 |
| 1:w:36:PHE:C | 1:w:339:THR:HG23 | 2.32 | 0.54 |
| 1:z:57:GLN:O | 1:z:61:LEU:HD22 | 2.08 | 0.54 |
| 1:F:272:LYS:HB2 | 1:F:272:LYS:NZ | 2.21 | 0.54 |
| 1:I:316:ASN:O | 1:I:319:ILE:HG22 | 2.07 | 0.54 |
| 1:S:176:TYR:N | 1:S:245:ILE:O | 2.36 | 0.54 |
| 1:U:290:SER:O | 1:U:294:ILE:HG13 | 2.08 | 0.54 |
| 1:m:287:ALA:O | 1:m:291:VAL:HG12 | 2.07 | 0.54 |
| 1:u:279:ILE:CG2 | 1:u:290:SER:HB3 | 2.38 | 0.54 |
| 1:l:25:GLN:OE1 | 1:z:364:GLN:NE2 | 2.41 | 0.54 |
| 1:2:38:ILE:HD11 | 1:2:48:LEU:HB2 | 1.90 | 0.54 |
| 1:J:162:LYS:HG2 | 1:J:304:HIS:NE2 | 2.23 | 0.54 |
| 1:P:50:ILE:O | 1:P:54:LEU:HG | 2.08 | 0.54 |
| 1:P:159:LEU:HD12 | 1:P:160:GLU:N | 2.23 | 0.54 |
| 1:P:222:LEU:O | 1:P:226:ILE:HG12 | 2.08 | 0.54 |
| 1:R:201:ASP:CG | 1:R:203:TYR:HD1 | 2.16 | 0.54 |
| 1:T:190:GLU:OE2 | 1:T:190:GLU:N | 2.24 | 0.54 |
| 1:h:315:PHE:O | 1:h:319:ILE:HG13 | 2.08 | 0.54 |
| 1:i:321:ASN:ND2 | 1:u:126:ILE:HG23 | 2.23 | 0.54 |
| 1:o:153:ASN:OD1 | 1:o:154:GLY:N | 2.41 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:r:111:ALA:O | 1:r:114:GLU:HG2 | 2.08 | 0.54 |
| 1:s:246:PHE:HD2 | 1:s:247:ALA:N | 2.06 | 0.54 |
| 1:v:57:GLN:O | 1:v:61:LEU:HG | 2.08 | 0.54 |
| 1:z:84:GLU:O | 1:z:88:ILE:HG12 | 2.07 | 0.54 |
| 1:2:150:GLY:HA3 | 1:2:155:GLU:HB2 | 1.90 | 0.54 |
| 1:3:210:ASN:O | 1:3:211:ILE:HD13 | 2.08 | 0.54 |
| 1:O:149:ILE:HG21 | 1:O:315:PHE:CE2 | 2.43 | 0.54 |
| 1:h:280:ASP:OD1 | 1:h:282:THR:HG23 | 2.07 | 0.54 |
| 1:j:79:GLU:HA | 1:j:82:MET:HG3 | 1.89 | 0.54 |
| 1:p:168:ASN:O | 1:p:171:MET:HB2 | 2.07 | 0.54 |
| 1:3:138:LEU:HB3 | 1:3:164:MET:HG3 | 1.89 | 0.53 |
| 1:D:300:TYR:O | 1:D:304:HIS:ND1 | 2.39 | 0.53 |
| 1:E:84:GLU:OE1 | 1:O:320:SER:HB2 | 2.08 | 0.53 |
| 1:E:109:ARG:HH12 | 1:E:284:VAL:HG22 | 1.73 | 0.53 |
| 1:F:181:GLY:C | 1:F:182:LYS:HD3 | 2.34 | 0.53 |
| 1:N:318:ALA:O | 1:N:322:LEU:HG | 2.08 | 0.53 |
| 1:S:162:LYS:HE2 | 1:S:304:HIS:CE1 | 2.43 | 0.53 |
| 1:c:201:ASP:HA | 1:c:252:VAL:HA | 1.90 | 0.53 |
| 1:l:340:ASP:O | 1:l:344:GLU:HG2 | 2.09 | 0.53 |
| 1:m:250:ASN:HD21 | 1:m:296:ALA:HB1 | 1.73 | 0.53 |
| 1:t:238:ASP:OD2 | 1:t:244:GLN:NE2 | 2.41 | 0.53 |
| 1:x:122:GLU:O | 1:x:126:ILE:HG13 | 2.08 | 0.53 |
| 1:x:287:ALA:O | 1:x:290:SER:OG | 2.21 | 0.53 |
| 1:A:214:LYS:N | 1:A:214:LYS:HD2 | 2.24 | 0.53 |
| 1:I:122:GLU:O | 1:I:126:ILE:HG13 | 2.08 | 0.53 |
| 1:J:4:ASN:C | 1:J:4:ASN:ND2 | 2.65 | 0.53 |
| 1:K:31:ARG:HH21 | 1:K:37:LYS:HB2 | 1.71 | 0.53 |
| 1:K:177:GLN:OE1 | 1:K:177:GLN:N | 2.40 | 0.53 |
| 1:O:164:MET:SD | 1:O:300:TYR:OH | 2.66 | 0.53 |
| 1:T:52:ASN:O | 1:T:56:VAL:HG22 | 2.09 | 0.53 |
| 1:T:79:GLU:HG2 | 1:T:305:ARG:HH21 | 1.74 | 0.53 |
| 1:k:53:ARG:NH1 | 1:w:133:GLY:O | 2.41 | 0.53 |
| 1:k:240:ASP:OD1 | 1:k:240:ASP:N | 2.39 | 0.53 |
| 1:l:38:ILE:CD1 | 1:l:337:LYS:HA | 2.38 | 0.53 |
| 1:m:257:GLU:N | 1:m:257:GLU:OE2 | 2.42 | 0.53 |
| 1:p:373:LEU:HD12 | 1:p:373:LEU:H | 1.73 | 0.53 |
| 1:B:219:ILE:HD11 | 1:B:243:LEU:HD13 | 1.90 | 0.53 |
| 1:D:69:ASN:O | 1:D:72:ILE:HG22 | 2.08 | 0.53 |
| 1:L:225:TYR:O | 1:L:229:GLN:HG3 | 2.08 | 0.53 |
| 1:R:214:LYS:O | 1:R:215:ALA:C | 2.50 | 0.53 |
| 1:R:232:LEU:HA | 1:R:251:LYS:NZ | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:232:LEU:HD13 | 1:R:251:LYS:NZ | 2.23 | 0.53 |
| 1:T:270:GLU:OE2 | 1:T:271:GLY:N | 2.41 | 0.53 |
| 1:c:139:ASN:C | 1:c:141:THR:H | 2.17 | 0.53 |
| 1:n:13:THR:HA | 1:n:16:ARG:HH12 | 1.74 | 0.53 |
| 1:o:244:GLN:C | 1:o:245:ILE:HD12 | 2.33 | 0.53 |
| 1:x:38:ILE:HD11 | 1:x:337:LYS:HA | 1.90 | 0.53 |
| 1:D:84:GLU:O | 1:D:88:ILE:HG12 | 2.08 | 0.53 |
| 1:I:112:ILE:HG22 | 1:I:281:VAL:HG21 | 1.89 | 0.53 |
| 1:O:29:MET:HG2 | 1:O:348:MET:HE2 | 1.91 | 0.53 |
| 1:k:84:GLU:OE2 | 1:k:87:ASN:ND2 | 2.33 | 0.53 |
| 1:n:137:LEU:HB3 | 1:n:138:LEU:HD23 | 1.91 | 0.53 |
| 1:o:51:SER:OG | 1:o:337:LYS:HD2 | 2.08 | 0.53 |
| 1:r:142:HIS:CG | 1:r:143:GLY:H | 2.26 | 0.53 |
| 1:s:218:ASP:OD1 | 1:s:219:ILE:N | 2.41 | 0.53 |
| 1:t:78:ALA:O | 1:t:82:MET:HG3 | 2.09 | 0.53 |
| 1:x:37:LYS:NZ | 1:x:336:ILE:O | 2.38 | 0.53 |
| 1:2:125:ARG:HD3 | 1:p:314:ARG:NH2 | 2.24 | 0.53 |
| 1:C:366:LYS:O | 1:C:369:PRO:HD2 | 2.09 | 0.53 |
| 1:E:153:ASN:OD1 | 1:l:288:GLN:NE2 | 2.42 | 0.53 |
| 1:E:353:ILE:HD11 | 1:Q:370:ASN:HD22 | 1.72 | 0.53 |
| 1:J:93:ARG:NE | 1:J:295:ASP:OD1 | 2.37 | 0.53 |
| 1:L:243:LEU:HD22 | 1:L:266:LEU:HD11 | 1.91 | 0.53 |
| 1:M:238:ASP:N | 1:M:242:LYS:O | 2.40 | 0.53 |
| 1:N:222:LEU:O | 1:N:226:ILE:HG12 | 2.09 | 0.53 |
| 1:N:251:LYS:HD2 | 1:N:251:LYS:O | 2.07 | 0.53 |
| 1:V:79:GLU:OE1 | 1:V:305:ARG:NH2 | 2.41 | 0.53 |
| 1:c:92:MET:HA | 1:c:92:MET:HE3 | 1.91 | 0.53 |
| 1:c:95:LEU:CD1 | 1:c:112:ILE:HG23 | 2.38 | 0.53 |
| 1:i:375:LEU:O | 1:i:375:LEU:HD12 | 2.09 | 0.53 |
| 1:o:199:LEU:HB3 | 1:o:256:VAL:HG22 | 1.89 | 0.53 |
| 1:E:192:LYS:HD2 | 1:E:265:GLU:HB2 | 1.91 | 0.53 |
| 1:E:288:GLN:HE21 | 1:P:154:GLY:H | 1.55 | 0.53 |
| 1:F:244:GLN:HE22 | 1:F:285:GLY:HA3 | 1.73 | 0.53 |
| 1:G:51:SER:HB2 | 1:G:337:LYS:HD2 | 1.89 | 0.53 |
| 1:K:321:ASN:O | 1:K:325:ILE:HG13 | 2.09 | 0.53 |
| 1:S:357:ALA:O | 1:S:361:ILE:HG13 | 2.09 | 0.53 |
| 1:h:12:MET:HE1 | 1:s:330:ASN:HD22 | 1.74 | 0.53 |
| 1:l:255:GLU:HG3 | 1:l:256:VAL:N | 2.24 | 0.53 |
| 1:m:40:SER:OG | 1:m:42:LYS:NZ | 2.41 | 0.53 |
| 1:t:247:ALA:HB1 | 1:t:252:VAL:HG21 | 1.90 | 0.53 |
| 1:x:272:LYS:HD2 | 1:x:273:LYS:H | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:x:287:ALA:O | 1:x:291:VAL:HG23 | 2.08 | 0.53 |
| 1:C:93:ARG:NE | 1:C:291:VAL:HG13 | 2.22 | 0.53 |
| 1:C:101:ASN:HD22 | 1:N:67:ASN:HB3 | 1.73 | 0.53 |
| 1:I:15:GLN:OE1 | 1:o:343:LYS:HD2 | 2.09 | 0.53 |
| 1:I:250:ASN:HD21 | 1:I:299:LYS:HG3 | 1.74 | 0.53 |
| 1:K:234:LYS:O | 1:K:245:ILE:HD12 | 2.09 | 0.53 |
| 1:M:193:ASN:HA | 1:M:262:LEU:HD21 | 1.91 | 0.53 |
| 1:N:147:PHE:N | 1:N:157:VAL:O | 2.31 | 0.53 |
| 1:P:108:GLU:O | 1:P:112:ILE:HG12 | 2.09 | 0.53 |
| 1:P:304:HIS:HA | 1:P:307:GLU:OE1 | 2.09 | 0.53 |
| 1:S:273:LYS:N | 1:S:273:LYS:HD3 | 2.24 | 0.53 |
| 1:U:300:TYR:CE1 | 1:U:304:HIS:HE1 | 2.27 | 0.53 |
| 1:l:194:ASP:CG | 1:l:261:GLY:H | 2.17 | 0.53 |
| 1:q:108:GLU:H | 1:q:108:GLU:CD | 2.17 | 0.53 |
| 1:2:350:LYS:O | 1:2:353:ILE:HG22 | 2.08 | 0.53 |
| 1:G:142:HIS:HD2 | 1:G:161:LEU:HD12 | 1.72 | 0.53 |
| 1:G:353:ILE:HD11 | 1:H:5:VAL:HG13 | 1.90 | 0.53 |
| 1:O:172:GLY:HA3 | 1:O:273:LYS:HZ2 | 1.73 | 0.53 |
| 1:O:231:ASP:OD2 | 1:O:232:LEU:N | 2.41 | 0.53 |
| 1:P:192:LYS:HA | 1:P:192:LYS:HE3 | 1.91 | 0.53 |
| 1:Q:149:ILE:HG21 | 1:Q:315:PHE:HE2 | 1.74 | 0.53 |
| 1:V:366:LYS:O | 1:V:369:PRO:HD2 | 2.08 | 0.53 |
| 1:l:201:ASP:OD1 | 1:l:207:GLN:NE2 | 2.42 | 0.53 |
| 1:p:6:ASN:CA | 1:z:350:LYS:HZ1 | 2.17 | 0.53 |
| 1:p:31:ARG:NH2 | 1:p:43:ASP:OD1 | 2.41 | 0.53 |
| 1:w:124:ASN:O | 1:w:128:GLU:HG2 | 2.09 | 0.53 |
| 1:w:178:ALA:HB2 | 1:w:268:LEU:HA | 1.91 | 0.53 |
| 1:z:169:LYS:HD2 | 1:z:169:LYS:N | 2.20 | 0.53 |
| 1:z:219:ILE:CD1 | 1:z:243:LEU:HD12 | 2.38 | 0.53 |
| 1:1:29:MET:HA | 1:1:29:MET:HE3 | 1.91 | 0.53 |
| 1:E:82:MET:O | 1:E:85:THR:OG1 | 2.22 | 0.53 |
| 1:H:169:LYS:HD2 | 1:H:169:LYS:N | 2.24 | 0.53 |
| 1:I:61:LEU:HD22 | 1:I:151:ALA:HB2 | 1.91 | 0.53 |
| 1:P:31:ARG:NH2 | 1:P:32:LEU:HA | 2.24 | 0.53 |
| 1:P:371:SER:O | 1:P:374:SER:OG | 2.27 | 0.53 |
| 1:S:246:PHE:HD1 | 1:S:292:ALA:HB1 | 1.74 | 0.53 |
| 1:T:92:MET:HA | 1:T:95:LEU:HD12 | 1.90 | 0.53 |
| 1:c:257:GLU:N | 1:c:257:GLU:OE2 | 2.41 | 0.53 |
| 1:l:290:SER:O | 1:l:294:ILE:HG13 | 2.09 | 0.53 |
| 1:n:27:THR:O | 1:n:31:ARG:HG3 | 2.09 | 0.53 |
| 1:t:313:ASN:HA | 1:t:316:ASN:OD1 | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:v:276:VAL:O | 1:v:279:ILE:HG12 | 2.08 | 0.53 |
| 1:x:276:VAL:O | 1:x:279:ILE:HG23 | 2.09 | 0.53 |
| 1:z:62:ASP:HA | 1:z:65:VAL:HG23 | 1.90 | 0.53 |
| 1:A:168:ASN:OD1 | 1:A:169:LYS:N | 2.42 | 0.53 |
| 1:F:142:HIS:CG | 1:F:143:GLY:H | 2.27 | 0.53 |
| 1:G:195:LEU:HB2 | 1:G:262:LEU:HD12 | 1.91 | 0.53 |
| 1:G:321:ASN:O | 1:G:325:ILE:HG13 | 2.09 | 0.53 |
| 1:I:174:VAL:HG22 | 1:I:273:LYS:HD2 | 1.91 | 0.53 |
| 1:I:349:THR:O | 1:I:353:ILE:HG13 | 2.09 | 0.53 |
| 1:L:88:ILE:HG21 | 1:L:123:LEU:HD21 | 1.90 | 0.53 |
| 1:M:31:ARG:HD3 | 1:M:37:LYS:HA | 1.89 | 0.53 |
| 1:S:150:GLY:HA3 | 1:S:155:GLU:HB2 | 1.91 | 0.53 |
| 1:U:25:GLN:NE2 | 1:U:352:GLN:HG3 | 2.24 | 0.53 |
| 1:U:195:LEU:C | 1:U:196:LYS:HD3 | 2.34 | 0.53 |
| 1:U:288:GLN:HE21 | 1:U:288:GLN:C | 2.17 | 0.53 |
| 1:h:348:MET:SD | 1:h:352:GLN:NE2 | 2.82 | 0.53 |
| 1:i:150:GLY:HA3 | 1:i:155:GLU:HB2 | 1.90 | 0.53 |
| 1:m:122:GLU:O | 1:m:126:ILE:HG22 | 2.08 | 0.53 |
| 1:p:26:GLN:HE21 | 1:p:26:GLN:C | 2.16 | 0.53 |
| 1:r:88:ILE:HG23 | 1:r:119:LEU:HD23 | 1.90 | 0.53 |
| 1:s:169:LYS:HB2 | 1:s:170:MET:HE2 | 1.91 | 0.53 |
| 1:2:203:TYR:CB | 1:2:205:GLN:HE22 | 2.22 | 0.52 |
| 1:A:109:ARG:HB3 | 1:A:282:THR:HA | 1.92 | 0.52 |
| 1:A:250:ASN:HD21 | 1:A:296:ALA:HB1 | 1.74 | 0.52 |
| 1:H:65:VAL:HB | 1:H:66:ARG:HH11 | 1.74 | 0.52 |
| 1:J:48:LEU:HD11 | 1:q:305:ARG:NH2 | 2.24 | 0.52 |
| 1:J:184:LYS:HG3 | 1:J:184:LYS:O | 2.09 | 0.52 |
| 1:J:307:GLU:OE2 | 1:K:114:GLU:HG2 | 2.10 | 0.52 |
| 1:Q:93:ARG:NH2 | 1:Q:295:ASP:OD1 | 2.42 | 0.52 |
| 1:S:272:LYS:HA | 1:S:272:LYS:HE2 | 1.91 | 0.52 |
| 1:j:59:ARG:NH1 | 1:u:94:ASP:OD2 | 2.43 | 0.52 |
| 1:l:109:ARG:HB3 | 1:l:282:THR:HA | 1.91 | 0.52 |
| 1:o:144:ALA:HB1 | 1:o:158:MET:HE1 | 1.91 | 0.52 |
| 1:1:51:SER:HB3 | 1:1:337:LYS:HD3 | 1.92 | 0.52 |
| 1:2:84:GLU:OE2 | 1:2:126:ILE:HG21 | 2.10 | 0.52 |
| 1:2:89:LEU:HA | 1:2:92:MET:CE | 2.40 | 0.52 |
| 1:2:321:ASN:O | 1:2:325:ILE:HG12 | 2.09 | 0.52 |
| 1:F:40:SER:OG | 1:F:42:LYS:NZ | 2.41 | 0.52 |
| 1:L:196:LYS:C | 1:L:197:ILE:HD13 | 2.35 | 0.52 |
| 1:Q:159:LEU:HD12 | 1:Q:160:GLU:N | 2.25 | 0.52 |
| 1:R:190:GLU:O | 1:R:192:LYS:N | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:190:GLU:HB2 | 1:U:215:ALA:HB2 | 1.90 | 0.52 |
| 1:i:350:LYS:NZ | 1:j:6:ASN:O | 2.42 | 0.52 |
| 1:j:13:THR:O | 1:j:17:TYR:HD1 | 1.92 | 0.52 |
| 1:j:37:LYS:NZ | 1:j:338:ASP:O | 2.29 | 0.52 |
| 1:j:49:GLN:HE22 | 1:j:53:ARG:HE | 1.57 | 0.52 |
| 1:l:108:GLU:O | 1:l:112:ILE:HD12 | 2.08 | 0.52 |
| 1:p:109:ARG:HB3 | 1:p:282:THR:HA | 1.92 | 0.52 |
| 1:w:192:LYS:HE2 | 1:w:192:LYS:HA | 1.91 | 0.52 |
| 1:1:332:SER:OG | 1:1:335:ARG:NH2 | 2.42 | 0.52 |
| 1:3:222:LEU:O | 1:3:226:ILE:HG12 | 2.09 | 0.52 |
| 1:A:58:SER:HA | 1:A:61:LEU:HD23 | 1.90 | 0.52 |
| 1:A:196:LYS:C | 1:A:197:ILE:HD12 | 2.34 | 0.52 |
| 1:G:164:MET:HE2 | 1:G:164:MET:HA | 1.91 | 0.52 |
| 1:H:37:LYS:NZ | 1:H:336:ILE:O | 2.38 | 0.52 |
| 1:H:289:GLU:O | 1:H:293:ILE:HG13 | 2.09 | 0.52 |
| 1:L:119:LEU:O | 1:L:123:LEU:HG | 2.10 | 0.52 |
| 1:R:176:TYR:HB2 | 1:R:245:ILE:CG2 | 2.40 | 0.52 |
| 1:R:223:ALA:HA | 1:R:226:ILE:HD12 | 1.89 | 0.52 |
| 1:S:349:THR:O | 1:S:353:ILE:HG12 | 2.10 | 0.52 |
| 1:U:91:ARG:O | 1:U:91:ARG:HD3 | 2.09 | 0.52 |
| 1:i:160:GLU:OE2 | 1:i:162:LYS:HD2 | 2.10 | 0.52 |
| 1:r:287:ALA:O | 1:r:291:VAL:HG12 | 2.08 | 0.52 |
| 1:z:162:LYS:HG2 | 1:z:304:HIS:CE1 | 2.44 | 0.52 |
| 1:1:163:ASP:C | 1:1:164:MET:HE2 | 2.35 | 0.52 |
| 1:F:279:ILE:HB | 1:F:290:SER:OG | 2.10 | 0.52 |
| 1:G:138:LEU:HD12 | 1:G:164:MET:HG3 | 1.92 | 0.52 |
| 1:I:53:ARG:NH2 | 1:q:134:GLY:H | 2.01 | 0.52 |
| 1:I:169:LYS:HD3 | 1:I:169:LYS:N | 2.23 | 0.52 |
| 1:K:153:ASN:ND2 | 1:r:288:GLN:OE1 | 2.37 | 0.52 |
| 1:Q:318:ALA:O | 1:Q:322:LEU:HG | 2.09 | 0.52 |
| 1:T:177:GLN:NE2 | 1:T:238:ASP:OD2 | 2.42 | 0.52 |
| 1:h:149:ILE:HG21 | 1:h:315:PHE:HE2 | 1.73 | 0.52 |
| 1:p:88:ILE:O | 1:p:92:MET:HG3 | 2.09 | 0.52 |
| 1:q:82:MET:HE2 | 1:q:308:LEU:HD12 | 1.91 | 0.52 |
| 1:t:52:ASN:O | 1:t:56:VAL:HG12 | 2.09 | 0.52 |
| 1:x:330:ASN:H | 1:x:330:ASN:HD22 | 1.58 | 0.52 |
| 1:1:93:ARG:HG2 | 1:1:294:ILE:HG21 | 1.91 | 0.52 |
| 1:A:195:LEU:HB2 | 1:A:262:LEU:HD12 | 1.92 | 0.52 |
| 1:L:231:ASP:O | 1:L:234:LYS:NZ | 2.42 | 0.52 |
| 1:L:332:SER:O | 1:L:336:ILE:HG13 | 2.09 | 0.52 |
| 1:N:276:VAL:O | 1:N:279:ILE:HG12 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:366:LYS:O | 1:c:369:PRO:HD2 | 2.10 | 0.52 |
| 1:h:201:ASP:OD2 | 1:h:205:GLN:HB2 | 2.10 | 0.52 |
| 1:w:109:ARG:HA | 1:w:112:ILE:HD12 | 1.90 | 0.52 |
| 1:w:344:GLU:O | 1:w:345:THR:C | 2.53 | 0.52 |
| 1:x:159:LEU:HD13 | 1:x:311:PHE:CE1 | 2.44 | 0.52 |
| 1:l:126:ILE:HG23 | 1:z:321:ASN:ND2 | 2.24 | 0.52 |
| 1:3:36:PHE:CD1 | 1:3:337:LYS:HD2 | 2.45 | 0.52 |
| 1:C:366:LYS:HB2 | 1:C:366:LYS:HZ3 | 1.74 | 0.52 |
| 1:D:171:MET:HE2 | 1:D:171:MET:N | 2.24 | 0.52 |
| 1:F:182:LYS:HD3 | 1:F:182:LYS:N | 2.24 | 0.52 |
| 1:J:196:LYS:NZ | 1:J:208:GLU:OE1 | 2.42 | 0.52 |
| 1:M:46:ALA:O | 1:M:50:ILE:HG12 | 2.10 | 0.52 |
| 1:O:31:ARG:HH21 | 1:O:37:LYS:HB2 | 1.74 | 0.52 |
| 1:O:173:GLY:HA3 | 1:O:246:PHE:CE1 | 2.45 | 0.52 |
| 1:S:117:THR:HA | 1:S:120:ASN:ND2 | 2.23 | 0.52 |
| 1:V:37:LYS:O | 1:V:37:LYS:HG2 | 2.10 | 0.52 |
| 1:h:232:LEU:HA | 1:h:251:LYS:NZ | 2.23 | 0.52 |
| 1:o:357:ALA:O | 1:o:361:ILE:HG12 | 2.10 | 0.52 |
| 1:p:38:ILE:HD11 | 1:p:44:ASP:HB3 | 1.90 | 0.52 |
| 1:q:369:PRO:HD2 | 1:q:370:ASN:H | 1.74 | 0.52 |
| 1:r:12:MET:HA | 1:r:15:GLN:OE1 | 2.10 | 0.52 |
| 1:r:38:ILE:HG23 | 1:r:43:ASP:HB2 | 1.91 | 0.52 |
| 1:r:159:LEU:HD12 | 1:r:160:GLU:N | 2.25 | 0.52 |
| 1:s:115:GLU:O | 1:s:119:LEU:HG | 2.09 | 0.52 |
| 1:t:25:GLN:O | 1:t:29:MET:HG3 | 2.10 | 0.52 |
| 1:t:31:ARG:NH1 | 1:t:37:LYS:O | 2.43 | 0.52 |
| 1:u:169:LYS:HE2 | 1:u:249:ASN:HB3 | 1.90 | 0.52 |
| 1:w:290:SER:O | 1:w:294:ILE:HD12 | 2.09 | 0.52 |
| 1:3:325:ILE:O | 1:3:329:VAL:HG23 | 2.09 | 0.52 |
| 1:A:149:ILE:HD12 | 1:A:315:PHE:HE2 | 1.75 | 0.52 |
| 1:B:199:LEU:HB3 | 1:B:256:VAL:HG22 | 1.92 | 0.52 |
| 1:D:366:LYS:O | 1:D:369:PRO:HD2 | 2.10 | 0.52 |
| 1:F:321:ASN:HD22 | 1:G:126:ILE:HG12 | 1.75 | 0.52 |
| 1:N:70:ASP:O | 1:N:73:SER:OG | 2.26 | 0.52 |
| 1:N:90:GLN:HG2 | 1:N:93:ARG:HH21 | 1.74 | 0.52 |
| 1:V:108:GLU:O | 1:V:112:ILE:HG12 | 2.09 | 0.52 |
| 1:p:25:GLN:O | 1:p:29:MET:HG3 | 2.10 | 0.52 |
| 1:s:5:VAL:HG22 | 1:s:372:ALA:HB1 | 1.91 | 0.52 |
| 1:x:257:GLU:OE1 | 1:x:257:GLU:N | 2.42 | 0.52 |
| 1:2:313:ASN:HA | 1:2:316:ASN:HD21 | 1.73 | 0.52 |
| 1:B:171:MET:HE1 | 1:B:300:TYR:HD2 | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:73:SER:OG | 1:R:335:ARG:NH2 | 2.42 | 0.52 |
| 1:L:274:VAL:HG11 | 1:L:289:GLU:OE2 | 2.09 | 0.52 |
| 1:N:4:ASN:C | 1:N:4:ASN:ND2 | 2.66 | 0.52 |
| 1:O:255:GLU:OE1 | 1:O:256:VAL:N | 2.42 | 0.52 |
| 1:Q:276:VAL:O | 1:Q:279:ILE:HG12 | 2.09 | 0.52 |
| 1:S:173:GLY:HA3 | 1:S:246:PHE:CE2 | 2.45 | 0.52 |
| 1:U:350:LYS:O | 1:U:354:LEU:HD12 | 2.10 | 0.52 |
| 1:k:184:LYS:HD2 | 1:k:184:LYS:O | 2.09 | 0.52 |
| 1:n:25:GLN:NE2 | 1:n:29:MET:SD | 2.76 | 0.52 |
| 1:q:91:ARG:O | 1:q:95:LEU:HD23 | 2.09 | 0.52 |
| 1:s:128:GLU:OE1 | 1:s:165:ARG:NH1 | 2.43 | 0.52 |
| 1:2:350:LYS:O | 1:2:354:LEU:HD22 | 2.10 | 0.52 |
| 1:3:55:ASN:HB2 | 1:3:333:LYS:HE2 | 1.92 | 0.52 |
| 1:C:327:GLU:OE1 | 1:N:16:ARG:NH1 | 2.36 | 0.52 |
| 1:D:223:ALA:HA | 1:D:226:ILE:HD12 | 1.92 | 0.52 |
| 1:D:244:GLN:NE2 | 1:D:289:GLU:OE1 | 2.41 | 0.52 |
| 1:H:167:ASP:OD2 | 1:H:167:ASP:N | 2.43 | 0.52 |
| 1:I:321:ASN:HB2 | 1:q:84:GLU:OE2 | 2.09 | 0.52 |
| 1:L:54:LEU:CD1 | 1:L:329:VAL:HG13 | 2.38 | 0.52 |
| 1:N:163:ASP:C | 1:N:164:MET:HE2 | 2.35 | 0.52 |
| 1:Q:108:GLU:O | 1:Q:112:ILE:HG12 | 2.09 | 0.52 |
| 1:U:37:LYS:HG2 | 1:U:337:LYS:O | 2.10 | 0.52 |
| 1:c:190:GLU:OE2 | 1:c:193:ASN:ND2 | 2.40 | 0.52 |
| 1:h:170:MET:HA | 1:h:170:MET:HE3 | 1.91 | 0.52 |
| 1:o:145:LYS:O | 1:o:158:MET:HG3 | 2.09 | 0.52 |
| 1:t:101:ASN:OD1 | 1:t:102:GLY:N | 2.43 | 0.52 |
| 1:u:166:SER:HB2 | 1:u:276:VAL:HB | 1.91 | 0.52 |
| 1:u:350:LYS:O | 1:u:354:LEU:HD23 | 2.09 | 0.52 |
| 1:v:162:LYS:H | 1:v:162:LYS:HD2 | 1.75 | 0.52 |
| 1:w:206:GLU:H | 1:w:206:GLU:CD | 2.18 | 0.52 |
| 1:x:210:ASN:C | 1:x:211:ILE:HD12 | 2.34 | 0.52 |
| 1:z:44:ASP:O | 1:z:48:LEU:HG | 2.10 | 0.52 |
| 1:2:162:LYS:HG3 | 1:2:304:HIS:ND1 | 2.25 | 0.52 |
| 1:2:173:GLY:HA3 | 1:2:246:PHE:CZ | 2.45 | 0.52 |
| 1:H:142:HIS:CG | 1:H:143:GLY:H | 2.27 | 0.52 |
| 1:S:113:GLN:HE22 | 1:S:281:VAL:H | 1.57 | 0.52 |
| 1:S:159:LEU:HD12 | 1:S:160:GLU:N | 2.25 | 0.52 |
| 1:V:176:TYR:OH | 1:V:255:GLU:OE1 | 2.27 | 0.52 |
| 1:c:70:ASP:O | 1:c:74:ILE:HG13 | 2.10 | 0.52 |
| 1:c:174:VAL:HB | 1:c:247:ALA:HB3 | 1.92 | 0.52 |
| 1:l:219:ILE:HG13 | 1:l:237:VAL:HG21 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:o:335:ARG:NH2 | 1:p:73:SER:OG | 2.39 | 0.52 |
| 1:w:28:SER:HA | 1:w:31:ARG:HG3 | 1.92 | 0.52 |
| 1:x:149:ILE:HG21 | 1:x:315:PHE:CE2 | 2.41 | 0.52 |
| 1:1:190:GLU:OE2 | 1:1:193:ASN:ND2 | 2.39 | 0.51 |
| 1:2:82:MET:O | 1:2:85:THR:OG1 | 2.26 | 0.51 |
| 1:3:79:GLU:HG3 | 1:3:305:ARG:HH21 | 1.75 | 0.51 |
| 1:3:327:GLU:OE1 | 1:r:12:MET:HB2 | 2.10 | 0.51 |
| 1:A:194:ASP:OD1 | 1:A:194:ASP:N | 2.43 | 0.51 |
| 1:B:37:LYS:NZ | 1:B:336:ILE:O | 2.37 | 0.51 |
| 1:B:285:GLY:O | 1:B:289:GLU:HG2 | 2.10 | 0.51 |
| 1:E:69:ASN:O | 1:E:72:ILE:HG22 | 2.10 | 0.51 |
| 1:E:257:GLU:OE1 | 1:E:258:PHE:N | 2.41 | 0.51 |
| 1:F:322:LEU:HA | 1:F:325:ILE:HD12 | 1.93 | 0.51 |
| 1:G:25:GLN:O | 1:G:29:MET:HG3 | 2.10 | 0.51 |
| 1:M:222:LEU:O | 1:M:226:ILE:HG12 | 2.10 | 0.51 |
| 1:Q:366:LYS:O | 1:Q:369:PRO:HD2 | 2.11 | 0.51 |
| 1:R:290:SER:O | 1:R:294:ILE:HG13 | 2.10 | 0.51 |
| 1:U:299:LYS:HD2 | 1:U:299:LYS:O | 2.08 | 0.51 |
| 1:j:179:GLU:O | 1:j:242:LYS:NZ | 2.43 | 0.51 |
| 1:m:85:THR:O | 1:m:89:LEU:HD13 | 2.10 | 0.51 |
| 1:o:153:ASN:HD21 | 1:z:288:GLN:HB3 | 1.75 | 0.51 |
| 1:r:37:LYS:HG2 | 1:r:337:LYS:O | 2.11 | 0.51 |
| 1:r:93:ARG:HB2 | 1:r:294:ILE:HG21 | 1.91 | 0.51 |
| 1:x:81:ALA:O | 1:x:85:THR:HG23 | 2.10 | 0.51 |
| 1:3:78:ALA:HB1 | 1:3:82:MET:HE3 | 1.92 | 0.51 |
| 1:D:158:MET:HE1 | 1:D:160:GLU:HB2 | 1.91 | 0.51 |
| 1:E:160:GLU:OE1 | 1:E:162:LYS:NZ | 2.28 | 0.51 |
| 1:G:6:ASN:ND2 | 1:n:35:GLY:O | 2.39 | 0.51 |
| 1:G:274:VAL:HG11 | 1:G:289:GLU:OE2 | 2.10 | 0.51 |
| 1:H:108:GLU:H | 1:H:108:GLU:CD | 2.18 | 0.51 |
| 1:J:233:VAL:HB | 1:J:245:ILE:HD11 | 1.92 | 0.51 |
| 1:L:236:SER:OG | 1:L:244:GLN:HG3 | 2.09 | 0.51 |
| 1:N:123:LEU:O | 1:N:126:ILE:HG22 | 2.10 | 0.51 |
| 1:N:171:MET:SD | 1:N:171:MET:N | 2.83 | 0.51 |
| 1:N:235:ALA:HA | 1:N:244:GLN:O | 2.10 | 0.51 |
| 1:O:144:ALA:C | 1:O:145:LYS:HD3 | 2.36 | 0.51 |
| 1:O:219:ILE:HD12 | 1:O:222:LEU:HD23 | 1.92 | 0.51 |
| 1:P:25:GLN:NE2 | 1:P:351:SER:OG | 2.44 | 0.51 |
| 1:U:367:GLN:HA | 1:U:367:GLN:OE1 | 2.11 | 0.51 |
| 1:l:162:LYS:HG2 | 1:l:304:HIS:CD2 | 2.45 | 0.51 |
| 1:r:73:SER:O | 1:r:77:THR:HG23 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:s:13:THR:HG21 | 1:t:30:GLU:OE1 | 2.10 | 0.51 |
| 1:u:321:ASN:ND2 | 1:v:126:ILE:HG23 | 2.25 | 0.51 |
| 1:v:18:LEU:HD12 | 1:v:22:ASN:ND2 | 2.25 | 0.51 |
| 1:x:321:ASN:O | 1:x:325:ILE:HG13 | 2.11 | 0.51 |
| 1:A:158:MET:HB2 | 1:h:220:GLU:OE1 | 2.10 | 0.51 |
| 1:E:314:ARG:NE | 1:F:122:GLU:OE1 | 2.41 | 0.51 |
| 1:F:61:LEU:HD23 | 1:F:151:ALA:HB2 | 1.93 | 0.51 |
| 1:K:334:SER:HB2 | 1:V:7:THR:HG21 | 1.93 | 0.51 |
| 1:P:168:ASN:OD1 | 1:P:170:MET:HE2 | 2.10 | 0.51 |
| 1:P:203:TYR:CB | 1:P:205:GLN:HE22 | 2.23 | 0.51 |
| 1:Q:279:ILE:HB | 1:Q:290:SER:OG | 2.11 | 0.51 |
| 1:R:192:LYS:HG3 | 1:R:261:GLY:O | 2.10 | 0.51 |
| 1:S:30:GLU:OE2 | 1:S:39:ASN:ND2 | 2.43 | 0.51 |
| 1:S:257:GLU:N | 1:S:257:GLU:OE1 | 2.42 | 0.51 |
| 1:k:11:ALA:C | 1:k:15:GLN:HE21 | 2.19 | 0.51 |
| 1:m:272:LYS:HD2 | 1:m:273:LYS:N | 2.24 | 0.51 |
| 1:o:232:LEU:HA | 1:o:251:LYS:NZ | 2.24 | 0.51 |
| 1:p:65:VAL:HG13 | 1:p:319:ILE:HD11 | 1.92 | 0.51 |
| 1:v:223:ALA:HA | 1:v:226:ILE:HD12 | 1.91 | 0.51 |
| 1:v:338:ASP:N | 1:v:338:ASP:OD1 | 2.44 | 0.51 |
| 1:x:12:MET:N | 1:x:12:MET:SD | 2.83 | 0.51 |
| 1:z:12:MET:O | 1:z:16:ARG:HG3 | 2.11 | 0.51 |
| 1:z:300:TYR:CE1 | 1:z:304:HIS:CD2 | 2.98 | 0.51 |
| 1:1:98:GLN:O | 1:1:98:GLN:NE2 | 2.34 | 0.51 |
| 1:H:138:LEU:HB3 | 1:H:164:MET:HG2 | 1.93 | 0.51 |
| 1:H:231:ASP:O | 1:H:251:LYS:NZ | 2.43 | 0.51 |
| 1:N:168:ASN:OD1 | 1:N:169:LYS:N | 2.43 | 0.51 |
| 1:N:290:SER:O | 1:N:293:ILE:HG22 | 2.10 | 0.51 |
| 1:R:52:ASN:O | 1:R:56:VAL:HG13 | 2.11 | 0.51 |
| 1:R:234:LYS:O | 1:R:245:ILE:HD12 | 2.11 | 0.51 |
| 1:T:128:GLU:OE2 | 1:T:165:ARG:NH1 | 2.43 | 0.51 |
| 1:U:120:ASN:OD1 | 1:U:124:ASN:ND2 | 2.44 | 0.51 |
| 1:n:54:LEU:HD12 | 1:n:329:VAL:HG13 | 1.90 | 0.51 |
| 1:n:91:ARG:O | 1:n:95:LEU:HG | 2.11 | 0.51 |
| 1:s:219:ILE:HD12 | 1:s:222:LEU:HD23 | 1.92 | 0.51 |
| 1:s:291:VAL:O | 1:s:294:ILE:HG22 | 2.10 | 0.51 |
| 1:t:55:ASN:O | 1:t:59:ARG:HG3 | 2.11 | 0.51 |
| 1:u:340:ASP:O | 1:u:344:GLU:HG2 | 2.11 | 0.51 |
| 1:x:350:LYS:O | 1:x:354:LEU:HD22 | 2.11 | 0.51 |
| 1:z:332:SER:HA | 1:z:335:ARG:HH12 | 1.74 | 0.51 |
| 1:3:162:LYS:HD3 | 1:3:304:HIS:HB3 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:343:LYS:HA | 1:A:343:LYS:HE2 | 1.93 | 0.51 |
| 1:C:92:MET:HE1 | 1:C:120:ASN:OD1 | 2.11 | 0.51 |
| 1:G:210:ASN:C | 1:G:211:ILE:HD12 | 2.36 | 0.51 |
| 1:H:35:GLY:O | 1:S:6:ASN:ND2 | 2.40 | 0.51 |
| 1:I:343:LYS:HE2 | 1:I:343:LYS:HA | 1.92 | 0.51 |
| 1:M:30:GLU:OE2 | 1:M:39:ASN:ND2 | 2.35 | 0.51 |
| 1:P:29:MET:HE2 | 1:P:29:MET:N | 2.26 | 0.51 |
| 1:Q:162:LYS:CD | 1:Q:304:HIS:HB3 | 2.39 | 0.51 |
| 1:T:88:ILE:HG22 | 1:T:92:MET:HE2 | 1.91 | 0.51 |
| 1:c:247:ALA:HB1 | 1:c:252:VAL:HG21 | 1.92 | 0.51 |
| 1:i:376:LEU:HD12 | 1:i:377:GLY:H | 1.75 | 0.51 |
| 1:u:105:SER:N | 1:u:108:GLU:OE2 | 2.38 | 0.51 |
| 1:z:34:SER:HB2 | 1:z:36:PHE:HD2 | 1.76 | 0.51 |
| 1:1:70:ASP:O | 1:1:74:ILE:HG12 | 2.11 | 0.51 |
| 1:1:169:LYS:HE2 | 1:1:169:LYS:HA | 1.92 | 0.51 |
| 1:3:19:ASN:HA | 1:3:22:ASN:ND2 | 2.25 | 0.51 |
| 1:C:50:ILE:HG22 | 1:C:54:LEU:HD11 | 1.92 | 0.51 |
| 1:C:205:GLN:NE2 | 1:C:206:GLU:O | 2.43 | 0.51 |
| 1:F:12:MET:SD | 1:m:327:GLU:HG2 | 2.51 | 0.51 |
| 1:G:59:ARG:HA | 1:G:62:ASP:OD1 | 2.11 | 0.51 |
| 1:I:82:MET:HE1 | 1:I:304:HIS:HB2 | 1.92 | 0.51 |
| 1:L:205:GLN:HB2 | 1:L:207:GLN:HE22 | 1.75 | 0.51 |
| 1:Q:162:LYS:NZ | 1:Q:307:GLU:HB2 | 2.25 | 0.51 |
| 1:S:246:PHE:CD1 | 1:S:292:ALA:HB1 | 2.45 | 0.51 |
| 1:S:276:VAL:O | 1:S:279:ILE:HG12 | 2.11 | 0.51 |
| 1:U:25:GLN:NE2 | 1:U:351:SER:HB2 | 2.26 | 0.51 |
| 1:m:304:HIS:HA | 1:m:307:GLU:OE2 | 2.11 | 0.51 |
| 1:q:335:ARG:HH11 | 1:q:335:ARG:HG3 | 1.76 | 0.51 |
| 1:r:125:ARG:HG2 | 1:r:125:ARG:HH11 | 1.76 | 0.51 |
| 1:v:52:ASN:HA | 1:v:55:ASN:HD22 | 1.76 | 0.51 |
| 1:w:27:THR:O | 1:w:31:ARG:HG3 | 2.11 | 0.51 |
| 1:w:92:MET:HG2 | 1:w:119:LEU:HD12 | 1.92 | 0.51 |
| 1:1:174:VAL:HG22 | 1:1:273:LYS:HD2 | 1.93 | 0.51 |
| 1:2:30:GLU:OE2 | 1:p:10:SER:HA | 2.11 | 0.51 |
| 1:2:143:GLY:HA3 | 1:2:145:LYS:HZ2 | 1.75 | 0.51 |
| 1:3:198:ASN:OD1 | 1:3:198:ASN:N | 2.44 | 0.51 |
| 1:D:111:ALA:HA | 1:D:114:GLU:OE2 | 2.11 | 0.51 |
| 1:U:192:LYS:HE2 | 1:U:261:GLY:O | 2.11 | 0.51 |
| 1:U:225:TYR:O | 1:U:229:GLN:HG2 | 2.10 | 0.51 |
| 1:m:300:TYR:CE2 | 1:m:304:HIS:NE2 | 2.79 | 0.51 |
| 1:n:170:MET:HG3 | 1:n:300:TYR:HE2 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:v:53:ARG:O | 1:v:57:GLN:HG2 | 2.11 | 0.51 |
| 1:v:92:MET:HE1 | 1:v:123:LEU:HD11 | 1.93 | 0.51 |
| 1:1:292:ALA:HA | 1:1:295:ASP:OD2 | 2.11 | 0.51 |
| 1:A:231:ASP:OD1 | 1:A:251:LYS:NZ | 2.40 | 0.51 |
| 1:B:97:LEU:HD23 | 1:B:291:VAL:HG21 | 1.92 | 0.51 |
| 1:H:38:ILE:HG13 | 1:H:38:ILE:O | 2.09 | 0.51 |
| 1:I:25:GLN:OE1 | 1:I:352:GLN:HG2 | 2.11 | 0.51 |
| 1:I:299:LYS:HD2 | 1:I:299:LYS:C | 2.36 | 0.51 |
| 1:J:38:ILE:HG23 | 1:J:337:LYS:HG3 | 1.93 | 0.51 |
| 1:L:177:GLN:HE21 | 1:L:244:GLN:HB3 | 1.76 | 0.51 |
| 1:N:142:HIS:CG | 1:N:143:GLY:H | 2.29 | 0.51 |
| 1:Q:294:ILE:O | 1:Q:298:LEU:HG | 2.11 | 0.51 |
| 1:T:125:ARG:HD2 | 1:T:125:ARG:C | 2.36 | 0.51 |
| 1:T:176:TYR:HB2 | 1:T:245:ILE:HB | 1.93 | 0.51 |
| 1:T:238:ASP:OD2 | 1:T:242:LYS:HB2 | 2.10 | 0.51 |
| 1:i:218:ASP:HB3 | 1:i:221:GLU:HG3 | 1.92 | 0.51 |
| 1:j:344:GLU:OE1 | 1:j:344:GLU:HA | 2.11 | 0.51 |
| 1:n:273:LYS:HD2 | 1:n:273:LYS:N | 2.25 | 0.51 |
| 1:o:63:VAL:HG11 | 1:z:97:LEU:HB2 | 1.92 | 0.51 |
| 1:q:196:LYS:O | 1:q:197:ILE:HD13 | 2.10 | 0.51 |
| 1:t:208:GLU:N | 1:t:208:GLU:OE2 | 2.44 | 0.51 |
| 1:u:250:ASN:HD21 | 1:u:299:LYS:HE2 | 1.76 | 0.51 |
| 1:w:170:MET:HA | 1:w:170:MET:HE3 | 1.93 | 0.51 |
| 1:x:321:ASN:OD1 | 1:x:325:ILE:HD11 | 2.11 | 0.51 |
| 1:2:142:HIS:CE1 | 1:2:161:LEU:HD12 | 2.45 | 0.51 |
| 1:A:276:VAL:HA | 1:A:279:ILE:HD11 | 1.91 | 0.51 |
| 1:B:50:ILE:O | 1:B:54:LEU:HD23 | 2.10 | 0.51 |
| 1:F:108:GLU:CG | 1:P:50:ILE:HD11 | 2.41 | 0.51 |
| 1:M:163:ASP:OD1 | 1:M:165:ARG:HG3 | 2.11 | 0.51 |
| 1:M:239:GLN:OE1 | 1:M:284:VAL:HB | 2.11 | 0.51 |
| 1:O:323:ASP:O | 1:O:327:GLU:HG2 | 2.11 | 0.51 |
| 1:Q:314:ARG:NE | 1:R:122:GLU:OE2 | 2.38 | 0.51 |
| 1:S:66:ARG:NE | 1:S:66:ARG:O | 2.44 | 0.51 |
| 1:U:163:ASP:C | 1:U:164:MET:HE2 | 2.36 | 0.51 |
| 1:c:89:LEU:HD21 | 1:c:298:LEU:HB2 | 1.91 | 0.51 |
| 1:h:9:VAL:O | 1:h:12:MET:HG2 | 2.11 | 0.51 |
| 1:j:182:LYS:HD3 | 1:j:186:TRP:CG | 2.45 | 0.51 |
| 1:l:143:GLY:HA3 | 1:l:145:LYS:HE2 | 1.91 | 0.51 |
| 1:l:290:SER:HA | 1:l:293:ILE:HD12 | 1.92 | 0.51 |
| 1:o:343:LYS:HA | 1:o:343:LYS:HE2 | 1.93 | 0.51 |
| 1:q:72:ILE:HG13 | 1:q:312:GLN:OE1 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:t:332:SER:O | 1:t:335:ARG:HG2 | 2.11 | 0.51 |
| 1:w:335:ARG:HD2 | 1:x:69:ASN:CB | 2.41 | 0.51 |
| 1:1:350:LYS:HA | 1:1:353:ILE:HD12 | 1.93 | 0.51 |
| 1:3:220:GLU:OE2 | 1:r:156:ALA:HB3 | 2.11 | 0.51 |
| 1:B:244:GLN:C | 1:B:245:ILE:HD12 | 2.36 | 0.51 |
| 1:G:88:ILE:HG23 | 1:G:119:LEU:HD22 | 1.93 | 0.51 |
| 1:H:304:HIS:HA | 1:H:307:GLU:HG3 | 1.92 | 0.51 |
| 1:K:23:SER:O | 1:K:26:GLN:HG3 | 2.11 | 0.51 |
| 1:N:46:ALA:O | 1:N:50:ILE:HG12 | 2.11 | 0.51 |
| 1:O:172:GLY:HA3 | 1:O:273:LYS:NZ | 2.26 | 0.51 |
| 1:P:227:ASN:OD1 | 1:P:234:LYS:HG3 | 2.11 | 0.51 |
| 1:Q:220:GLU:HA | 1:Q:237:VAL:HG21 | 1.91 | 0.51 |
| 1:c:170:MET:N | 1:c:170:MET:SD | 2.83 | 0.51 |
| 1:j:158:MET:HE3 | 1:u:220:GLU:HG2 | 1.92 | 0.51 |
| 1:k:195:LEU:HD13 | 1:k:262:LEU:HB2 | 1.93 | 0.51 |
| 1:1:150:GLY:HA3 | 1:1:155:GLU:CD | 2.36 | 0.50 |
| 1:1:188:VAL:HG23 | 1:1:217:ASP:O | 2.12 | 0.50 |
| 1:C:76:GLN:OE1 | 1:C:76:GLN:HA | 2.10 | 0.50 |
| 1:C:343:LYS:HB3 | 1:C:343:LYS:NZ | 2.24 | 0.50 |
| 1:J:115:GLU:O | 1:J:119:LEU:HD22 | 2.11 | 0.50 |
| 1:L:27:THR:O | 1:L:31:ARG:HG3 | 2.11 | 0.50 |
| 1:N:54:LEU:HA | 1:N:57:GLN:HG3 | 1.93 | 0.50 |
| 1:U:25:GLN:NE2 | 1:U:348:MET:O | 2.44 | 0.50 |
| 1:n:361:ILE:HD13 | 1:z:32:LEU:HD12 | 1.92 | 0.50 |
| 1:r:168:ASN:OD1 | 1:r:170:MET:N | 2.43 | 0.50 |
| 1:s:82:MET:O | 1:s:85:THR:OG1 | 2.27 | 0.50 |
| 1:s:253:GLU:OE1 | 1:s:254:GLY:N | 2.43 | 0.50 |
| 1:v:177:GLN:HE22 | 1:v:179:GLU:HA | 1.76 | 0.50 |
| 1:x:66:ARG:HA | 1:x:69:ASN:OD1 | 2.11 | 0.50 |
| 1:1:152:ASP:N | 1:1:155:GLU:OE2 | 2.42 | 0.50 |
| 1:3:79:GLU:O | 1:3:305:ARG:NH2 | 2.44 | 0.50 |
| 1:A:6:ASN:ND2 | 1:h:35:GLY:O | 2.42 | 0.50 |
| 1:D:202:SER:HA | 1:D:253:GLU:HG3 | 1.92 | 0.50 |
| 1:F:163:ASP:O | 1:F:164:MET:HE2 | 2.10 | 0.50 |
| 1:G:159:LEU:HB2 | 1:G:311:PHE:HE1 | 1.75 | 0.50 |
| 1:G:361:ILE:HD11 | 1:o:29:MET:HG2 | 1.93 | 0.50 |
| 1:H:356:GLN:O | 1:H:359:SER:OG | 2.26 | 0.50 |
| 1:K:82:MET:HG2 | 1:K:164:MET:HE3 | 1.93 | 0.50 |
| 1:L:111:ALA:HA | 1:L:114:GLU:HG2 | 1.92 | 0.50 |
| 1:L:276:VAL:O | 1:L:279:ILE:HG12 | 2.12 | 0.50 |
| 1:N:323:ASP:O | 1:N:327:GLU:HG3 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:122:GLU:HB2 | 1:c:314:ARG:CD | 2.41 | 0.50 |
| 1:u:50:ILE:O | 1:u:54:LEU:HG | 2.10 | 0.50 |
| 1:u:111:ALA:HA | 1:u:114:GLU:OE2 | 2.10 | 0.50 |
| 1:u:238:ASP:OD1 | 1:u:239:GLN:NE2 | 2.43 | 0.50 |
| 1:z:109:ARG:HB3 | 1:z:282:THR:HA | 1.93 | 0.50 |
| 1:1:151:ALA:N | 1:1:155:GLU:OE2 | 2.44 | 0.50 |
| 1:1:332:SER:HA | 1:1:335:ARG:HE | 1.76 | 0.50 |
| 1:J:366:LYS:NZ | 1:T:377:GLY:O | 2.44 | 0.50 |
| 1:N:300:TYR:CZ | 1:N:304:HIS:HE1 | 2.30 | 0.50 |
| 1:P:176:TYR:HB2 | 1:P:245:ILE:HG23 | 1.91 | 0.50 |
| 1:P:219:ILE:HD11 | 1:P:243:LEU:HD23 | 1.93 | 0.50 |
| 1:S:144:ALA:HB1 | 1:S:158:MET:CE | 2.41 | 0.50 |
| 1:T:171:MET:HA | 1:T:171:MET:HE3 | 1.94 | 0.50 |
| 1:h:159:LEU:HD13 | 1:h:311:PHE:CE2 | 2.47 | 0.50 |
| 1:m:69:ASN:HA | 1:m:72:ILE:HD12 | 1.94 | 0.50 |
| 1:m:106:LYS:HE2 | 1:m:106:LYS:HA | 1.93 | 0.50 |
| 1:n:153:ASN:OD1 | 1:n:154:GLY:N | 2.44 | 0.50 |
| 1:p:169:LYS:HD2 | 1:p:169:LYS:O | 2.11 | 0.50 |
| 1:p:185:ASP:OD1 | 1:p:185:ASP:N | 2.33 | 0.50 |
| 1:t:57:GLN:O | 1:t:61:LEU:HG | 2.11 | 0.50 |
| 1:t:325:ILE:O | 1:t:329:VAL:HG22 | 2.11 | 0.50 |
| 1:z:74:ILE:O | 1:z:77:THR:OG1 | 2.24 | 0.50 |
| 1:2:149:ILE:HG21 | 1:2:315:PHE:CE2 | 2.46 | 0.50 |
| 1:A:73:SER:OG | 1:V:335:ARG:NH2 | 2.45 | 0.50 |
| 1:D:227:ASN:OD1 | 1:D:234:LYS:HD3 | 2.12 | 0.50 |
| 1:F:318:ALA:O | 1:F:322:LEU:HG | 2.11 | 0.50 |
| 1:I:161:LEU:C | 1:I:162:LYS:HD2 | 2.37 | 0.50 |
| 1:R:59:ARG:HA | 1:R:62:ASP:OD2 | 2.11 | 0.50 |
| 1:R:316:ASN:HA | 1:R:319:ILE:HD12 | 1.94 | 0.50 |
| 1:S:238:ASP:OD2 | 1:S:242:LYS:HB2 | 2.11 | 0.50 |
| 1:h:94:ASP:OD2 | 1:h:95:LEU:N | 2.45 | 0.50 |
| 1:i:37:LYS:NZ | 1:i:336:ILE:O | 2.45 | 0.50 |
| 1:k:128:GLU:OE1 | 1:k:165:ARG:NH1 | 2.43 | 0.50 |
| 1:m:70:ASP:O | 1:m:74:ILE:HG12 | 2.12 | 0.50 |
| 1:n:70:ASP:O | 1:n:74:ILE:HG13 | 2.11 | 0.50 |
| 1:t:299:LYS:NZ | 1:t:303:SER:HB2 | 2.26 | 0.50 |
| 1:1:214:LYS:HB2 | 1:1:217:ASP:OD1 | 2.12 | 0.50 |
| 1:2:350:LYS:HA | 1:2:353:ILE:HG22 | 1.93 | 0.50 |
| 1:B:61:LEU:HD12 | 1:B:322:LEU:HB3 | 1.91 | 0.50 |
| 1:C:190:GLU:H | 1:C:190:GLU:CD | 2.18 | 0.50 |
| 1:C:222:LEU:HG | 1:C:226:ILE:HD11 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:89:LEU:HA | 1:D:92:MET:HE3 | 1.92 | 0.50 |
| 1:E:288:GLN:HG3 | 1:P:153:ASN:OD1 | 2.12 | 0.50 |
| 1:M:239:GLN:HE22 | 1:M:285:GLY:H | 1.58 | 0.50 |
| 1:O:27:THR:O | 1:O:31:ARG:HG3 | 2.11 | 0.50 |
| 1:S:36:PHE:CD1 | 1:S:337:LYS:HG2 | 2.46 | 0.50 |
| 1:i:88:ILE:O | 1:i:92:MET:HG3 | 2.11 | 0.50 |
| 1:j:49:GLN:HE22 | 1:j:53:ARG:NE | 2.09 | 0.50 |
| 1:j:93:ARG:NH1 | 1:j:295:ASP:OD1 | 2.44 | 0.50 |
| 1:o:82:MET:HB2 | 1:o:305:ARG:HD3 | 1.93 | 0.50 |
| 1:s:68:ALA:O | 1:s:72:ILE:HG13 | 2.11 | 0.50 |
| 1:v:84:GLU:OE1 | 1:v:84:GLU:HA | 2.12 | 0.50 |
| 1:2:239:GLN:NE2 | 1:2:240:ASP:OD1 | 2.38 | 0.50 |
| 1:2:299:LYS:O | 1:2:299:LYS:HD2 | 2.12 | 0.50 |
| 1:K:4:ASN:ND2 | 1:K:7:THR:HB | 2.26 | 0.50 |
| 1:K:219:ILE:HG22 | 1:K:237:VAL:HG21 | 1.92 | 0.50 |
| 1:L:82:MET:HE1 | 1:L:308:LEU:HD11 | 1.94 | 0.50 |
| 1:N:69:ASN:HA | 1:N:72:ILE:HD12 | 1.94 | 0.50 |
| 1:l:95:LEU:HB3 | 1:l:112:ILE:CG2 | 2.41 | 0.50 |
| 1:n:36:PHE:HA | 1:n:338:ASP:HA | 1.92 | 0.50 |
| 1:p:174:VAL:HG23 | 1:p:249:ASN:OD1 | 2.11 | 0.50 |
| 1:p:348:MET:O | 1:p:352:GLN:HG3 | 2.12 | 0.50 |
| 1:t:108:GLU:O | 1:t:112:ILE:HG13 | 2.12 | 0.50 |
| 1:u:84:GLU:HA | 1:u:87:ASN:OD1 | 2.11 | 0.50 |
| 1:1:302:ASP:OD1 | 1:1:302:ASP:N | 2.43 | 0.50 |
| 1:3:50:ILE:O | 1:3:54:LEU:HG | 2.12 | 0.50 |
| 1:3:321:ASN:OD1 | 1:3:325:ILE:HD11 | 2.11 | 0.50 |
| 1:A:375:LEU:HD11 | 1:B:362:LEU:HD23 | 1.93 | 0.50 |
| 1:G:333:LYS:HA | 1:G:336:ILE:HD12 | 1.94 | 0.50 |
| 1:H:159:LEU:HB2 | 1:H:311:PHE:HE1 | 1.74 | 0.50 |
| 1:I:84:GLU:HA | 1:I:84:GLU:OE2 | 2.12 | 0.50 |
| 1:I:160:GLU:HG2 | 1:I:162:LYS:NZ | 2.26 | 0.50 |
| 1:J:88:ILE:O | 1:J:92:MET:HG3 | 2.12 | 0.50 |
| 1:O:113:GLN:OE1 | 1:O:281:VAL:HG22 | 2.12 | 0.50 |
| 1:P:106:LYS:HE3 | 1:P:109:ARG:HD2 | 1.93 | 0.50 |
| 1:Q:69:ASN:O | 1:Q:72:ILE:HG22 | 2.12 | 0.50 |
| 1:S:84:GLU:O | 1:S:88:ILE:HG13 | 2.12 | 0.50 |
| 1:h:3:VAL:HG12 | 1:h:372:ALA:HB2 | 1.93 | 0.50 |
| 1:j:170:MET:HA | 1:j:170:MET:HE3 | 1.93 | 0.50 |
| 1:k:50:ILE:O | 1:k:54:LEU:HD23 | 2.11 | 0.50 |
| 1:k:79:GLU:OE1 | 1:k:305:ARG:NH2 | 2.39 | 0.50 |
| 1:m:164:MET:HE1 | 1:m:304:HIS:HD2 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:u:223:ALA:HA | 1:u:226:ILE:HD12 | 1.94 | 0.50 |
| 1:1:219:ILE:HG23 | 1:1:220:GLU:OE2 | 2.12 | 0.50 |
| 1:3:231:ASP:O | 1:3:234:LYS:NZ | 2.40 | 0.50 |
| 1:H:171:MET:HA | 1:H:171:MET:HE3 | 1.92 | 0.50 |
| 1:H:177:GLN:N | 1:H:272:LYS:HZ1 | 2.09 | 0.50 |
| 1:H:300:TYR:HE1 | 1:H:304:HIS:NE2 | 2.09 | 0.50 |
| 1:I:163:ASP:C | 1:I:164:MET:HE2 | 2.37 | 0.50 |
| 1:R:267:GLY:O | 1:R:268:LEU:HD23 | 2.11 | 0.50 |
| 1:q:313:ASN:HA | 1:q:316:ASN:HD22 | 1.76 | 0.50 |
| 1:s:31:ARG:HD2 | 1:s:344:GLU:OE2 | 2.12 | 0.50 |
| 1:1:95:LEU:HD22 | 1:1:112:ILE:HD11 | 1.93 | 0.50 |
| 1:3:218:ASP:O | 1:3:222:LEU:N | 2.43 | 0.50 |
| 1:J:321:ASN:O | 1:J:325:ILE:HG12 | 2.12 | 0.50 |
| 1:M:27:THR:HG22 | 1:M:31:ARG:NH1 | 2.27 | 0.50 |
| 1:M:69:ASN:HA | 1:M:72:ILE:HD12 | 1.94 | 0.50 |
| 1:Q:343:LYS:HB2 | 1:Q:343:LYS:NZ | 2.27 | 0.50 |
| 1:S:171:MET:HE1 | 1:S:300:TYR:HD2 | 1.77 | 0.50 |
| 1:c:222:LEU:O | 1:c:226:ILE:HG22 | 2.11 | 0.50 |
| 1:c:316:ASN:O | 1:c:319:ILE:HG22 | 2.12 | 0.50 |
| 1:i:223:ALA:O | 1:i:227:ASN:ND2 | 2.45 | 0.50 |
| 1:j:144:ALA:HB2 | 1:j:160:GLU:HG2 | 1.93 | 0.50 |
| 1:k:78:ALA:O | 1:k:82:MET:HG3 | 2.12 | 0.50 |
| 1:q:300:TYR:O | 1:q:304:HIS:ND1 | 2.44 | 0.50 |
| 1:v:85:THR:HA | 1:v:88:ILE:HD12 | 1.92 | 0.50 |
| 1:x:28:SER:OG | 1:x:348:MET:HB2 | 2.12 | 0.50 |
| 1:z:246:PHE:HD1 | 1:z:247:ALA:N | 2.10 | 0.50 |
| 1:z:294:ILE:O | 1:z:298:LEU:HD12 | 2.10 | 0.50 |
| 1:1:9:VAL:HA | 1:1:12:MET:HE2 | 1.94 | 0.49 |
| 1:2:125:ARG:HG2 | 1:2:125:ARG:HH11 | 1.76 | 0.49 |
| 1:B:142:HIS:CG | 1:B:143:GLY:H | 2.29 | 0.49 |
| 1:B:305:ARG:HE | 1:M:48:LEU:HD11 | 1.77 | 0.49 |
| 1:D:171:MET:HE1 | 1:D:300:TYR:CE2 | 2.47 | 0.49 |
| 1:H:366:LYS:O | 1:H:369:PRO:HD2 | 2.12 | 0.49 |
| 1:J:125:ARG:NH1 | 1:J:129:THR:HG21 | 2.27 | 0.49 |
| 1:K:13:THR:O | 1:K:17:TYR:HD2 | 1.94 | 0.49 |
| 1:L:105:SER:OG | 1:L:106:LYS:N | 2.45 | 0.49 |
| 1:N:128:GLU:OE2 | 1:N:165:ARG:NH1 | 2.45 | 0.49 |
| 1:Q:300:TYR:CD1 | 1:Q:304:HIS:CE1 | 3.00 | 0.49 |
| 1:R:31:ARG:NH2 | 1:R:37:LYS:O | 2.44 | 0.49 |
| 1:R:162:LYS:HD3 | 1:R:304:HIS:ND1 | 2.27 | 0.49 |
| 1:T:38:ILE:HG13 | 1:T:43:ASP:HB2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:j:114:GLU:OE1 | 1:j:114:GLU:HA | 2.12 | 0.49 |
| 1:u:257:GLU:N | 1:u:257:GLU:OE2 | 2.45 | 0.49 |
| 1:3:196:LYS:HZ1 | 1:3:210:ASN:HD21 | 1.59 | 0.49 |
| 1:3:196:LYS:NZ | 1:3:210:ASN:HD21 | 2.10 | 0.49 |
| 1:I:128:GLU:OE1 | 1:I:128:GLU:HA | 2.11 | 0.49 |
| 1:K:171:MET:HB3 | 1:K:276:VAL:HG23 | 1.94 | 0.49 |
| 1:L:196:LYS:HZ2 | 1:L:208:GLU:CD | 2.20 | 0.49 |
| 1:M:239:GLN:NE2 | 1:M:285:GLY:H | 2.11 | 0.49 |
| 1:M:267:GLY:O | 1:M:268:LEU:HD23 | 2.12 | 0.49 |
| 1:S:108:GLU:CD | 1:S:108:GLU:H | 2.20 | 0.49 |
| 1:i:78:ALA:O | 1:i:82:MET:HG3 | 2.11 | 0.49 |
| 1:i:239:GLN:HG3 | 1:i:284:VAL:HB | 1.93 | 0.49 |
| 1:i:300:TYR:CE1 | 1:i:304:HIS:CE1 | 3.00 | 0.49 |
| 1:l:84:GLU:O | 1:l:88:ILE:HG12 | 2.11 | 0.49 |
| 1:n:131:SER:HB3 | 1:n:136:LYS:HD3 | 1.93 | 0.49 |
| 1:q:79:GLU:OE1 | 1:q:305:ARG:HD2 | 2.13 | 0.49 |
| 1:u:219:ILE:HG13 | 1:u:237:VAL:HG21 | 1.92 | 0.49 |
| 1:x:23:SER:HA | 1:x:26:GLN:OE1 | 2.12 | 0.49 |
| 1:x:31:ARG:HD3 | 1:x:37:LYS:HA | 1.93 | 0.49 |
| 1:z:29:MET:HA | 1:z:32:LEU:HG | 1.94 | 0.49 |
| 1:1:111:ALA:HA | 1:1:114:GLU:OE2 | 2.12 | 0.49 |
| 1:1:159:LEU:HD23 | 1:1:160:GLU:N | 2.27 | 0.49 |
| 1:2:89:LEU:HA | 1:2:92:MET:HE3 | 1.94 | 0.49 |
| 1:3:28:SER:O | 1:3:32:LEU:HG | 2.12 | 0.49 |
| 1:F:233:VAL:HG23 | 1:F:245:ILE:HD11 | 1.94 | 0.49 |
| 1:G:184:LYS:HD2 | 1:R:158:MET:SD | 2.52 | 0.49 |
| 1:K:203:TYR:OH | 1:h:106:LYS:NZ | 2.44 | 0.49 |
| 1:M:332:SER:O | 1:M:336:ILE:HD12 | 2.11 | 0.49 |
| 1:N:85:THR:O | 1:N:89:LEU:HD23 | 2.11 | 0.49 |
| 1:P:68:ALA:O | 1:P:72:ILE:HG12 | 2.12 | 0.49 |
| 1:P:95:LEU:HD22 | 1:P:112:ILE:HG23 | 1.94 | 0.49 |
| 1:P:196:LYS:HB2 | 1:P:259:SER:OG | 2.11 | 0.49 |
| 1:R:357:ALA:O | 1:R:361:ILE:HG12 | 2.12 | 0.49 |
| 1:U:57:GLN:O | 1:U:61:LEU:HG | 2.12 | 0.49 |
| 1:U:83:ASN:HA | 1:U:305:ARG:HH12 | 1.77 | 0.49 |
| 1:U:98:GLN:OE1 | 1:U:98:GLN:HA | 2.12 | 0.49 |
| 1:U:334:SER:HA | 1:U:338:ASP:OD2 | 2.11 | 0.49 |
| 1:i:244:GLN:C | 1:i:245:ILE:HD12 | 2.37 | 0.49 |
| 1:q:91:ARG:NH1 | 1:q:94:ASP:OD2 | 2.45 | 0.49 |
| 1:r:321:ASN:O | 1:r:325:ILE:HG13 | 2.13 | 0.49 |
| 1:t:246:PHE:CD2 | 1:t:292:ALA:HB1 | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:u:328:ASN:OD1 | 1:v:76:GLN:HG2 | 2.12 | 0.49 |
| 1:v:59:ARG:HA | 1:v:62:ASP:OD1 | 2.12 | 0.49 |
| 1:1:47:GLY:HA2 | 1:1:50:ILE:HG22 | 1.94 | 0.49 |
| 1:1:262:LEU:O | 1:1:266:LEU:HG | 2.13 | 0.49 |
| 1:A:328:ASN:OD1 | 1:B:76:GLN:HG2 | 2.11 | 0.49 |
| 1:E:246:PHE:HB2 | 1:E:289:GLU:OE2 | 2.13 | 0.49 |
| 1:F:108:GLU:HG2 | 1:P:50:ILE:HD11 | 1.94 | 0.49 |
| 1:H:159:LEU:HD12 | 1:H:160:GLU:H | 1.77 | 0.49 |
| 1:N:202:SER:HA | 1:N:253:GLU:HG2 | 1.94 | 0.49 |
| 1:P:168:ASN:HD21 | 1:P:170:MET:HE1 | 1.77 | 0.49 |
| 1:S:117:THR:HA | 1:S:120:ASN:HD22 | 1.77 | 0.49 |
| 1:T:205:GLN:NE2 | 1:T:206:GLU:O | 2.46 | 0.49 |
| 1:U:128:GLU:OE2 | 1:U:165:ARG:NH1 | 2.44 | 0.49 |
| 1:c:193:ASN:HA | 1:c:262:LEU:HD21 | 1.93 | 0.49 |
| 1:h:312:GLN:O | 1:h:316:ASN:ND2 | 2.39 | 0.49 |
| 1:l:51:SER:HA | 1:l:54:LEU:HD12 | 1.93 | 0.49 |
| 1:m:209:ILE:HG22 | 1:m:211:ILE:HD11 | 1.94 | 0.49 |
| 1:n:45:ALA:O | 1:n:49:GLN:HG3 | 2.12 | 0.49 |
| 1:z:26:GLN:HA | 1:z:29:MET:HE1 | 1.95 | 0.49 |
| 1:z:37:LYS:NZ | 1:z:336:ILE:O | 2.45 | 0.49 |
| 1:z:106:LYS:O | 1:z:110:VAL:HG23 | 2.13 | 0.49 |
| 1:B:357:ALA:O | 1:B:361:ILE:HG12 | 2.13 | 0.49 |
| 1:F:303:SER:O | 1:F:307:GLU:OE2 | 2.31 | 0.49 |
| 1:M:27:THR:HG22 | 1:M:31:ARG:HH12 | 1.78 | 0.49 |
| 1:O:88:ILE:HG23 | 1:O:119:LEU:HD22 | 1.93 | 0.49 |
| 1:k:3:VAL:O | 1:k:4:ASN:C | 2.54 | 0.49 |
| 1:k:52:ASN:O | 1:k:56:VAL:HG23 | 2.12 | 0.49 |
| 1:s:319:ILE:HA | 1:s:322:LEU:HD12 | 1.95 | 0.49 |
| 1:t:187:ASN:OD1 | 1:t:187:ASN:N | 2.46 | 0.49 |
| 1:t:250:ASN:ND2 | 1:t:250:ASN:C | 2.71 | 0.49 |
| 1:u:57:GLN:O | 1:u:61:LEU:HG | 2.12 | 0.49 |
| 1:u:88:ILE:HG23 | 1:u:119:LEU:HD22 | 1.95 | 0.49 |
| 1:v:31:ARG:NH2 | 1:v:37:LYS:HB2 | 2.27 | 0.49 |
| 1:3:142:HIS:CG | 1:3:143:GLY:N | 2.80 | 0.49 |
| 1:3:288:GLN:OE1 | 1:r:153:ASN:ND2 | 2.40 | 0.49 |
| 1:A:12:MET:O | 1:A:15:GLN:HG2 | 2.13 | 0.49 |
| 1:B:82:MET:HE1 | 1:B:304:HIS:HB3 | 1.95 | 0.49 |
| 1:C:287:ALA:O | 1:C:290:SER:OG | 2.29 | 0.49 |
| 1:F:321:ASN:O | 1:F:325:ILE:HD12 | 2.13 | 0.49 |
| 1:L:162:LYS:HB2 | 1:L:164:MET:CE | 2.42 | 0.49 |
| 1:O:190:GLU:CD | 1:O:190:GLU:H | 2.20 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:192:LYS:O | 1:S:192:LYS:HG3 | 2.13 | 0.49 |
| 1:U:144:ALA:HB2 | 1:U:160:GLU:OE1 | 2.12 | 0.49 |
| 1:j:334:SER:HA | 1:j:338:ASP:OD1 | 2.13 | 0.49 |
| 1:n:262:LEU:O | 1:n:266:LEU:HG | 2.12 | 0.49 |
| 1:v:32:LEU:HD21 | 1:v:344:GLU:HG2 | 1.95 | 0.49 |
| 1:w:111:ALA:HA | 1:w:114:GLU:OE2 | 2.13 | 0.49 |
| 1:H:84:GLU:O | 1:H:88:ILE:HG13 | 2.12 | 0.49 |
| 1:I:111:ALA:HA | 1:I:114:GLU:OE1 | 2.13 | 0.49 |
| 1:I:146:SER:HA | 1:I:158:MET:HA | 1.94 | 0.49 |
| 1:J:294:ILE:O | 1:J:298:LEU:HG | 2.13 | 0.49 |
| 1:K:281:VAL:HG12 | 1:K:287:ALA:HA | 1.94 | 0.49 |
| 1:L:108:GLU:O | 1:L:112:ILE:HG12 | 2.13 | 0.49 |
| 1:L:320:SER:HA | 1:L:323:ASP:OD2 | 2.12 | 0.49 |
| 1:M:188:VAL:HG23 | 1:M:217:ASP:O | 2.13 | 0.49 |
| 1:O:25:GLN:O | 1:O:28:SER:OG | 2.30 | 0.49 |
| 1:O:179:GLU:OE1 | 1:O:180:SER:OG | 2.28 | 0.49 |
| 1:T:176:TYR:OH | 1:T:255:GLU:OE2 | 2.29 | 0.49 |
| 1:c:113:GLN:OE1 | 1:c:281:VAL:HG22 | 2.13 | 0.49 |
| 1:n:108:GLU:OE2 | 1:n:108:GLU:N | 2.36 | 0.49 |
| 1:o:12:MET:HA | 1:o:15:GLN:OE1 | 2.13 | 0.49 |
| 1:r:176:TYR:HB2 | 1:r:245:ILE:HG22 | 1.95 | 0.49 |
| 1:s:122:GLU:O | 1:s:126:ILE:HG13 | 2.13 | 0.49 |
| 1:x:79:GLU:HA | 1:x:82:MET:CE | 2.43 | 0.49 |
| 1:z:9:VAL:O | 1:z:13:THR:HG23 | 2.13 | 0.49 |
| 1:1:26:GLN:CG | 1:z:10:SER:HB3 | 2.43 | 0.49 |
| 1:2:292:ALA:HA | 1:2:295:ASP:OD2 | 2.12 | 0.49 |
| 1:B:111:ALA:HA | 1:B:114:GLU:OE1 | 2.13 | 0.49 |
| 1:C:117:THR:HA | 1:C:120:ASN:HD22 | 1.77 | 0.49 |
| 1:F:16:ARG:NE | 1:m:327:GLU:OE2 | 2.38 | 0.49 |
| 1:G:159:LEU:HB2 | 1:G:311:PHE:CE1 | 2.48 | 0.49 |
| 1:K:68:ALA:O | 1:K:72:ILE:HG13 | 2.11 | 0.49 |
| 1:L:51:SER:HB2 | 1:L:333:LYS:HZ2 | 1.77 | 0.49 |
| 1:O:62:ASP:O | 1:O:66:ARG:HG3 | 2.13 | 0.49 |
| 1:P:184:LYS:HE2 | 1:P:219:ILE:HG22 | 1.94 | 0.49 |
| 1:Q:91:ARG:NE | 1:Q:95:LEU:HD21 | 2.27 | 0.49 |
| 1:c:177:GLN:NE2 | 1:c:178:ALA:N | 2.60 | 0.49 |
| 1:h:262:LEU:O | 1:h:265:GLU:N | 2.46 | 0.49 |
| 1:l:38:ILE:HD12 | 1:l:337:LYS:HA | 1.94 | 0.49 |
| 1:n:358:SER:O | 1:n:361:ILE:HG22 | 2.13 | 0.49 |
| 1:p:214:LYS:HB2 | 1:p:217:ASP:OD1 | 2.13 | 0.49 |
| 1:r:239:GLN:HE21 | 1:r:240:ASP:CG | 2.21 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:w:277:ASP:N | 1:w:277:ASP:OD1 | 2.44 | 0.49 |
| 1:w:346:THR:O | 1:w:347:ALA:C | 2.55 | 0.49 |
| 1:z:131:SER:HB3 | 1:z:136:LYS:HD2 | 1.95 | 0.49 |
| 1:z:174:VAL:HG13 | 1:z:273:LYS:HD2 | 1.94 | 0.49 |
| 1:1:343:LYS:HA | 1:1:343:LYS:HE2 | 1.95 | 0.49 |
| 1:3:168:ASN:HD21 | 1:3:170:MET:CE | 2.26 | 0.49 |
| 1:B:137:LEU:HB2 | 1:B:138:LEU:HD22 | 1.95 | 0.49 |
| 1:G:63:VAL:HA | 1:G:66:ARG:NH1 | 2.28 | 0.49 |
| 1:H:66:ARG:H | 1:H:66:ARG:HD2 | 1.78 | 0.49 |
| 1:L:195:LEU:HD12 | 1:L:196:LYS:N | 2.28 | 0.49 |
| 1:R:351:SER:HA | 1:R:354:LEU:HD12 | 1.95 | 0.49 |
| 1:U:236:SER:OG | 1:U:244:GLN:HB2 | 2.13 | 0.49 |
| 1:c:92:MET:HE1 | 1:c:116:VAL:HA | 1.93 | 0.49 |
| 1:h:159:LEU:HD12 | 1:h:160:GLU:N | 2.27 | 0.49 |
| 1:i:348:MET:O | 1:i:352:GLN:HG3 | 2.11 | 0.49 |
| 1:k:228:GLY:HA2 | 1:l:136:LYS:NZ | 2.28 | 0.49 |
| 1:l:139:ASN:OD1 | 1:l:141:THR:HG22 | 2.12 | 0.49 |
| 1:r:183:GLY:C | 1:r:185:ASP:H | 2.21 | 0.49 |
| 1:s:170:MET:HE2 | 1:s:170:MET:N | 2.27 | 0.49 |
| 1:t:86:THR:O | 1:t:90:GLN:HG2 | 2.13 | 0.49 |
| 1:v:308:LEU:O | 1:v:312:GLN:HG3 | 2.13 | 0.49 |
| 1:z:362:LEU:HD12 | 1:z:362:LEU:O | 2.13 | 0.49 |
| 1:1:80:GLY:HA2 | 1:z:324:ASN:HD21 | 1.78 | 0.49 |
| 1:1:208:GLU:O | 1:1:209:ILE:HD13 | 2.13 | 0.49 |
| 1:3:170:MET:HG3 | 1:3:249:ASN:HD22 | 1.76 | 0.49 |
| 1:A:68:ALA:O | 1:A:72:ILE:HG13 | 2.13 | 0.49 |
| 1:C:190:GLU:OE2 | 1:C:190:GLU:N | 2.28 | 0.49 |
| 1:D:196:LYS:C | 1:D:197:ILE:HD13 | 2.38 | 0.49 |
| 1:E:288:GLN:NE2 | 1:P:153:ASN:OD1 | 2.46 | 0.49 |
| 1:F:104:ASN:O | 1:F:109:ARG:NH2 | 2.44 | 0.49 |
| 1:I:300:TYR:CE1 | 1:I:304:HIS:NE2 | 2.81 | 0.49 |
| 1:J:184:LYS:CD | 1:U:158:MET:HE1 | 2.42 | 0.49 |
| 1:K:84:GLU:O | 1:K:88:ILE:HG12 | 2.13 | 0.49 |
| 1:M:214:LYS:HD3 | 1:M:216:GLY:H | 1.77 | 0.49 |
| 1:N:49:GLN:O | 1:N:53:ARG:HG2 | 2.12 | 0.49 |
| 1:h:70:ASP:OD2 | 1:s:101:ASN:ND2 | 2.42 | 0.49 |
| 1:j:297:ALA:O | 1:j:301:VAL:HG22 | 2.13 | 0.49 |
| 1:k:157:VAL:CG2 | 1:k:314:ARG:HH22 | 2.18 | 0.49 |
| 1:k:349:THR:O | 1:k:353:ILE:HG12 | 2.13 | 0.49 |
| 1:l:164:MET:HE1 | 1:l:301:VAL:HG12 | 1.95 | 0.49 |
| 1:n:5:VAL:HG22 | 1:n:372:ALA:HB1 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:r:217:ASP:OD1 | 1:r:217:ASP:N | 2.45 | 0.49 |
| 1:t:28:SER:O | 1:t:32:LEU:HG | 2.13 | 0.49 |
| 1:x:290:SER:O | 1:x:294:ILE:HG12 | 2.12 | 0.49 |
| 1:3:172:GLY:HA2 | 1:3:275:THR:HA | 1.96 | 0.48 |
| 1:B:168:ASN:O | 1:B:171:MET:HB2 | 2.13 | 0.48 |
| 1:E:29:MET:O | 1:E:32:LEU:HB3 | 2.12 | 0.48 |
| 1:E:168:ASN:HB3 | 1:E:171:MET:HG2 | 1.95 | 0.48 |
| 1:G:173:GLY:HA3 | 1:G:246:PHE:CZ | 2.48 | 0.48 |
| 1:G:272:LYS:HD3 | 1:G:272:LYS:C | 2.38 | 0.48 |
| 1:H:49:GLN:O | 1:H:53:ARG:HG2 | 2.13 | 0.48 |
| 1:I:192:LYS:NZ | 1:I:265:GLU:OE1 | 2.31 | 0.48 |
| 1:J:82:MET:HE1 | 1:J:304:HIS:HB3 | 1.95 | 0.48 |
| 1:K:142:HIS:CG | 1:K:143:GLY:H | 2.30 | 0.48 |
| 1:K:290:SER:O | 1:K:293:ILE:HG22 | 2.12 | 0.48 |
| 1:O:122:GLU:OE1 | 1:O:125:ARG:NH2 | 2.45 | 0.48 |
| 1:S:194:ASP:CG | 1:S:261:GLY:H | 2.21 | 0.48 |
| 1:T:332:SER:O | 1:T:336:ILE:HD12 | 2.13 | 0.48 |
| 1:V:53:ARG:HG2 | 1:V:53:ARG:HH11 | 1.78 | 0.48 |
| 1:c:95:LEU:HD21 | 1:c:115:GLU:HB3 | 1.95 | 0.48 |
| 1:h:108:GLU:CD | 1:h:108:GLU:H | 2.21 | 0.48 |
| 1:i:366:LYS:HD2 | 1:s:349:THR:HG21 | 1.94 | 0.48 |
| 1:n:246:PHE:HZ | 1:n:293:ILE:HD13 | 1.76 | 0.48 |
| 1:o:171:MET:SD | 1:o:300:TYR:CD1 | 3.06 | 0.48 |
| 1:p:58:SER:HA | 1:p:61:LEU:HD12 | 1.94 | 0.48 |
| 1:p:248:GLY:O | 1:p:252:VAL:HG12 | 2.13 | 0.48 |
| 1:p:369:PRO:HD2 | 1:p:370:ASN:N | 2.23 | 0.48 |
| 1:t:169:LYS:HD3 | 1:t:169:LYS:N | 2.28 | 0.48 |
| 1:u:273:LYS:HD3 | 1:u:273:LYS:N | 2.28 | 0.48 |
| 1:w:84:GLU:HA | 1:w:87:ASN:HD22 | 1.76 | 0.48 |
| 1:z:184:LYS:NZ | 1:z:218:ASP:OD1 | 2.42 | 0.48 |
| 1:2:72:ILE:HD11 | 1:2:319:ILE:HD11 | 1.94 | 0.48 |
| 1:3:93:ARG:NH2 | 1:r:151:ALA:O | 2.45 | 0.48 |
| 1:D:161:LEU:HA | 1:D:162:LYS:NZ | 2.28 | 0.48 |
| 1:E:357:ALA:O | 1:E:361:ILE:HG12 | 2.13 | 0.48 |
| 1:G:108:GLU:O | 1:G:112:ILE:HG13 | 2.13 | 0.48 |
| 1:H:162:LYS:O | 1:H:164:MET:HE2 | 2.13 | 0.48 |
| 1:H:316:ASN:HA | 1:H:319:ILE:HD12 | 1.95 | 0.48 |
| 1:I:49:GLN:HE22 | 1:p:302:ASP:HB2 | 1.77 | 0.48 |
| 1:J:47:GLY:HA2 | 1:J:50:ILE:HD12 | 1.94 | 0.48 |
| 1:N:151:ALA:N | 1:N:155:GLU:OE1 | 2.45 | 0.48 |
| 1:P:191:GLY:O | 1:P:192:LYS:HE3 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:Q:319:ILE:HA | 1:Q:322:LEU:HD12 | 1.95 | 0.48 |
| 1:R:220:GLU:CG | 1:R:237:VAL:HG11 | 2.43 | 0.48 |
| 1:S:316:ASN:O | 1:S:319:ILE:HG12 | 2.13 | 0.48 |
| 1:o:240:ASP:HB3 | 1:o:242:LYS:HG3 | 1.94 | 0.48 |
| 1:r:205:GLN:HG2 | 1:r:206:GLU:N | 2.27 | 0.48 |
| 1:s:69:ASN:HA | 1:s:72:ILE:HD12 | 1.95 | 0.48 |
| 1:w:299:LYS:HD2 | 1:w:299:LYS:C | 2.38 | 0.48 |
| 1:x:196:LYS:HD3 | 1:x:196:LYS:N | 2.27 | 0.48 |
| 1:2:17:TYR:HD1 | 1:3:33:SER:HB3 | 1.78 | 0.48 |
| 1:A:79:GLU:OE1 | 1:A:305:ARG:NE | 2.46 | 0.48 |
| 1:D:277:ASP:N | 1:D:277:ASP:OD1 | 2.45 | 0.48 |
| 1:F:210:ASN:C | 1:F:211:ILE:HD12 | 2.38 | 0.48 |
| 1:G:31:ARG:HH11 | 1:G:31:ARG:HG2 | 1.77 | 0.48 |
| 1:K:106:LYS:NZ | 1:K:282:THR:O | 2.45 | 0.48 |
| 1:O:91:ARG:O | 1:O:95:LEU:HG | 2.13 | 0.48 |
| 1:P:28:SER:HB2 | 1:P:29:MET:HE2 | 1.95 | 0.48 |
| 1:k:314:ARG:HD2 | 1:w:118:ALA:O | 2.12 | 0.48 |
| 1:l:91:ARG:O | 1:l:95:LEU:HG | 2.13 | 0.48 |
| 1:l:287:ALA:O | 1:l:291:VAL:HG23 | 2.12 | 0.48 |
| 1:p:15:GLN:HE22 | 1:z:343:LYS:HZ3 | 1.59 | 0.48 |
| 1:q:322:LEU:HA | 1:q:325:ILE:HD12 | 1.95 | 0.48 |
| 1:r:59:ARG:HA | 1:r:62:ASP:OD2 | 2.13 | 0.48 |
| 1:s:276:VAL:O | 1:s:279:ILE:HG12 | 2.12 | 0.48 |
| 1:u:251:LYS:HG2 | 1:u:251:LYS:O | 2.14 | 0.48 |
| 1:v:244:GLN:NE2 | 1:v:289:GLU:OE1 | 2.46 | 0.48 |
| 1:w:169:LYS:HE2 | 1:w:169:LYS:HA | 1.95 | 0.48 |
| 1:x:160:GLU:OE1 | 1:x:161:LEU:N | 2.47 | 0.48 |
| 1:z:190:GLU:OE2 | 1:z:190:GLU:N | 2.25 | 0.48 |
| 1:z:196:LYS:HB2 | 1:z:259:SER:OG | 2.13 | 0.48 |
| 1:B:170:MET:HE1 | 1:B:250:ASN:HB3 | 1.96 | 0.48 |
| 1:D:108:GLU:HG2 | 1:N:50:ILE:HD11 | 1.96 | 0.48 |
| 1:D:226:ILE:HA | 1:D:229:GLN:HG2 | 1.95 | 0.48 |
| 1:F:162:LYS:HE3 | 1:F:304:HIS:CG | 2.47 | 0.48 |
| 1:G:55:ASN:O | 1:G:59:ARG:HG3 | 2.14 | 0.48 |
| 1:H:65:VAL:HG13 | 1:H:319:ILE:HG23 | 1.95 | 0.48 |
| 1:J:170:MET:HE2 | 1:J:170:MET:HA | 1.94 | 0.48 |
| 1:L:37:LYS:NZ | 1:L:336:ILE:O | 2.41 | 0.48 |
| 1:O:169:LYS:HG3 | 1:O:170:MET:HE3 | 1.95 | 0.48 |
| 1:R:84:GLU:O | 1:R:88:ILE:HD12 | 2.13 | 0.48 |
| 1:R:192:LYS:HA | 1:R:261:GLY:CA | 2.39 | 0.48 |
| 1:U:79:GLU:HA | 1:U:82:MET:HE3 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:i:304:HIS:HA | 1:i:307:GLU:CD | 2.38 | 0.48 |
| 1:n:139:ASN:OD1 | 1:n:141:THR:HG22 | 2.12 | 0.48 |
| 1:n:275:THR:OG1 | 1:n:277:ASP:OD1 | 2.26 | 0.48 |
| 1:n:287:ALA:O | 1:n:290:SER:OG | 2.25 | 0.48 |
| 1:o:37:LYS:HG2 | 1:o:337:LYS:O | 2.12 | 0.48 |
| 1:q:185:ASP:N | 1:q:185:ASP:OD1 | 2.46 | 0.48 |
| 1:r:239:GLN:CD | 1:r:239:GLN:H | 2.21 | 0.48 |
| 1:t:332:SER:O | 1:t:336:ILE:HG12 | 2.14 | 0.48 |
| 1:t:368:ALA:HB3 | 1:t:369:PRO:HD3 | 1.95 | 0.48 |
| 1:1:315:PHE:O | 1:1:319:ILE:HG13 | 2.13 | 0.48 |
| 1:B:144:ALA:O | 1:B:145:LYS:HD2 | 2.14 | 0.48 |
| 1:B:256:VAL:HG12 | 1:B:258:PHE:CE1 | 2.48 | 0.48 |
| 1:D:162:LYS:HG3 | 1:D:304:HIS:HD2 | 1.78 | 0.48 |
| 1:E:194:ASP:OD1 | 1:E:261:GLY:N | 2.34 | 0.48 |
| 1:H:192:LYS:NZ | 1:H:261:GLY:HA2 | 2.29 | 0.48 |
| 1:L:59:ARG:HA | 1:L:62:ASP:OD1 | 2.14 | 0.48 |
| 1:L:69:ASN:O | 1:L:72:ILE:HG22 | 2.13 | 0.48 |
| 1:L:144:ALA:HB1 | 1:L:158:MET:SD | 2.54 | 0.48 |
| 1:L:238:ASP:OD1 | 1:L:238:ASP:N | 2.47 | 0.48 |
| 1:Q:300:TYR:O | 1:Q:304:HIS:ND1 | 2.47 | 0.48 |
| 1:S:85:THR:HA | 1:S:88:ILE:HD12 | 1.96 | 0.48 |
| 1:S:188:VAL:HG23 | 1:S:217:ASP:O | 2.12 | 0.48 |
| 1:h:227:ASN:HD21 | 1:h:235:ALA:HB3 | 1.79 | 0.48 |
| 1:i:280:ASP:OD1 | 1:i:282:THR:HG23 | 2.13 | 0.48 |
| 1:i:343:LYS:NZ | 1:i:343:LYS:HB2 | 2.28 | 0.48 |
| 1:l:3:VAL:HG12 | 1:w:342:ALA:HB2 | 1.95 | 0.48 |
| 1:o:2:ALA:N | 1:z:340:ASP:OD1 | 2.46 | 0.48 |
| 1:q:159:LEU:HD23 | 1:q:160:GLU:N | 2.28 | 0.48 |
| 1:s:22:ASN:O | 1:s:26:GLN:HG3 | 2.12 | 0.48 |
| 1:t:365:ALA:O | 1:t:369:PRO:HD3 | 2.13 | 0.48 |
| 1:u:176:TYR:OH | 1:u:255:GLU:OE1 | 2.25 | 0.48 |
| 1:w:194:ASP:CG | 1:w:261:GLY:H | 2.22 | 0.48 |
| 1:z:31:ARG:NH2 | 1:z:43:ASP:OD1 | 2.47 | 0.48 |
| 1:B:113:GLN:HB2 | 1:B:281:VAL:HG22 | 1.95 | 0.48 |
| 1:E:122:GLU:OE1 | 1:O:314:ARG:NE | 2.31 | 0.48 |
| 1:J:169:LYS:H | 1:J:169:LYS:CD | 2.26 | 0.48 |
| 1:L:366:LYS:O | 1:L:369:PRO:HD2 | 2.13 | 0.48 |
| 1:N:4:ASN:ND2 | 1:N:4:ASN:O | 2.45 | 0.48 |
| 1:O:223:ALA:O | 1:O:226:ILE:HG22 | 2.14 | 0.48 |
| 1:i:299:LYS:NZ | 1:i:303:SER:HB2 | 2.29 | 0.48 |
| 1:l:223:ALA:HA | 1:l:226:ILE:HD12 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:n:4:ASN:HD21 | 1:n:6:ASN:HB2 | 1.78 | 0.48 |
| 1:n:26:GLN:HA | 1:n:29:MET:HE2 | 1.94 | 0.48 |
| 1:o:31:ARG:HD3 | 1:o:344:GLU:OE2 | 2.14 | 0.48 |
| 1:o:196:LYS:HD3 | 1:o:209:ILE:O | 2.14 | 0.48 |
| 1:p:243:LEU:HD13 | 1:p:266:LEU:HD13 | 1.96 | 0.48 |
| 1:u:348:MET:O | 1:u:352:GLN:HG2 | 2.13 | 0.48 |
| 1:x:173:GLY:HA3 | 1:x:246:PHE:CZ | 2.49 | 0.48 |
| 1:z:205:GLN:NE2 | 1:z:206:GLU:H | 2.12 | 0.48 |
| 1:2:203:TYR:HB2 | 1:2:205:GLN:HE22 | 1.79 | 0.48 |
| 1:2:305:ARG:NH1 | 1:q:48:LEU:HD11 | 2.29 | 0.48 |
| 1:3:26:GLN:NE2 | 1:3:29:MET:SD | 2.84 | 0.48 |
| 1:A:125:ARG:HG2 | 1:A:125:ARG:HH11 | 1.79 | 0.48 |
| 1:C:78:ALA:O | 1:C:82:MET:HG2 | 2.14 | 0.48 |
| 1:C:220:GLU:H | 1:C:220:GLU:HG2 | 1.47 | 0.48 |
| 1:D:25:GLN:O | 1:D:29:MET:HG3 | 2.14 | 0.48 |
| 1:D:175:SER:O | 1:D:271:GLY:HA2 | 2.13 | 0.48 |
| 1:H:243:LEU:HD23 | 1:H:244:GLN:N | 2.28 | 0.48 |
| 1:J:210:ASN:O | 1:J:211:ILE:HD13 | 2.13 | 0.48 |
| 1:N:68:ALA:O | 1:N:72:ILE:HG13 | 2.13 | 0.48 |
| 1:N:126:ILE:O | 1:N:130:THR:OG1 | 2.30 | 0.48 |
| 1:N:149:ILE:HD11 | 1:O:125:ARG:HH12 | 1.79 | 0.48 |
| 1:N:195:LEU:HB2 | 1:N:262:LEU:HB2 | 1.95 | 0.48 |
| 1:O:25:GLN:O | 1:O:29:MET:HG3 | 2.13 | 0.48 |
| 1:O:91:ARG:NH1 | 1:O:95:LEU:HD21 | 2.28 | 0.48 |
| 1:O:175:SER:O | 1:O:271:GLY:HA2 | 2.13 | 0.48 |
| 1:P:239:GLN:NE2 | 1:P:240:ASP:OD1 | 2.29 | 0.48 |
| 1:Q:239:GLN:CD | 1:Q:239:GLN:H | 2.21 | 0.48 |
| 1:U:87:ASN:O | 1:U:90:GLN:HG3 | 2.14 | 0.48 |
| 1:U:233:VAL:HG13 | 1:U:246:PHE:O | 2.14 | 0.48 |
| 1:V:338:ASP:OD1 | 1:V:339:THR:N | 2.47 | 0.48 |
| 1:o:250:ASN:C | 1:o:250:ASN:OD1 | 2.57 | 0.48 |
| 1:p:316:ASN:O | 1:p:319:ILE:HG22 | 2.14 | 0.48 |
| 1:r:105:SER:OG | 1:r:106:LYS:N | 2.47 | 0.48 |
| 1:t:32:LEU:HD23 | 1:t:344:GLU:HG2 | 1.96 | 0.48 |
| 1:x:79:GLU:HA | 1:x:82:MET:HE1 | 1.95 | 0.48 |
| 1:2:184:LYS:NZ | 1:2:218:ASP:OD2 | 2.34 | 0.48 |
| 1:2:220:GLU:OE1 | 1:2:220:GLU:HA | 2.13 | 0.48 |
| 1:A:30:GLU:CD | 1:A:39:ASN:HD22 | 2.21 | 0.48 |
| 1:C:49:GLN:HA | 1:C:52:ASN:ND2 | 2.27 | 0.48 |
| 1:D:5:VAL:HG13 | 1:k:341:PHE:CE1 | 2.49 | 0.48 |
| 1:D:159:LEU:HD23 | 1:D:160:GLU:N | 2.29 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:214:LYS:HD3 | 1:T:165:ARG:HH22 | 1.77 | 0.48 |
| 1:L:177:GLN:NE2 | 1:L:244:GLN:HB3 | 2.28 | 0.48 |
| 1:P:192:LYS:O | 1:P:262:LEU:HD13 | 2.14 | 0.48 |
| 1:Q:79:GLU:HA | 1:Q:82:MET:HE2 | 1.95 | 0.48 |
| 1:Q:371:SER:O | 1:Q:374:SER:OG | 2.30 | 0.48 |
| 1:c:109:ARG:HB3 | 1:c:282:THR:HA | 1.95 | 0.48 |
| 1:i:52:ASN:O | 1:i:56:VAL:HG23 | 2.14 | 0.48 |
| 1:n:149:ILE:O | 1:n:149:ILE:HG13 | 2.13 | 0.48 |
| 1:n:162:LYS:HE3 | 1:n:300:TYR:OH | 2.14 | 0.48 |
| 1:t:27:THR:CG2 | 1:t:31:ARG:HE | 2.27 | 0.48 |
| 1:t:343:LYS:HZ3 | 1:u:15:GLN:HE22 | 1.60 | 0.48 |
| 1:x:320:SER:O | 1:x:323:ASP:OD2 | 2.31 | 0.48 |
| 1:x:320:SER:O | 1:x:324:ASN:OD1 | 2.31 | 0.48 |
| 1:z:273:LYS:N | 1:z:273:LYS:HD3 | 2.29 | 0.48 |
| 1:2:31:ARG:HD3 | 1:2:37:LYS:HA | 1.96 | 0.48 |
| 1:A:321:ASN:O | 1:A:325:ILE:HG13 | 2.14 | 0.48 |
| 1:B:40:SER:OG | 1:B:42:LYS:NZ | 2.44 | 0.48 |
| 1:C:6:ASN:N | 1:C:6:ASN:OD1 | 2.45 | 0.48 |
| 1:F:302:ASP:OD1 | 1:F:302:ASP:N | 2.47 | 0.48 |
| 1:I:299:LYS:HD2 | 1:I:299:LYS:O | 2.13 | 0.48 |
| 1:J:81:ALA:O | 1:J:85:THR:HG23 | 2.13 | 0.48 |
| 1:M:276:VAL:O | 1:M:279:ILE:HG12 | 2.12 | 0.48 |
| 1:R:28:SER:HA | 1:R:344:GLU:OE2 | 2.13 | 0.48 |
| 1:S:262:LEU:O | 1:S:266:LEU:HG | 2.14 | 0.48 |
| 1:S:364:GLN:OE1 | 1:S:364:GLN:HA | 2.14 | 0.48 |
| 1:U:150:GLY:HA3 | 1:U:155:GLU:HB2 | 1.96 | 0.48 |
| 1:U:219:ILE:HG13 | 1:U:220:GLU:N | 2.27 | 0.48 |
| 1:c:94:ASP:OD1 | 1:c:95:LEU:N | 2.46 | 0.48 |
| 1:j:177:GLN:N | 1:j:177:GLN:OE1 | 2.46 | 0.48 |
| 1:k:287:ALA:HA | 1:k:290:SER:OG | 2.14 | 0.48 |
| 1:o:173:GLY:HA3 | 1:o:246:PHE:CZ | 2.49 | 0.48 |
| 1:p:12:MET:HG3 | 1:z:343:LYS:HZ1 | 1.78 | 0.48 |
| 1:q:239:GLN:CD | 1:q:239:GLN:H | 2.22 | 0.48 |
| 1:r:49:GLN:HA | 1:r:52:ASN:OD1 | 2.13 | 0.48 |
| 1:s:130:THR:HG21 | 1:s:138:LEU:HD23 | 1.96 | 0.48 |
| 1:u:162:LYS:HZ1 | 1:u:304:HIS:HB3 | 1.77 | 0.48 |
| 1:u:238:ASP:OD2 | 1:u:242:LYS:HB2 | 2.14 | 0.48 |
| 1:z:9:VAL:HG23 | 1:z:12:MET:HE1 | 1.95 | 0.48 |
| 1:1:287:ALA:O | 1:1:291:VAL:HG23 | 2.13 | 0.48 |
| 1:B:89:LEU:HA | 1:B:92:MET:HG3 | 1.95 | 0.48 |
| 1:D:23:SER:O | 1:D:27:THR:HG22 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:37:LYS:NZ | 1:D:336:ILE:O | 2.41 | 0.48 |
| 1:I:240:ASP:HB2 | 1:I:242:LYS:HG3 | 1.95 | 0.48 |
| 1:J:125:ARG:HD3 | 1:T:314:ARG:NH2 | 2.28 | 0.48 |
| 1:M:170:MET:N | 1:M:170:MET:SD | 2.86 | 0.48 |
| 1:P:31:ARG:NH1 | 1:P:36:PHE:O | 2.46 | 0.48 |
| 1:P:70:ASP:O | 1:P:73:SER:OG | 2.28 | 0.48 |
| 1:R:211:ILE:HG22 | 1:R:212:SER:O | 2.14 | 0.48 |
| 1:c:194:ASP:O | 1:c:261:GLY:N | 2.47 | 0.48 |
| 1:j:321:ASN:O | 1:j:325:ILE:HG13 | 2.14 | 0.48 |
| 1:l:236:SER:HB3 | 1:l:288:GLN:HG3 | 1.95 | 0.48 |
| 1:n:199:LEU:HB3 | 1:n:256:VAL:HG22 | 1.96 | 0.48 |
| 1:t:84:GLU:O | 1:t:88:ILE:HG12 | 2.14 | 0.48 |
| 1:t:330:ASN:HA | 1:t:333:LYS:HE2 | 1.95 | 0.48 |
| 1:u:376:LEU:HD12 | 1:u:377:GLY:N | 2.29 | 0.48 |
| 1:w:221:GLU:N | 1:w:221:GLU:OE2 | 2.47 | 0.48 |
| 1:2:366:LYS:NZ | 1:p:375:LEU:O | 2.45 | 0.47 |
| 1:3:199:LEU:HD13 | 1:3:252:VAL:HG22 | 1.94 | 0.47 |
| 1:B:212:SER:O | 1:B:214:LYS:NZ | 2.38 | 0.47 |
| 1:D:138:LEU:HB3 | 1:D:164:MET:HG2 | 1.95 | 0.47 |
| 1:D:375:LEU:O | 1:D:377:GLY:N | 2.47 | 0.47 |
| 1:H:168:ASN:ND2 | 1:H:300:TYR:OH | 2.47 | 0.47 |
| 1:I:101:ASN:HB2 | 1:T:67:ASN:OD1 | 2.14 | 0.47 |
| 1:J:361:ILE:HD11 | 1:V:376:LEU:HD11 | 1.95 | 0.47 |
| 1:K:49:GLN:HG2 | 1:K:53:ARG:NH2 | 2.29 | 0.47 |
| 1:L:246:PHE:HZ | 1:L:293:ILE:HG13 | 1.78 | 0.47 |
| 1:M:83:ASN:OD1 | 1:M:83:ASN:C | 2.57 | 0.47 |
| 1:N:273:LYS:C | 1:N:273:LYS:HD3 | 2.39 | 0.47 |
| 1:P:219:ILE:HD11 | 1:P:243:LEU:CD2 | 2.44 | 0.47 |
| 1:S:115:GLU:O | 1:S:119:LEU:HG | 2.14 | 0.47 |
| 1:S:294:ILE:O | 1:S:298:LEU:HD23 | 2.14 | 0.47 |
| 1:U:159:LEU:HD22 | 1:U:311:PHE:CE1 | 2.49 | 0.47 |
| 1:U:209:ILE:HG22 | 1:U:211:ILE:HD11 | 1.95 | 0.47 |
| 1:m:12:MET:O | 1:m:15:GLN:HG2 | 2.14 | 0.47 |
| 1:v:357:ALA:O | 1:v:361:ILE:HG12 | 2.14 | 0.47 |
| 1:x:48:LEU:O | 1:x:52:ASN:ND2 | 2.47 | 0.47 |
| 1:C:69:ASN:HB3 | 1:M:335:ARG:HD3 | 1.97 | 0.47 |
| 1:K:314:ARG:NE | 1:h:122:GLU:OE1 | 2.47 | 0.47 |
| 1:M:22:ASN:H | 1:M:22:ASN:HD22 | 1.62 | 0.47 |
| 1:N:152:ASP:N | 1:N:155:GLU:OE1 | 2.45 | 0.47 |
| 1:O:349:THR:O | 1:O:353:ILE:HD12 | 2.15 | 0.47 |
| 1:P:147:PHE:HE1 | 1:P:159:LEU:HD23 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:91:ARG:CZ | 1:Q:95:LEU:HD21 | 2.44 | 0.47 |
| 1:R:276:VAL:O | 1:R:279:ILE:HG12 | 2.14 | 0.47 |
| 1:R:299:LYS:NZ | 1:c:49:GLN:OE1 | 2.46 | 0.47 |
| 1:T:31:ARG:HD3 | 1:T:37:LYS:HA | 1.95 | 0.47 |
| 1:V:201:ASP:HB3 | 1:V:207:GLN:NE2 | 2.29 | 0.47 |
| 1:j:4:ASN:OD1 | 1:j:4:ASN:O | 2.32 | 0.47 |
| 1:k:28:SER:O | 1:k:32:LEU:HD23 | 2.14 | 0.47 |
| 1:k:201:ASP:OD2 | 1:k:203:TYR:HB2 | 2.14 | 0.47 |
| 1:l:202:SER:HB3 | 1:l:251:LYS:C | 2.39 | 0.47 |
| 1:l:311:PHE:CE1 | 1:l:315:PHE:HE1 | 2.32 | 0.47 |
| 1:n:178:ALA:HB3 | 1:n:242:LYS:HB3 | 1.96 | 0.47 |
| 1:s:166:SER:OG | 1:s:277:ASP:OD2 | 2.29 | 0.47 |
| 1:t:65:VAL:HG12 | 1:t:66:ARG:NH2 | 2.30 | 0.47 |
| 1:z:159:LEU:HD12 | 1:z:160:GLU:H | 1.78 | 0.47 |
| 1:z:162:LYS:N | 1:z:162:LYS:HD3 | 2.28 | 0.47 |
| 1:z:208:GLU:O | 1:z:209:ILE:HD13 | 2.14 | 0.47 |
| 1:1:243:LEU:HD23 | 1:1:244:GLN:N | 2.28 | 0.47 |
| 1:B:110:VAL:HG12 | 1:B:114:GLU:OE2 | 2.14 | 0.47 |
| 1:D:162:LYS:HG3 | 1:D:304:HIS:CD2 | 2.50 | 0.47 |
| 1:G:208:GLU:OE2 | 1:G:210:ASN:ND2 | 2.47 | 0.47 |
| 1:L:91:ARG:O | 1:L:91:ARG:HD3 | 2.15 | 0.47 |
| 1:P:364:GLN:HA | 1:P:367:GLN:OE1 | 2.14 | 0.47 |
| 1:U:25:GLN:CD | 1:U:352:GLN:HG3 | 2.39 | 0.47 |
| 1:h:12:MET:O | 1:h:16:ARG:HG3 | 2.13 | 0.47 |
| 1:o:12:MET:O | 1:o:16:ARG:HG3 | 2.14 | 0.47 |
| 1:o:144:ALA:HB1 | 1:o:158:MET:CE | 2.45 | 0.47 |
| 1:q:30:GLU:OE1 | 1:q:31:ARG:HG3 | 2.15 | 0.47 |
| 1:q:349:THR:O | 1:q:353:ILE:HG12 | 2.14 | 0.47 |
| 1:r:77:THR:HG21 | 1:r:132:PHE:CD2 | 2.48 | 0.47 |
| 1:r:218:ASP:O | 1:r:222:LEU:N | 2.44 | 0.47 |
| 1:u:12:MET:O | 1:u:16:ARG:HG3 | 2.14 | 0.47 |
| 1:v:88:ILE:HG23 | 1:v:119:LEU:HD22 | 1.96 | 0.47 |
| 1:v:208:GLU:O | 1:v:209:ILE:HD13 | 2.14 | 0.47 |
| 1:B:160:GLU:OE2 | 1:B:162:LYS:HD3 | 2.14 | 0.47 |
| 1:E:25:GLN:HB3 | 1:E:351:SER:HB2 | 1.95 | 0.47 |
| 1:F:125:ARG:NH1 | 1:F:129:THR:HG21 | 2.29 | 0.47 |
| 1:H:56:VAL:HG22 | 1:o:90:GLN:OE1 | 2.14 | 0.47 |
| 1:H:108:GLU:OE1 | 1:H:108:GLU:N | 2.36 | 0.47 |
| 1:I:108:GLU:H | 1:I:108:GLU:CD | 2.22 | 0.47 |
| 1:K:149:ILE:HD11 | 1:h:125:ARG:HE | 1.80 | 0.47 |
| 1:K:239:GLN:H | 1:K:239:GLN:CD | 2.22 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:97:LEU:HD23 | 1:O:291:VAL:HG21 | 1.96 | 0.47 |
| 1:P:163:ASP:OD1 | 1:P:165:ARG:HG2 | 2.14 | 0.47 |
| 1:Q:249:ASN:HA | 1:Q:252:VAL:O | 2.14 | 0.47 |
| 1:T:188:VAL:HB | 1:T:216:GLY:H | 1.79 | 0.47 |
| 1:V:85:THR:O | 1:V:89:LEU:HD13 | 2.14 | 0.47 |
| 1:j:332:SER:O | 1:j:336:ILE:HD12 | 2.14 | 0.47 |
| 1:l:220:GLU:OE1 | 1:l:237:VAL:HB | 2.14 | 0.47 |
| 1:t:61:LEU:O | 1:t:65:VAL:HG23 | 2.15 | 0.47 |
| 1:v:159:LEU:HD13 | 1:v:311:PHE:CE1 | 2.49 | 0.47 |
| 1:1:126:ILE:O | 1:1:130:THR:HG23 | 2.14 | 0.47 |
| 1:1:238:ASP:OD1 | 1:1:242:LYS:HG2 | 2.14 | 0.47 |
| 1:2:270:GLU:O | 1:2:272:LYS:HD3 | 2.14 | 0.47 |
| 1:B:168:ASN:OD1 | 1:B:170:MET:HB2 | 2.15 | 0.47 |
| 1:B:169:LYS:HD2 | 1:B:169:LYS:O | 2.15 | 0.47 |
| 1:F:332:SER:O | 1:F:336:ILE:HG12 | 2.14 | 0.47 |
| 1:H:6:ASN:HD22 | 1:H:6:ASN:H | 1.59 | 0.47 |
| 1:J:139:ASN:O | 1:J:141:THR:HG23 | 2.14 | 0.47 |
| 1:K:106:LYS:HE2 | 1:K:106:LYS:HA | 1.96 | 0.47 |
| 1:L:325:ILE:O | 1:L:329:VAL:HG23 | 2.14 | 0.47 |
| 1:O:122:GLU:O | 1:O:126:ILE:HG12 | 2.14 | 0.47 |
| 1:O:253:GLU:N | 1:O:253:GLU:OE2 | 2.46 | 0.47 |
| 1:P:9:VAL:O | 1:P:13:THR:HG23 | 2.15 | 0.47 |
| 1:P:28:SER:O | 1:P:31:ARG:HB3 | 2.14 | 0.47 |
| 1:T:193:ASN:HA | 1:T:262:LEU:HD21 | 1.97 | 0.47 |
| 1:T:332:SER:HA | 1:T:335:ARG:HG3 | 1.95 | 0.47 |
| 1:V:164:MET:HE2 | 1:V:304:HIS:HD2 | 1.80 | 0.47 |
| 1:c:177:GLN:OE1 | 1:c:244:GLN:HB3 | 2.15 | 0.47 |
| 1:i:53:ARG:HH11 | 1:i:53:ARG:HB2 | 1.79 | 0.47 |
| 1:k:231:ASP:OD1 | 1:k:231:ASP:N | 2.32 | 0.47 |
| 1:l:113:GLN:OE1 | 1:l:281:VAL:HG22 | 2.14 | 0.47 |
| 1:s:321:ASN:HD21 | 1:t:126:ILE:HG23 | 1.79 | 0.47 |
| 1:t:164:MET:HA | 1:t:164:MET:HE3 | 1.97 | 0.47 |
| 1:v:85:THR:O | 1:v:89:LEU:HD13 | 2.14 | 0.47 |
| 1:w:113:GLN:OE1 | 1:w:281:VAL:HG22 | 2.14 | 0.47 |
| 1:z:207:GLN:N | 1:z:207:GLN:OE1 | 2.47 | 0.47 |
| 1:C:64:ALA:HB1 | 1:C:149:ILE:O | 2.14 | 0.47 |
| 1:F:321:ASN:OD1 | 1:F:325:ILE:HD11 | 2.14 | 0.47 |
| 1:F:350:LYS:O | 1:F:354:LEU:HG | 2.14 | 0.47 |
| 1:G:170:MET:HE2 | 1:G:170:MET:N | 2.30 | 0.47 |
| 1:I:179:GLU:HG2 | 1:I:180:SER:N | 2.30 | 0.47 |
| 1:K:109:ARG:HB3 | 1:K:282:THR:HA | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:109:ARG:HB3 | 1:M:282:THR:HA | 1.95 | 0.47 |
| 1:N:13:THR:HG1 | 1:N:17:TYR:HE2 | 1.62 | 0.47 |
| 1:N:214:LYS:HG2 | 1:N:215:ALA:O | 2.15 | 0.47 |
| 1:O:118:ALA:HA | 1:O:121:ASP:OD1 | 2.14 | 0.47 |
| 1:P:149:ILE:HD11 | 1:Q:125:ARG:NH1 | 2.28 | 0.47 |
| 1:S:159:LEU:HD12 | 1:S:160:GLU:H | 1.79 | 0.47 |
| 1:U:105:SER:OG | 1:U:108:GLU:OE1 | 2.22 | 0.47 |
| 1:V:106:LYS:HZ2 | 1:V:282:THR:HB | 1.80 | 0.47 |
| 1:V:164:MET:HE1 | 1:V:301:VAL:HG12 | 1.97 | 0.47 |
| 1:V:297:ALA:O | 1:V:301:VAL:HG22 | 2.14 | 0.47 |
| 1:V:321:ASN:C | 1:V:321:ASN:OD1 | 2.56 | 0.47 |
| 1:c:68:ALA:O | 1:c:72:ILE:HG12 | 2.15 | 0.47 |
| 1:h:334:SER:OG | 1:h:338:ASP:OD2 | 2.27 | 0.47 |
| 1:h:366:LYS:O | 1:h:369:PRO:HD2 | 2.14 | 0.47 |
| 1:i:147:PHE:N | 1:i:157:VAL:O | 2.45 | 0.47 |
| 1:j:25:GLN:O | 1:j:29:MET:HG3 | 2.14 | 0.47 |
| 1:l:109:ARG:HA | 1:l:112:ILE:HD12 | 1.97 | 0.47 |
| 1:l:338:ASP:OD2 | 1:l:338:ASP:N | 2.48 | 0.47 |
| 1:m:233:VAL:HG23 | 1:m:245:ILE:HD11 | 1.97 | 0.47 |
| 1:n:122:GLU:OE1 | 1:n:125:ARG:NH1 | 2.47 | 0.47 |
| 1:n:368:ALA:HB3 | 1:n:369:PRO:HD3 | 1.97 | 0.47 |
| 1:o:158:MET:CE | 1:z:184:LYS:HG2 | 2.45 | 0.47 |
| 1:r:205:GLN:OE1 | 1:r:207:GLN:HG2 | 2.14 | 0.47 |
| 1:1:5:VAL:HG12 | 1:1:6:ASN:OD1 | 2.13 | 0.47 |
| 1:1:178:ALA:O | 1:1:242:LYS:HD3 | 2.15 | 0.47 |
| 1:2:162:LYS:NZ | 1:2:304:HIS:HB3 | 2.30 | 0.47 |
| 1:B:30:GLU:OE2 | 1:B:39:ASN:ND2 | 2.25 | 0.47 |
| 1:C:108:GLU:CD | 1:C:108:GLU:H | 2.22 | 0.47 |
| 1:E:350:LYS:HB2 | 1:E:350:LYS:NZ | 2.29 | 0.47 |
| 1:G:102:GLY:O | 1:R:145:LYS:NZ | 2.42 | 0.47 |
| 1:H:184:LYS:HE2 | 1:H:184:LYS:HA | 1.95 | 0.47 |
| 1:H:357:ALA:O | 1:H:361:ILE:HG12 | 2.13 | 0.47 |
| 1:I:88:ILE:CG2 | 1:I:119:LEU:HD12 | 2.38 | 0.47 |
| 1:J:169:LYS:HD3 | 1:J:169:LYS:N | 2.30 | 0.47 |
| 1:K:366:LYS:O | 1:K:369:PRO:HD2 | 2.15 | 0.47 |
| 1:M:18:LEU:HD12 | 1:M:22:ASN:HD21 | 1.80 | 0.47 |
| 1:M:96:SER:O | 1:M:99:SER:OG | 2.26 | 0.47 |
| 1:O:168:ASN:OD1 | 1:O:169:LYS:N | 2.47 | 0.47 |
| 1:P:82:MET:O | 1:P:86:THR:HG23 | 2.14 | 0.47 |
| 1:Q:70:ASP:O | 1:Q:74:ILE:HG13 | 2.15 | 0.47 |
| 1:Q:81:ALA:O | 1:Q:85:THR:HG23 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:197:ILE:HB | 1:Q:209:ILE:HG23 | 1.96 | 0.47 |
| 1:R:88:ILE:O | 1:R:92:MET:HG3 | 2.14 | 0.47 |
| 1:R:192:LYS:C | 1:R:262:LEU:HD23 | 2.40 | 0.47 |
| 1:R:195:LEU:HD12 | 1:R:262:LEU:HD12 | 1.97 | 0.47 |
| 1:S:328:ASN:OD1 | 1:T:76:GLN:HG2 | 2.15 | 0.47 |
| 1:T:198:ASN:HB2 | 1:T:257:GLU:HG2 | 1.96 | 0.47 |
| 1:T:350:LYS:HE3 | 1:U:6:ASN:HA | 1.95 | 0.47 |
| 1:c:289:GLU:OE1 | 1:c:293:ILE:HD11 | 2.14 | 0.47 |
| 1:h:152:ASP:OD2 | 1:s:93:ARG:NH2 | 2.34 | 0.47 |
| 1:l:162:LYS:HD3 | 1:l:162:LYS:N | 2.30 | 0.47 |
| 1:l:343:LYS:HE2 | 1:l:343:LYS:HA | 1.96 | 0.47 |
| 1:n:155:GLU:OE1 | 1:z:129:THR:HG22 | 2.15 | 0.47 |
| 1:o:300:TYR:CD2 | 1:o:304:HIS:NE2 | 2.82 | 0.47 |
| 1:r:59:ARG:O | 1:r:63:VAL:HG22 | 2.14 | 0.47 |
| 1:r:111:ALA:HA | 1:r:114:GLU:OE1 | 2.15 | 0.47 |
| 1:r:161:LEU:HD23 | 1:r:162:LYS:N | 2.30 | 0.47 |
| 1:v:67:ASN:HA | 1:v:70:ASP:OD2 | 2.14 | 0.47 |
| 1:z:26:GLN:HA | 1:z:29:MET:CE | 2.44 | 0.47 |
| 1:z:162:LYS:HE3 | 1:z:304:HIS:HB3 | 1.96 | 0.47 |
| 1:D:194:ASP:O | 1:D:195:LEU:HD23 | 2.15 | 0.47 |
| 1:F:16:ARG:HH21 | 1:m:327:GLU:CD | 2.22 | 0.47 |
| 1:K:27:THR:O | 1:K:31:ARG:HG2 | 2.14 | 0.47 |
| 1:L:37:LYS:HG2 | 1:L:337:LYS:O | 2.14 | 0.47 |
| 1:M:13:THR:HG22 | 1:M:17:TYR:HE1 | 1.80 | 0.47 |
| 1:j:160:GLU:OE1 | 1:j:161:LEU:N | 2.48 | 0.47 |
| 1:r:273:LYS:HD3 | 1:r:274:VAL:N | 2.30 | 0.47 |
| 1:t:122:GLU:O | 1:t:126:ILE:HG13 | 2.15 | 0.47 |
| 1:t:125:ARG:HG2 | 1:t:125:ARG:HH11 | 1.79 | 0.47 |
| 1:w:125:ARG:HD2 | 1:w:129:THR:HG21 | 1.97 | 0.47 |
| 1:1:173:GLY:HA3 | 1:1:246:PHE:CE1 | 2.50 | 0.47 |
| 1:3:368:ALA:HB3 | 1:3:369:PRO:HD3 | 1.96 | 0.47 |
| 1:A:227:ASN:ND2 | 1:L:155:GLU:OE1 | 2.48 | 0.47 |
| 1:C:244:GLN:O | 1:C:245:ILE:HD13 | 2.15 | 0.47 |
| 1:E:61:LEU:CD2 | 1:E:151:ALA:HB2 | 2.44 | 0.47 |
| 1:H:32:LEU:HD11 | 1:H:344:GLU:HB3 | 1.97 | 0.47 |
| 1:H:300:TYR:CE1 | 1:H:304:HIS:NE2 | 2.83 | 0.47 |
| 1:Q:97:LEU:HD23 | 1:Q:97:LEU:HA | 1.72 | 0.47 |
| 1:Q:147:PHE:CE1 | 1:Q:159:LEU:HD23 | 2.50 | 0.47 |
| 1:R:185:ASP:OD1 | 1:R:185:ASP:N | 2.48 | 0.47 |
| 1:T:146:SER:HA | 1:T:158:MET:HA | 1.96 | 0.47 |
| 1:V:170:MET:HE1 | 1:V:250:ASN:ND2 | 2.26 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:120:ASN:HD21 | 1:h:277:ASP:HA | 1.80 | 0.47 |
| 1:i:69:ASN:HA | 1:i:72:ILE:HD12 | 1.97 | 0.47 |
| 1:i:357:ALA:O | 1:i:361:ILE:HG13 | 2.15 | 0.47 |
| 1:k:3:VAL:HG23 | 1:k:5:VAL:H | 1.80 | 0.47 |
| 1:m:170:MET:HA | 1:m:170:MET:HE3 | 1.97 | 0.47 |
| 1:m:239:GLN:H | 1:m:239:GLN:CD | 2.23 | 0.47 |
| 1:t:343:LYS:HD2 | 1:u:15:GLN:NE2 | 2.30 | 0.47 |
| 1:x:335:ARG:HH11 | 1:x:335:ARG:HG3 | 1.80 | 0.47 |
| 1:2:111:ALA:O | 1:2:115:GLU:OE2 | 2.33 | 0.47 |
| 1:3:220:GLU:OE1 | 1:3:237:VAL:HB | 2.14 | 0.47 |
| 1:B:300:TYR:CE1 | 1:B:304:HIS:CD2 | 3.03 | 0.47 |
| 1:F:166:SER:HB2 | 1:F:276:VAL:HB | 1.97 | 0.47 |
| 1:H:61:LEU:HB2 | 1:H:326:ASN:OD1 | 2.14 | 0.47 |
| 1:I:214:LYS:N | 1:I:217:ASP:OD2 | 2.48 | 0.47 |
| 1:J:270:GLU:OE2 | 1:J:273:LYS:NZ | 2.46 | 0.47 |
| 1:L:92:MET:HB2 | 1:L:294:ILE:HD12 | 1.97 | 0.47 |
| 1:O:125:ARG:HD2 | 1:O:125:ARG:C | 2.40 | 0.47 |
| 1:O:173:GLY:HA3 | 1:O:246:PHE:HE1 | 1.79 | 0.47 |
| 1:Q:50:ILE:O | 1:Q:54:LEU:HG | 2.15 | 0.47 |
| 1:R:373:LEU:HD12 | 1:R:373:LEU:O | 2.15 | 0.47 |
| 1:T:79:GLU:HA | 1:T:82:MET:HE3 | 1.97 | 0.47 |
| 1:V:238:ASP:OD2 | 1:V:242:LYS:HB2 | 2.15 | 0.47 |
| 1:h:362:LEU:HD12 | 1:h:362:LEU:O | 2.14 | 0.47 |
| 1:j:64:ALA:HB1 | 1:j:149:ILE:O | 2.15 | 0.47 |
| 1:k:3:VAL:CG1 | 1:v:341:PHE:H | 2.28 | 0.47 |
| 1:t:13:THR:HG23 | 1:t:17:TYR:CZ | 2.50 | 0.47 |
| 1:z:246:PHE:CD1 | 1:z:247:ALA:N | 2.83 | 0.47 |
| 1:2:84:GLU:OE2 | 1:2:126:ILE:HD13 | 2.15 | 0.46 |
| 1:2:162:LYS:HG3 | 1:2:304:HIS:CE1 | 2.49 | 0.46 |
| 1:A:70:ASP:OD1 | 1:A:70:ASP:N | 2.42 | 0.46 |
| 1:C:72:ILE:CD1 | 1:C:312:GLN:HG2 | 2.45 | 0.46 |
| 1:C:164:MET:HE1 | 1:C:304:HIS:CD2 | 2.43 | 0.46 |
| 1:I:292:ALA:HB2 | 1:T:153:ASN:ND2 | 2.30 | 0.46 |
| 1:K:51:SER:HB2 | 1:K:337:LYS:HD2 | 1.97 | 0.46 |
| 1:M:104:ASN:O | 1:M:109:ARG:NH2 | 2.38 | 0.46 |
| 1:N:238:ASP:OD2 | 1:N:242:LYS:NZ | 2.49 | 0.46 |
| 1:O:36:PHE:CD1 | 1:O:337:LYS:HG2 | 2.50 | 0.46 |
| 1:Q:205:GLN:HB2 | 1:Q:207:GLN:HE22 | 1.79 | 0.46 |
| 1:R:35:GLY:O | 1:c:6:ASN:ND2 | 2.45 | 0.46 |
| 1:S:158:MET:SD | 1:S:158:MET:C | 2.98 | 0.46 |
| 1:S:250:ASN:C | 1:S:250:ASN:OD1 | 2.59 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:i:144:ALA:O | 1:i:145:LYS:HD3 | 2.16 | 0.46 |
| 1:k:7:THR:HG21 | 1:v:334:SER:HB2 | 1.96 | 0.46 |
| 1:t:148:GLN:NE2 | 1:t:150:GLY:H | 2.12 | 0.46 |
| 1:x:46:ALA:O | 1:x:49:GLN:HG3 | 2.15 | 0.46 |
| 1:z:244:GLN:C | 1:z:245:ILE:HD12 | 2.40 | 0.46 |
| 1:1:72:ILE:HG23 | 1:1:312:GLN:HG3 | 1.97 | 0.46 |
| 1:B:157:VAL:HG22 | 1:B:158:MET:N | 2.31 | 0.46 |
| 1:F:366:LYS:HD3 | 1:l:349:THR:HG21 | 1.97 | 0.46 |
| 1:G:234:LYS:NZ | 1:R:153:ASN:O | 2.48 | 0.46 |
| 1:Q:201:ASP:OD2 | 1:Q:207:GLN:NE2 | 2.48 | 0.46 |
| 1:R:194:ASP:O | 1:R:262:LEU:HG | 2.14 | 0.46 |
| 1:S:208:GLU:HG2 | 1:S:209:ILE:N | 2.29 | 0.46 |
| 1:h:162:LYS:HD3 | 1:h:162:LYS:N | 2.29 | 0.46 |
| 1:h:246:PHE:CZ | 1:h:293:ILE:HD13 | 2.47 | 0.46 |
| 1:i:139:ASN:OD1 | 1:i:140:GLY:N | 2.49 | 0.46 |
| 1:j:31:ARG:NH2 | 1:j:37:LYS:HB2 | 2.30 | 0.46 |
| 1:k:201:ASP:OD1 | 1:k:202:SER:N | 2.48 | 0.46 |
| 1:m:332:SER:O | 1:m:336:ILE:HD12 | 2.15 | 0.46 |
| 1:r:176:TYR:OH | 1:r:255:GLU:OE1 | 2.30 | 0.46 |
| 1:t:340:ASP:OD1 | 1:t:343:LYS:HG2 | 2.15 | 0.46 |
| 1:v:105:SER:OG | 1:v:106:LYS:N | 2.47 | 0.46 |
| 1:w:37:LYS:HZ3 | 1:w:340:ASP:H | 1.61 | 0.46 |
| 1:2:63:VAL:HG13 | 1:2:66:ARG:NH2 | 2.31 | 0.46 |
| 1:B:38:ILE:HG22 | 1:B:337:LYS:HG3 | 1.97 | 0.46 |
| 1:B:72:ILE:HD12 | 1:B:72:ILE:HA | 1.84 | 0.46 |
| 1:D:152:ASP:N | 1:D:155:GLU:OE2 | 2.44 | 0.46 |
| 1:F:209:ILE:HD12 | 1:F:209:ILE:N | 2.31 | 0.46 |
| 1:G:268:LEU:HD23 | 1:G:268:LEU:HA | 1.80 | 0.46 |
| 1:J:79:GLU:OE2 | 1:J:305:ARG:HD2 | 2.15 | 0.46 |
| 1:K:25:GLN:C | 1:K:25:GLN:OE1 | 2.59 | 0.46 |
| 1:M:222:LEU:HD12 | 1:M:226:ILE:HD11 | 1.97 | 0.46 |
| 1:N:139:ASN:OD1 | 1:N:141:THR:HG22 | 2.14 | 0.46 |
| 1:O:150:GLY:HA3 | 1:O:155:GLU:HB2 | 1.96 | 0.46 |
| 1:Q:12:MET:HE2 | 1:Q:12:MET:HB2 | 1.84 | 0.46 |
| 1:R:116:VAL:HA | 1:R:119:LEU:HD12 | 1.98 | 0.46 |
| 1:S:49:GLN:O | 1:S:53:ARG:HG3 | 2.16 | 0.46 |
| 1:c:177:GLN:HE21 | 1:c:178:ALA:N | 2.14 | 0.46 |
| 1:c:266:LEU:HD23 | 1:c:266:LEU:HA | 1.80 | 0.46 |
| 1:i:105:SER:OG | 1:i:106:LYS:N | 2.48 | 0.46 |
| 1:m:169:LYS:NZ | 1:m:249:ASN:OD1 | 2.44 | 0.46 |
| 1:n:194:ASP:CG | 1:n:261:GLY:H | 2.23 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:n:350:LYS:NZ | 1:o:6:ASN:OD1 | 2.29 | 0.46 |
| 1:r:176:TYR:HB2 | 1:r:245:ILE:CG2 | 2.45 | 0.46 |
| 1:s:27:THR:HG23 | 1:s:31:ARG:HH21 | 1.79 | 0.46 |
| 1:v:239:GLN:H | 1:v:239:GLN:CD | 2.22 | 0.46 |
| 1:1:179:GLU:CD | 1:1:179:GLU:H | 2.21 | 0.46 |
| 1:F:367:GLN:HA | 1:F:370:ASN:OD1 | 2.15 | 0.46 |
| 1:G:27:THR:HG22 | 1:G:31:ARG:HD2 | 1.96 | 0.46 |
| 1:H:61:LEU:HD22 | 1:H:151:ALA:HB2 | 1.98 | 0.46 |
| 1:H:236:SER:O | 1:H:244:GLN:N | 2.46 | 0.46 |
| 1:M:93:ARG:HE | 1:M:291:VAL:HG13 | 1.79 | 0.46 |
| 1:R:124:ASN:O | 1:R:128:GLU:HG2 | 2.15 | 0.46 |
| 1:R:209:ILE:HD11 | 1:R:232:LEU:HG | 1.98 | 0.46 |
| 1:S:111:ALA:HA | 1:S:114:GLU:OE1 | 2.15 | 0.46 |
| 1:S:356:GLN:O | 1:S:359:SER:OG | 2.31 | 0.46 |
| 1:T:235:ALA:HB1 | 1:T:243:LEU:HD11 | 1.98 | 0.46 |
| 1:V:11:ALA:O | 1:V:15:GLN:HG2 | 2.15 | 0.46 |
| 1:i:332:SER:O | 1:i:336:ILE:HG13 | 2.16 | 0.46 |
| 1:n:335:ARG:NH2 | 1:z:73:SER:OG | 2.45 | 0.46 |
| 1:o:158:MET:HG3 | 1:o:159:LEU:N | 2.31 | 0.46 |
| 1:q:276:VAL:O | 1:q:279:ILE:HG12 | 2.14 | 0.46 |
| 1:r:5:VAL:HG23 | 1:r:5:VAL:O | 2.16 | 0.46 |
| 1:t:262:LEU:HD23 | 1:t:262:LEU:HA | 1.78 | 0.46 |
| 1:u:13:THR:O | 1:u:17:TYR:HD1 | 1.99 | 0.46 |
| 1:w:50:ILE:O | 1:w:54:LEU:HG | 2.15 | 0.46 |
| 1:z:9:VAL:HA | 1:z:12:MET:HE1 | 1.97 | 0.46 |
| 1:z:190:GLU:H | 1:z:190:GLU:CD | 2.20 | 0.46 |
| 1:B:184:LYS:HE3 | 1:M:144:ALA:HB2 | 1.98 | 0.46 |
| 1:C:93:ARG:HH12 | 1:N:56:VAL:HG11 | 1.81 | 0.46 |
| 1:D:171:MET:HE1 | 1:D:300:TYR:CD2 | 2.51 | 0.46 |
| 1:E:37:LYS:HD3 | 1:E:37:LYS:C | 2.41 | 0.46 |
| 1:G:163:ASP:OD1 | 1:G:165:ARG:HG3 | 2.16 | 0.46 |
| 1:R:170:MET:HE2 | 1:R:170:MET:N | 2.29 | 0.46 |
| 1:R:220:GLU:HG3 | 1:R:237:VAL:HG11 | 1.98 | 0.46 |
| 1:S:11:ALA:C | 1:S:15:GLN:HE21 | 2.23 | 0.46 |
| 1:h:185:ASP:OD1 | 1:h:185:ASP:N | 2.48 | 0.46 |
| 1:l:23:SER:OG | 1:l:24:ALA:N | 2.48 | 0.46 |
| 1:r:136:LYS:HD3 | 1:r:136:LYS:N | 2.30 | 0.46 |
| 1:t:286:GLY:O | 1:t:289:GLU:HG3 | 2.16 | 0.46 |
| 1:u:240:ASP:OD1 | 1:u:240:ASP:N | 2.39 | 0.46 |
| 1:z:79:GLU:CD | 1:z:305:ARG:HE | 2.23 | 0.46 |
| 1:1:35:GLY:HA2 | 1:1:341:PHE:CZ | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:1:126:ILE:HG23 | 1:z:321:ASN:HD21 | 1.81 | 0.46 |
| 1:1:214:LYS:HB2 | 1:1:217:ASP:CG | 2.41 | 0.46 |
| 1:E:125:ARG:NH1 | 1:E:129:THR:HG21 | 2.30 | 0.46 |
| 1:G:239:GLN:CD | 1:G:239:GLN:H | 2.24 | 0.46 |
| 1:H:42:LYS:NZ | 1:H:42:LYS:HB3 | 2.31 | 0.46 |
| 1:H:218:ASP:C | 1:H:218:ASP:OD2 | 2.59 | 0.46 |
| 1:J:305:ARG:HH21 | 1:U:48:LEU:HD21 | 1.80 | 0.46 |
| 1:L:159:LEU:HD12 | 1:L:160:GLU:N | 2.31 | 0.46 |
| 1:N:63:VAL:O | 1:N:67:ASN:OD1 | 2.34 | 0.46 |
| 1:N:301:VAL:O | 1:N:305:ARG:HG2 | 2.15 | 0.46 |
| 1:P:104:ASN:OD1 | 1:P:109:ARG:NH2 | 2.48 | 0.46 |
| 1:Q:270:GLU:OE2 | 1:Q:273:LYS:NZ | 2.49 | 0.46 |
| 1:T:61:LEU:HD22 | 1:T:151:ALA:HB2 | 1.97 | 0.46 |
| 1:T:96:SER:HB2 | 1:T:291:VAL:HG22 | 1.97 | 0.46 |
| 1:T:185:ASP:OD1 | 1:T:185:ASP:N | 2.49 | 0.46 |
| 1:T:208:GLU:O | 1:T:209:ILE:HD13 | 2.14 | 0.46 |
| 1:U:147:PHE:N | 1:U:157:VAL:O | 2.38 | 0.46 |
| 1:h:271:GLY:O | 1:h:273:LYS:NZ | 2.37 | 0.46 |
| 1:j:376:LEU:H | 1:j:376:LEU:HD12 | 1.81 | 0.46 |
| 1:l:149:ILE:HG21 | 1:l:315:PHE:HE2 | 1.80 | 0.46 |
| 1:m:38:ILE:O | 1:m:337:LYS:NZ | 2.47 | 0.46 |
| 1:n:31:ARG:NH2 | 1:n:37:LYS:HB2 | 2.31 | 0.46 |
| 1:p:221:GLU:OE2 | 1:p:221:GLU:N | 2.40 | 0.46 |
| 1:r:48:LEU:O | 1:r:51:SER:OG | 2.27 | 0.46 |
| 1:r:231:ASP:OD1 | 1:r:232:LEU:N | 2.49 | 0.46 |
| 1:v:19:ASN:OD1 | 1:v:20:ASN:N | 2.49 | 0.46 |
| 1:v:52:ASN:HA | 1:v:55:ASN:ND2 | 2.30 | 0.46 |
| 1:w:220:GLU:OE2 | 1:w:220:GLU:N | 2.49 | 0.46 |
| 1:x:94:ASP:N | 1:x:94:ASP:OD1 | 2.47 | 0.46 |
| 1:z:115:GLU:N | 1:z:115:GLU:OE1 | 2.48 | 0.46 |
| 1:z:201:ASP:OD2 | 1:z:203:TYR:HD2 | 1.99 | 0.46 |
| 1:1:174:VAL:N | 1:1:247:ALA:O | 2.48 | 0.46 |
| 1:3:335:ARG:HA | 1:r:4:ASN:HD21 | 1.80 | 0.46 |
| 1:3:350:LYS:O | 1:3:354:LEU:HG | 2.16 | 0.46 |
| 1:C:30:GLU:CD | 1:C:39:ASN:HD22 | 2.22 | 0.46 |
| 1:E:335:ARG:HB2 | 1:E:335:ARG:CZ | 2.45 | 0.46 |
| 1:K:32:LEU:HD11 | 1:K:341:PHE:CD2 | 2.51 | 0.46 |
| 1:L:201:ASP:OD2 | 1:L:207:GLN:NE2 | 2.48 | 0.46 |
| 1:N:188:VAL:HG23 | 1:N:217:ASP:O | 2.16 | 0.46 |
| 1:O:343:LYS:HE3 | 1:O:343:LYS:HB2 | 1.78 | 0.46 |
| 1:T:142:HIS:CE1 | 1:T:161:LEU:HD12 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:i:238:ASP:N | 1:i:238:ASP:OD1 | 2.49 | 0.46 |
| 1:j:336:ILE:HD12 | 1:j:336:ILE:H | 1.80 | 0.46 |
| 1:l:187:ASN:C | 1:l:187:ASN:OD1 | 2.59 | 0.46 |
| 1:n:232:LEU:HD13 | 1:n:251:LYS:HZ3 | 1.81 | 0.46 |
| 1:r:92:MET:HE3 | 1:r:92:MET:HB2 | 1.83 | 0.46 |
| 1:s:38:ILE:HG23 | 1:s:43:ASP:HB2 | 1.97 | 0.46 |
| 1:s:361:ILE:HD12 | 1:s:361:ILE:HA | 1.81 | 0.46 |
| 1:v:70:ASP:O | 1:v:74:ILE:HG12 | 2.16 | 0.46 |
| 1:1:89:LEU:HA | 1:1:92:MET:HG3 | 1.97 | 0.46 |
| 1:3:233:VAL:HG23 | 1:3:246:PHE:O | 2.14 | 0.46 |
| 1:B:22:ASN:O | 1:B:26:GLN:HG2 | 2.15 | 0.46 |
| 1:C:125:ARG:HG2 | 1:C:125:ARG:HH11 | 1.81 | 0.46 |
| 1:C:208:GLU:OE1 | 1:C:208:GLU:N | 2.48 | 0.46 |
| 1:C:209:ILE:HG22 | 1:C:211:ILE:HD11 | 1.98 | 0.46 |
| 1:E:218:ASP:HB3 | 1:E:221:GLU:OE2 | 2.16 | 0.46 |
| 1:G:5:VAL:HG23 | 1:n:341:PHE:CE2 | 2.51 | 0.46 |
| 1:I:256:VAL:HG12 | 1:I:258:PHE:CE2 | 2.51 | 0.46 |
| 1:N:177:GLN:HG3 | 1:N:244:GLN:HA | 1.98 | 0.46 |
| 1:P:347:ALA:O | 1:P:351:SER:OG | 2.32 | 0.46 |
| 1:Q:226:ILE:HA | 1:Q:229:GLN:HG2 | 1.97 | 0.46 |
| 1:V:26:GLN:OE1 | 1:V:26:GLN:HA | 2.14 | 0.46 |
| 1:c:248:GLY:O | 1:c:252:VAL:HG22 | 2.16 | 0.46 |
| 1:h:335:ARG:NH1 | 1:i:73:SER:OG | 2.49 | 0.46 |
| 1:l:3:VAL:O | 1:l:3:VAL:HG13 | 2.15 | 0.46 |
| 1:p:12:MET:HG3 | 1:z:343:LYS:NZ | 2.31 | 0.46 |
| 1:r:177:GLN:NE2 | 1:r:178:ALA:O | 2.48 | 0.46 |
| 1:r:210:ASN:O | 1:r:211:ILE:HD13 | 2.16 | 0.46 |
| 1:u:15:GLN:O | 1:u:19:ASN:OD1 | 2.34 | 0.46 |
| 1:v:82:MET:HG3 | 1:v:82:MET:H | 1.57 | 0.46 |
| 1:w:192:LYS:O | 1:w:262:LEU:HG | 2.15 | 0.46 |
| 1:w:346:THR:O | 1:w:349:THR:OG1 | 2.31 | 0.46 |
| 1:x:174:VAL:HG22 | 1:x:273:LYS:HG3 | 1.98 | 0.46 |
| 1:z:210:ASN:OD1 | 1:z:210:ASN:N | 2.47 | 0.46 |
| 1:z:318:ALA:O | 1:z:322:LEU:HD23 | 2.16 | 0.46 |
| 1:1:91:ARG:O | 1:1:95:LEU:HG | 2.16 | 0.46 |
| 1:1:121:ASP:HA | 1:1:124:ASN:OD1 | 2.16 | 0.46 |
| 1:2:325:ILE:HA | 1:2:328:ASN:HD22 | 1.81 | 0.46 |
| 1:A:274:VAL:HG11 | 1:A:289:GLU:OE2 | 2.16 | 0.46 |
| 1:B:88:ILE:HG23 | 1:B:119:LEU:HD22 | 1.98 | 0.46 |
| 1:D:250:ASN:C | 1:D:250:ASN:OD1 | 2.59 | 0.46 |
| 1:E:211:ILE:HG12 | 1:E:226:ILE:CD1 | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:250:ASN:OD1 | 1:E:251:LYS:NZ | 2.49 | 0.46 |
| 1:E:334:SER:HA | 1:E:338:ASP:OD1 | 2.16 | 0.46 |
| 1:E:371:SER:O | 1:E:374:SER:OG | 2.34 | 0.46 |
| 1:G:27:THR:O | 1:G:31:ARG:HG3 | 2.15 | 0.46 |
| 1:G:175:SER:O | 1:G:271:GLY:HA2 | 2.16 | 0.46 |
| 1:I:214:LYS:HB2 | 1:I:217:ASP:OD1 | 2.15 | 0.46 |
| 1:K:176:TYR:HB2 | 1:K:245:ILE:CG2 | 2.45 | 0.46 |
| 1:M:120:ASN:ND2 | 1:M:277:ASP:HA | 2.28 | 0.46 |
| 1:M:239:GLN:CD | 1:M:285:GLY:H | 2.24 | 0.46 |
| 1:O:366:LYS:O | 1:O:369:PRO:HD2 | 2.16 | 0.46 |
| 1:P:67:ASN:O | 1:P:70:ASP:OD2 | 2.34 | 0.46 |
| 1:P:122:GLU:O | 1:P:126:ILE:HG12 | 2.16 | 0.46 |
| 1:V:177:GLN:HE22 | 1:V:272:LYS:HE2 | 1.80 | 0.46 |
| 1:V:292:ALA:HA | 1:V:295:ASP:OD2 | 2.16 | 0.46 |
| 1:k:72:ILE:O | 1:k:76:GLN:HG2 | 2.16 | 0.46 |
| 1:l:79:GLU:HA | 1:l:82:MET:HG3 | 1.98 | 0.46 |
| 1:m:185:ASP:OD1 | 1:m:185:ASP:N | 2.48 | 0.46 |
| 1:p:364:GLN:OE1 | 1:p:364:GLN:N | 2.49 | 0.46 |
| 1:s:114:GLU:OE1 | 1:s:114:GLU:HA | 2.16 | 0.46 |
| 1:u:232:LEU:HD22 | 1:u:251:LYS:HZ3 | 1.81 | 0.46 |
| 1:v:132:PHE:CD1 | 1:v:132:PHE:C | 2.94 | 0.46 |
| 1:w:162:LYS:HE2 | 1:w:304:HIS:ND1 | 2.30 | 0.46 |
| 1:x:168:ASN:OD1 | 1:x:169:LYS:N | 2.49 | 0.46 |
| 1:z:38:ILE:HG13 | 1:z:43:ASP:HB2 | 1.97 | 0.46 |
| 1:2:176:TYR:OH | 1:2:255:GLU:OE1 | 2.24 | 0.46 |
| 1:A:85:THR:HA | 1:A:88:ILE:HD12 | 1.98 | 0.46 |
| 1:D:99:SER:HB2 | 1:D:112:ILE:HG21 | 1.98 | 0.46 |
| 1:E:125:ARG:HH11 | 1:E:129:THR:HG21 | 1.80 | 0.46 |
| 1:F:55:ASN:O | 1:F:59:ARG:HG3 | 2.16 | 0.46 |
| 1:G:167:ASP:OD1 | 1:G:167:ASP:N | 2.38 | 0.46 |
| 1:K:176:TYR:HB2 | 1:K:245:ILE:HG22 | 1.97 | 0.46 |
| 1:L:194:ASP:O | 1:L:261:GLY:N | 2.49 | 0.46 |
| 1:c:91:ARG:HA | 1:c:94:ASP:OD2 | 2.16 | 0.46 |
| 1:c:125:ARG:O | 1:c:129:THR:OG1 | 2.30 | 0.46 |
| 1:c:131:SER:HB3 | 1:c:136:LYS:HE3 | 1.98 | 0.46 |
| 1:i:152:ASP:OD2 | 1:t:234:LYS:NZ | 2.49 | 0.46 |
| 1:k:238:ASP:C | 1:k:238:ASP:OD1 | 2.59 | 0.46 |
| 1:n:240:ASP:OD1 | 1:n:242:LYS:HG3 | 2.16 | 0.46 |
| 1:o:63:VAL:HG22 | 1:o:66:ARG:HH22 | 1.81 | 0.46 |
| 1:s:321:ASN:O | 1:s:325:ILE:HG13 | 2.16 | 0.46 |
| 1:t:38:ILE:HD13 | 1:t:337:LYS:HA | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:t:205:GLN:CD | 1:t:205:GLN:N | 2.74 | 0.46 |
| 1:u:203:TYR:HB3 | 1:u:205:GLN:HE21 | 1.81 | 0.46 |
| 1:u:232:LEU:HD22 | 1:u:251:LYS:NZ | 2.31 | 0.46 |
| 1:x:219:ILE:HD12 | 1:x:237:VAL:HG11 | 1.98 | 0.46 |
| 1:z:232:LEU:HD13 | 1:z:251:LYS:HE3 | 1.97 | 0.46 |
| 1:1:148:GLN:NE2 | 1:1:152:ASP:O | 2.49 | 0.45 |
| 1:E:85:THR:O | 1:E:89:LEU:HD13 | 2.15 | 0.45 |
| 1:E:131:SER:HB3 | 1:E:136:LYS:HD3 | 1.98 | 0.45 |
| 1:F:49:GLN:HG2 | 1:F:53:ARG:NH2 | 2.31 | 0.45 |
| 1:G:52:ASN:O | 1:G:56:VAL:HG23 | 2.16 | 0.45 |
| 1:G:66:ARG:HA | 1:G:69:ASN:OD1 | 2.16 | 0.45 |
| 1:J:218:ASP:HB3 | 1:J:221:GLU:OE1 | 2.16 | 0.45 |
| 1:K:199:LEU:HD13 | 1:K:252:VAL:HG22 | 1.97 | 0.45 |
| 1:M:88:ILE:HG23 | 1:M:119:LEU:HD22 | 1.97 | 0.45 |
| 1:R:223:ALA:O | 1:R:227:ASN:ND2 | 2.49 | 0.45 |
| 1:S:112:ILE:HG13 | 1:S:112:ILE:H | 1.63 | 0.45 |
| 1:V:287:ALA:HA | 1:V:290:SER:OG | 2.16 | 0.45 |
| 1:l:38:ILE:HD11 | 1:l:336:ILE:O | 2.16 | 0.45 |
| 1:m:137:LEU:C | 1:m:138:LEU:HD23 | 2.41 | 0.45 |
| 1:n:82:MET:O | 1:n:85:THR:OG1 | 2.32 | 0.45 |
| 1:q:332:SER:O | 1:q:336:ILE:HD12 | 2.16 | 0.45 |
| 1:r:368:ALA:O | 1:r:371:SER:OG | 2.27 | 0.45 |
| 1:s:14:ALA:HB3 | 1:s:362:LEU:HD23 | 1.98 | 0.45 |
| 1:t:210:ASN:O | 1:t:211:ILE:HD13 | 2.15 | 0.45 |
| 1:u:159:LEU:HD12 | 1:u:160:GLU:H | 1.81 | 0.45 |
| 1:u:173:GLY:HA3 | 1:u:246:PHE:CZ | 2.52 | 0.45 |
| 1:x:48:LEU:HG | 1:x:52:ASN:HD21 | 1.81 | 0.45 |
| 1:x:184:LYS:H | 1:x:184:LYS:HD2 | 1.81 | 0.45 |
| 1:z:287:ALA:O | 1:z:290:SER:HB2 | 2.16 | 0.45 |
| 1:1:184:LYS:NZ | 1:1:219:ILE:HG22 | 2.31 | 0.45 |
| 1:2:115:GLU:OE2 | 1:2:115:GLU:N | 2.48 | 0.45 |
| 1:3:193:ASN:OD1 | 1:3:193:ASN:N | 2.49 | 0.45 |
| 1:J:120:ASN:ND2 | 1:J:277:ASP:HA | 2.31 | 0.45 |
| 1:J:314:ARG:HH22 | 1:K:121:ASP:HB2 | 1.80 | 0.45 |
| 1:P:22:ASN:O | 1:P:26:GLN:HB2 | 2.16 | 0.45 |
| 1:P:336:ILE:HG23 | 1:Q:66:ARG:HH21 | 1.81 | 0.45 |
| 1:Q:160:GLU:OE1 | 1:Q:161:LEU:N | 2.49 | 0.45 |
| 1:R:163:ASP:OD1 | 1:R:164:MET:N | 2.50 | 0.45 |
| 1:T:113:GLN:OE1 | 1:T:281:VAL:HG22 | 2.15 | 0.45 |
| 1:T:273:LYS:HD3 | 1:T:273:LYS:N | 2.32 | 0.45 |
| 1:V:368:ALA:HB3 | 1:V:369:PRO:HD3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:128:GLU:O | 1:c:136:LYS:HE2 | 2.17 | 0.45 |
| 1:t:159:LEU:HD12 | 1:t:160:GLU:N | 2.30 | 0.45 |
| 1:v:171:MET:HB3 | 1:v:276:VAL:HG23 | 1.97 | 0.45 |
| 1:w:256:VAL:HG23 | 1:w:258:PHE:HE1 | 1.80 | 0.45 |
| 1:z:233:VAL:HG12 | 1:z:247:ALA:HB2 | 1.98 | 0.45 |
| 1:1:93:ARG:HD3 | 1:1:291:VAL:HG13 | 1.99 | 0.45 |
| 1:1:214:LYS:HD3 | 1:1:214:LYS:N | 2.30 | 0.45 |
| 1:2:169:LYS:HB3 | 1:2:170:MET:CE | 2.45 | 0.45 |
| 1:B:199:LEU:HD11 | 1:B:232:LEU:HD23 | 1.97 | 0.45 |
| 1:C:177:GLN:NE2 | 1:C:289:GLU:OE2 | 2.50 | 0.45 |
| 1:G:227:ASN:ND2 | 1:G:235:ALA:H | 2.15 | 0.45 |
| 1:J:55:ASN:OD1 | 1:J:59:ARG:NH2 | 2.46 | 0.45 |
| 1:K:210:ASN:O | 1:K:211:ILE:HD13 | 2.15 | 0.45 |
| 1:K:232:LEU:HD23 | 1:K:232:LEU:HA | 1.73 | 0.45 |
| 1:K:303:SER:OG | 1:K:304:HIS:HD2 | 2.00 | 0.45 |
| 1:L:246:PHE:CD2 | 1:L:247:ALA:N | 2.84 | 0.45 |
| 1:L:321:ASN:ND2 | 1:L:325:ILE:HD11 | 2.32 | 0.45 |
| 1:N:59:ARG:O | 1:N:63:VAL:HG23 | 2.16 | 0.45 |
| 1:O:232:LEU:HA | 1:O:251:LYS:NZ | 2.31 | 0.45 |
| 1:Q:195:LEU:HD22 | 1:Q:211:ILE:HD13 | 1.97 | 0.45 |
| 1:T:148:GLN:NE2 | 1:T:150:GLY:O | 2.45 | 0.45 |
| 1:U:236:SER:N | 1:U:244:GLN:O | 2.50 | 0.45 |
| 1:i:151:ALA:N | 1:i:155:GLU:OE1 | 2.49 | 0.45 |
| 1:k:42:LYS:HB2 | 1:v:312:GLN:NE2 | 2.32 | 0.45 |
| 1:l:50:ILE:O | 1:l:54:LEU:HG | 2.17 | 0.45 |
| 1:n:152:ASP:HB3 | 1:n:155:GLU:OE2 | 2.16 | 0.45 |
| 1:o:281:VAL:O | 1:o:281:VAL:HG22 | 2.16 | 0.45 |
| 1:q:104:ASN:O | 1:q:109:ARG:NH2 | 2.32 | 0.45 |
| 1:q:274:VAL:HG21 | 1:q:293:ILE:HD11 | 1.99 | 0.45 |
| 1:t:38:ILE:HG23 | 1:t:43:ASP:HB2 | 1.99 | 0.45 |
| 1:u:214:LYS:HB2 | 1:u:217:ASP:OD2 | 2.16 | 0.45 |
| 1:u:234:LYS:HA | 1:u:234:LYS:HE2 | 1.98 | 0.45 |
| 1:v:128:GLU:OE1 | 1:v:165:ARG:NH1 | 2.50 | 0.45 |
| 1:v:211:ILE:N | 1:v:211:ILE:HD12 | 2.30 | 0.45 |
| 1:w:37:LYS:HG2 | 1:w:338:ASP:O | 2.17 | 0.45 |
| 1:w:222:LEU:HD22 | 1:w:226:ILE:HD11 | 1.98 | 0.45 |
| 1:x:170:MET:HE1 | 1:x:250:ASN:CB | 2.39 | 0.45 |
| 1:3:65:VAL:O | 1:3:69:ASN:OD1 | 2.34 | 0.45 |
| 1:D:184:LYS:O | 1:D:184:LYS:HD2 | 2.16 | 0.45 |
| 1:E:334:SER:HB2 | 1:P:7:THR:HG21 | 1.99 | 0.45 |
| 1:L:139:ASN:C | 1:L:139:ASN:OD1 | 2.59 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:176:TYR:OH | 1:L:255:GLU:OE1 | 2.32 | 0.45 |
| 1:O:166:SER:HB2 | 1:O:276:VAL:HB | 1.98 | 0.45 |
| 1:P:236:SER:O | 1:P:243:LEU:HD13 | 2.17 | 0.45 |
| 1:Q:240:ASP:OD2 | 1:Q:242:LYS:HG3 | 2.16 | 0.45 |
| 1:T:93:ARG:HG3 | 1:T:93:ARG:HH11 | 1.80 | 0.45 |
| 1:U:272:LYS:HD3 | 1:U:272:LYS:N | 2.30 | 0.45 |
| 1:c:178:ALA:HA | 1:c:268:LEU:HA | 1.98 | 0.45 |
| 1:c:354:LEU:HD12 | 1:c:354:LEU:HA | 1.72 | 0.45 |
| 1:h:232:LEU:HA | 1:h:251:LYS:HZ1 | 1.81 | 0.45 |
| 1:i:144:ALA:H | 1:i:145:LYS:HZ2 | 1.64 | 0.45 |
| 1:j:273:LYS:HA | 1:j:273:LYS:HD3 | 1.85 | 0.45 |
| 1:k:125:ARG:HH11 | 1:k:129:THR:HG21 | 1.82 | 0.45 |
| 1:o:85:THR:HG23 | 1:o:123:LEU:HD21 | 1.98 | 0.45 |
| 1:o:111:ALA:HA | 1:o:114:GLU:OE2 | 2.16 | 0.45 |
| 1:q:344:GLU:OE2 | 1:q:344:GLU:HA | 2.16 | 0.45 |
| 1:s:314:ARG:NH2 | 1:t:121:ASP:OD2 | 2.44 | 0.45 |
| 1:t:26:GLN:O | 1:t:30:GLU:OE2 | 2.35 | 0.45 |
| 1:u:166:SER:O | 1:u:275:THR:OG1 | 2.35 | 0.45 |
| 1:v:175:SER:O | 1:v:271:GLY:HA2 | 2.17 | 0.45 |
| 1:w:157:VAL:HG12 | 1:w:158:MET:N | 2.31 | 0.45 |
| 1:l:76:GLN:HB3 | 1:z:328:ASN:OD1 | 2.17 | 0.45 |
| 1:B:350:LYS:NZ | 1:C:6:ASN:O | 2.49 | 0.45 |
| 1:C:122:GLU:HB2 | 1:M:314:ARG:HG3 | 1.98 | 0.45 |
| 1:D:225:TYR:O | 1:D:229:GLN:NE2 | 2.40 | 0.45 |
| 1:L:299:LYS:HA | 1:L:299:LYS:HE3 | 1.99 | 0.45 |
| 1:M:270:GLU:OE1 | 1:M:273:LYS:NZ | 2.49 | 0.45 |
| 1:O:174:VAL:HG23 | 1:O:249:ASN:OD1 | 2.17 | 0.45 |
| 1:O:319:ILE:HA | 1:O:322:LEU:HD12 | 1.98 | 0.45 |
| 1:P:66:ARG:NH1 | 1:P:66:ARG:HB3 | 2.32 | 0.45 |
| 1:Q:195:LEU:HD21 | 1:Q:197:ILE:HG12 | 1.98 | 0.45 |
| 1:R:93:ARG:HB2 | 1:R:294:ILE:HG21 | 1.97 | 0.45 |
| 1:T:196:LYS:HB2 | 1:T:259:SER:OG | 2.16 | 0.45 |
| 1:U:250:ASN:HD21 | 1:U:299:LYS:HE3 | 1.80 | 0.45 |
| 1:i:50:ILE:O | 1:i:54:LEU:HG | 2.17 | 0.45 |
| 1:j:250:ASN:HD21 | 1:j:299:LYS:HB2 | 1.81 | 0.45 |
| 1:q:52:ASN:O | 1:q:56:VAL:HG23 | 2.16 | 0.45 |
| 1:t:179:GLU:H | 1:t:179:GLU:CD | 2.23 | 0.45 |
| 1:w:318:ALA:O | 1:w:322:LEU:HG | 2.17 | 0.45 |
| 1:z:92:MET:HG2 | 1:z:119:LEU:HD12 | 1.98 | 0.45 |
| 1:B:93:ARG:HG2 | 1:B:294:ILE:CG2 | 2.46 | 0.45 |
| 1:C:72:ILE:HD12 | 1:C:312:GLN:HG2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:82:MET:O | 1:D:85:THR:OG1 | 2.28 | 0.45 |
| 1:E:287:ALA:O | 1:E:291:VAL:HG23 | 2.16 | 0.45 |
| 1:H:217:ASP:N | 1:H:217:ASP:OD1 | 2.48 | 0.45 |
| 1:I:190:GLU:CD | 1:I:191:GLY:N | 2.74 | 0.45 |
| 1:I:343:LYS:HD2 | 1:J:15:GLN:OE1 | 2.17 | 0.45 |
| 1:J:335:ARG:HH11 | 1:J:335:ARG:HG3 | 1.80 | 0.45 |
| 1:K:290:SER:O | 1:K:294:ILE:HG13 | 2.16 | 0.45 |
| 1:N:55:ASN:O | 1:N:59:ARG:HG2 | 2.17 | 0.45 |
| 1:O:50:ILE:HG22 | 1:O:54:LEU:CD2 | 2.47 | 0.45 |
| 1:Q:93:ARG:HB2 | 1:Q:294:ILE:HG21 | 1.99 | 0.45 |
| 1:R:205:GLN:HB2 | 1:R:207:GLN:HE22 | 1.81 | 0.45 |
| 1:T:88:ILE:HG23 | 1:T:119:LEU:HD22 | 1.97 | 0.45 |
| 1:T:225:TYR:O | 1:T:229:GLN:HG2 | 2.17 | 0.45 |
| 1:U:61:LEU:O | 1:U:65:VAL:HG23 | 2.16 | 0.45 |
| 1:V:37:LYS:HE2 | 1:V:37:LYS:HB3 | 1.75 | 0.45 |
| 1:V:91:ARG:HH11 | 1:V:91:ARG:HA | 1.82 | 0.45 |
| 1:c:225:TYR:O | 1:c:229:GLN:HG2 | 2.17 | 0.45 |
| 1:i:152:ASP:N | 1:i:155:GLU:OE1 | 2.47 | 0.45 |
| 1:n:334:SER:HA | 1:n:338:ASP:OD1 | 2.17 | 0.45 |
| 1:p:193:ASN:HA | 1:p:262:LEU:HD21 | 1.99 | 0.45 |
| 1:q:128:GLU:HA | 1:q:128:GLU:OE2 | 2.16 | 0.45 |
| 1:q:253:GLU:OE2 | 1:q:253:GLU:HA | 2.17 | 0.45 |
| 1:q:357:ALA:O | 1:q:361:ILE:HG13 | 2.17 | 0.45 |
| 1:u:61:LEU:HD23 | 1:u:151:ALA:HB2 | 1.99 | 0.45 |
| 1:u:222:LEU:HG | 1:u:226:ILE:HD11 | 1.98 | 0.45 |
| 1:u:232:LEU:O | 1:u:251:LYS:HE2 | 2.17 | 0.45 |
| 1:v:99:SER:HB3 | 1:v:112:ILE:HD13 | 1.98 | 0.45 |
| 1:v:201:ASP:N | 1:v:205:GLN:O | 2.32 | 0.45 |
| 1:A:196:LYS:HB3 | 1:A:208:GLU:OE2 | 2.17 | 0.45 |
| 1:H:144:ALA:HB1 | 1:H:158:MET:HE2 | 1.97 | 0.45 |
| 1:H:328:ASN:CG | 1:I:76:GLN:HE21 | 2.21 | 0.45 |
| 1:I:93:ARG:HB2 | 1:I:294:ILE:HG21 | 1.99 | 0.45 |
| 1:K:313:ASN:ND2 | 1:h:115:GLU:OE2 | 2.34 | 0.45 |
| 1:L:196:LYS:N | 1:L:259:SER:O | 2.37 | 0.45 |
| 1:N:188:VAL:HB | 1:N:215:ALA:HA | 1.98 | 0.45 |
| 1:O:159:LEU:HD22 | 1:O:311:PHE:CZ | 2.52 | 0.45 |
| 1:O:214:LYS:HD3 | 1:O:214:LYS:N | 2.31 | 0.45 |
| 1:P:316:ASN:HA | 1:P:319:ILE:HD12 | 1.98 | 0.45 |
| 1:Q:108:GLU:H | 1:Q:108:GLU:CD | 2.25 | 0.45 |
| 1:R:350:LYS:O | 1:R:354:LEU:HG | 2.16 | 0.45 |
| 1:T:5:VAL:HG12 | 1:T:6:ASN:N | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:196:LYS:HD3 | 1:U:196:LYS:N | 2.32 | 0.45 |
| 1:c:196:LYS:N | 1:c:259:SER:O | 2.44 | 0.45 |
| 1:c:307:GLU:OE2 | 1:c:308:LEU:HD23 | 2.16 | 0.45 |
| 1:h:276:VAL:O | 1:h:279:ILE:HG12 | 2.17 | 0.45 |
| 1:i:52:ASN:ND2 | 1:t:302:ASP:OD1 | 2.47 | 0.45 |
| 1:l:22:ASN:CG | 1:l:23:SER:N | 2.74 | 0.45 |
| 1:l:311:PHE:CE1 | 1:l:315:PHE:CE1 | 3.04 | 0.45 |
| 1:m:244:GLN:HE22 | 1:m:285:GLY:HA3 | 1.82 | 0.45 |
| 1:m:349:THR:O | 1:m:353:ILE:HG13 | 2.17 | 0.45 |
| 1:n:4:ASN:CG | 1:n:6:ASN:H | 2.25 | 0.45 |
| 1:n:142:HIS:HD2 | 1:n:143:GLY:O | 2.00 | 0.45 |
| 1:q:248:GLY:HA3 | 1:q:251:LYS:HE3 | 1.99 | 0.45 |
| 1:s:238:ASP:OD1 | 1:s:242:LYS:HB2 | 2.16 | 0.45 |
| 1:x:25:GLN:OE1 | 1:x:25:GLN:C | 2.60 | 0.45 |
| 1:x:174:VAL:HG23 | 1:x:249:ASN:ND2 | 2.30 | 0.45 |
| 1:A:92:MET:HE2 | 1:A:92:MET:HB3 | 1.76 | 0.45 |
| 1:C:50:ILE:O | 1:C:54:LEU:HD12 | 2.16 | 0.45 |
| 1:C:318:ALA:O | 1:C:322:LEU:HD22 | 2.17 | 0.45 |
| 1:F:154:GLY:HA3 | 1:m:227:ASN:HD22 | 1.81 | 0.45 |
| 1:F:232:LEU:HD13 | 1:F:251:LYS:HE2 | 1.98 | 0.45 |
| 1:G:366:LYS:O | 1:G:369:PRO:HD2 | 2.17 | 0.45 |
| 1:H:109:ARG:HB3 | 1:H:282:THR:HA | 1.99 | 0.45 |
| 1:K:11:ALA:O | 1:K:15:GLN:HG2 | 2.17 | 0.45 |
| 1:M:208:GLU:N | 1:M:208:GLU:OE2 | 2.49 | 0.45 |
| 1:N:115:GLU:N | 1:N:115:GLU:OE2 | 2.49 | 0.45 |
| 1:Q:270:GLU:OE1 | 1:Q:271:GLY:N | 2.49 | 0.45 |
| 1:T:208:GLU:C | 1:T:209:ILE:HD13 | 2.42 | 0.45 |
| 1:V:232:LEU:HD23 | 1:V:232:LEU:HA | 1.78 | 0.45 |
| 1:c:240:ASP:OD1 | 1:c:242:LYS:HE3 | 2.16 | 0.45 |
| 1:i:170:MET:HE2 | 1:i:170:MET:HA | 1.99 | 0.45 |
| 1:i:251:LYS:HE2 | 1:i:251:LYS:HB2 | 1.93 | 0.45 |
| 1:j:93:ARG:HE | 1:j:93:ARG:HB3 | 1.54 | 0.45 |
| 1:j:122:GLU:OE2 | 1:j:125:ARG:NH2 | 2.38 | 0.45 |
| 1:j:194:ASP:OD1 | 1:j:194:ASP:N | 2.49 | 0.45 |
| 1:k:208:GLU:C | 1:k:209:ILE:HD13 | 2.41 | 0.45 |
| 1:m:250:ASN:ND2 | 1:m:296:ALA:HB1 | 2.31 | 0.45 |
| 1:n:13:THR:HA | 1:n:16:ARG:NH1 | 2.31 | 0.45 |
| 1:n:108:GLU:H | 1:n:108:GLU:CD | 2.15 | 0.45 |
| 1:p:26:GLN:NE2 | 1:p:26:GLN:C | 2.75 | 0.45 |
| 1:q:123:LEU:HD23 | 1:q:123:LEU:HA | 1.83 | 0.45 |
| 1:r:47:GLY:HA2 | 1:r:336:ILE:HD11 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:r:314:ARG:HD2 | 1:s:118:ALA:O | 2.17 | 0.45 |
| 1:s:37:LYS:HG2 | 1:s:337:LYS:O | 2.16 | 0.45 |
| 1:u:12:MET:HA | 1:u:15:GLN:OE1 | 2.17 | 0.45 |
| 1:w:25:GLN:O | 1:w:29:MET:HG2 | 2.16 | 0.45 |
| 1:x:185:ASP:OD2 | 1:x:185:ASP:N | 2.50 | 0.45 |
| 1:z:65:VAL:HG13 | 1:z:319:ILE:HG23 | 1.99 | 0.45 |
| 1:z:196:LYS:HE2 | 1:z:196:LYS:HB3 | 1.63 | 0.45 |
| 1:B:318:ALA:O | 1:B:322:LEU:HG | 2.17 | 0.45 |
| 1:C:368:ALA:O | 1:C:371:SER:OG | 2.35 | 0.45 |
| 1:D:350:LYS:O | 1:D:354:LEU:HG | 2.17 | 0.45 |
| 1:J:113:GLN:OE1 | 1:J:281:VAL:HG22 | 2.17 | 0.45 |
| 1:K:170:MET:HA | 1:K:249:ASN:ND2 | 2.32 | 0.45 |
| 1:M:120:ASN:HA | 1:M:123:LEU:HG | 1.99 | 0.45 |
| 1:R:92:MET:HA | 1:R:95:LEU:HD12 | 1.99 | 0.45 |
| 1:R:233:VAL:HG23 | 1:R:245:ILE:HD11 | 1.98 | 0.45 |
| 1:R:299:LYS:HA | 1:R:299:LYS:HE3 | 1.98 | 0.45 |
| 1:T:89:LEU:HA | 1:T:92:MET:HE3 | 1.98 | 0.45 |
| 1:c:341:PHE:O | 1:c:345:THR:HG23 | 2.16 | 0.45 |
| 1:n:18:LEU:HG | 1:n:22:ASN:HD21 | 1.82 | 0.45 |
| 1:s:246:PHE:CD2 | 1:s:247:ALA:N | 2.84 | 0.45 |
| 1:u:210:ASN:OD1 | 1:u:210:ASN:N | 2.47 | 0.45 |
| 1:v:3:VAL:HG13 | 1:v:3:VAL:O | 2.17 | 0.45 |
| 1:x:176:TYR:OH | 1:x:255:GLU:OE1 | 2.20 | 0.45 |
| 1:1:91:ARG:HA | 1:1:91:ARG:HH11 | 1.82 | 0.45 |
| 1:1:218:ASP:HB3 | 1:1:221:GLU:CD | 2.42 | 0.45 |
| 1:1:368:ALA:HB3 | 1:1:369:PRO:HD3 | 1.99 | 0.45 |
| 1:2:90:GLN:OE1 | 1:q:55:ASN:ND2 | 2.36 | 0.45 |
| 1:A:4:ASN:ND2 | 1:h:338:ASP:OD2 | 2.50 | 0.45 |
| 1:A:361:ILE:HD11 | 1:B:32:LEU:HB3 | 1.98 | 0.45 |
| 1:D:362:LEU:O | 1:D:366:LYS:HG2 | 2.17 | 0.45 |
| 1:H:289:GLU:OE2 | 1:H:293:ILE:HD11 | 2.16 | 0.45 |
| 1:O:169:LYS:HA | 1:O:273:LYS:NZ | 2.32 | 0.45 |
| 1:S:28:SER:HA | 1:S:344:GLU:OE1 | 2.17 | 0.45 |
| 1:T:173:GLY:HA3 | 1:T:246:PHE:CE1 | 2.38 | 0.45 |
| 1:V:201:ASP:HB3 | 1:V:207:GLN:HE22 | 1.82 | 0.45 |
| 1:c:230:THR:O | 1:c:234:LYS:NZ | 2.50 | 0.45 |
| 1:c:334:SER:OG | 1:c:338:ASP:OD2 | 2.28 | 0.45 |
| 1:h:158:MET:HE2 | 1:h:160:GLU:HB3 | 1.98 | 0.45 |
| 1:i:231:ASP:OD2 | 1:i:231:ASP:N | 2.50 | 0.45 |
| 1:j:173:GLY:HA3 | 1:j:246:PHE:CE1 | 2.52 | 0.45 |
| 1:j:232:LEU:HA | 1:j:251:LYS:HZ1 | 1.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:k:25:GLN:OE1 | 1:k:352:GLN:HG2 | 2.17 | 0.45 |
| 1:n:187:ASN:C | 1:n:187:ASN:OD1 | 2.60 | 0.45 |
| 1:o:238:ASP:OD2 | 1:o:239:GLN:NE2 | 2.50 | 0.45 |
| 1:p:112:ILE:O | 1:p:116:VAL:HG23 | 2.17 | 0.45 |
| 1:q:83:ASN:OD1 | 1:q:305:ARG:NH1 | 2.42 | 0.45 |
| 1:r:199:LEU:HD21 | 1:r:232:LEU:HD13 | 1.97 | 0.45 |
| 1:t:29:MET:HG3 | 1:t:348:MET:HE1 | 1.99 | 0.45 |
| 1:v:225:TYR:O | 1:v:229:GLN:HG2 | 2.16 | 0.45 |
| 1:w:218:ASP:OD1 | 1:w:220:GLU:N | 2.50 | 0.45 |
| 1:2:331:ALA:O | 1:2:335:ARG:HG3 | 2.17 | 0.44 |
| 1:A:184:LYS:HE3 | 1:L:158:MET:HG3 | 1.99 | 0.44 |
| 1:G:165:ARG:HB3 | 1:G:165:ARG:NH1 | 2.32 | 0.44 |
| 1:H:218:ASP:OD2 | 1:H:220:GLU:N | 2.50 | 0.44 |
| 1:I:373:LEU:HD12 | 1:I:373:LEU:O | 2.16 | 0.44 |
| 1:M:195:LEU:HD12 | 1:M:196:LYS:N | 2.32 | 0.44 |
| 1:N:163:ASP:O | 1:N:164:MET:HE2 | 2.17 | 0.44 |
| 1:Q:262:LEU:O | 1:Q:266:LEU:HG | 2.17 | 0.44 |
| 1:Q:300:TYR:CE1 | 1:Q:304:HIS:CE1 | 3.05 | 0.44 |
| 1:S:90:GLN:NE2 | 1:S:94:ASP:OD2 | 2.50 | 0.44 |
| 1:S:181:GLY:N | 1:S:242:LYS:HZ2 | 2.15 | 0.44 |
| 1:m:68:ALA:HA | 1:m:315:PHE:HE1 | 1.81 | 0.44 |
| 1:n:177:GLN:OE1 | 1:n:177:GLN:N | 2.50 | 0.44 |
| 1:n:331:ALA:O | 1:n:334:SER:OG | 2.31 | 0.44 |
| 1:n:333:LYS:HA | 1:n:336:ILE:HG22 | 1.99 | 0.44 |
| 1:o:63:VAL:HG13 | 1:o:66:ARG:NH2 | 2.32 | 0.44 |
| 1:p:297:ALA:O | 1:p:301:VAL:HG22 | 2.17 | 0.44 |
| 1:r:340:ASP:HB3 | 1:r:343:LYS:HG3 | 1.99 | 0.44 |
| 1:s:272:LYS:H | 1:s:272:LYS:HD2 | 1.81 | 0.44 |
| 1:x:63:VAL:HA | 1:x:66:ARG:HH12 | 1.81 | 0.44 |
| 1:z:178:ALA:HB3 | 1:z:242:LYS:HB3 | 1.99 | 0.44 |
| 1:1:106:LYS:O | 1:1:110:VAL:HG23 | 2.18 | 0.44 |
| 1:A:8:ASN:ND2 | 1:A:365:ALA:O | 2.50 | 0.44 |
| 1:C:150:GLY:HA3 | 1:C:155:GLU:HB2 | 2.00 | 0.44 |
| 1:D:93:ARG:HD3 | 1:O:56:VAL:CG2 | 2.48 | 0.44 |
| 1:E:9:VAL:O | 1:E:13:THR:HG23 | 2.17 | 0.44 |
| 1:J:148:GLN:OE1 | 1:J:148:GLN:HA | 2.18 | 0.44 |
| 1:M:177:GLN:CD | 1:M:242:LYS:HB3 | 2.42 | 0.44 |
| 1:M:193:ASN:OD1 | 1:M:193:ASN:C | 2.60 | 0.44 |
| 1:M:364:GLN:OE1 | 1:M:364:GLN:HA | 2.17 | 0.44 |
| 1:Q:115:GLU:O | 1:Q:119:LEU:HD12 | 2.17 | 0.44 |
| 1:Q:304:HIS:HA | 1:Q:307:GLU:OE1 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:153:ASN:OD1 | 1:R:154:GLY:N | 2.50 | 0.44 |
| 1:S:231:ASP:O | 1:S:251:LYS:NZ | 2.50 | 0.44 |
| 1:T:139:ASN:OD1 | 1:T:141:THR:HG22 | 2.18 | 0.44 |
| 1:i:82:MET:HE1 | 1:i:304:HIS:HB2 | 1.99 | 0.44 |
| 1:i:222:LEU:O | 1:i:226:ILE:HG13 | 2.18 | 0.44 |
| 1:l:187:ASN:ND2 | 1:l:216:GLY:HA2 | 2.32 | 0.44 |
| 1:m:312:GLN:O | 1:m:316:ASN:ND2 | 2.50 | 0.44 |
| 1:o:300:TYR:CE2 | 1:o:304:HIS:NE2 | 2.80 | 0.44 |
| 1:s:219:ILE:O | 1:s:222:LEU:HB3 | 2.17 | 0.44 |
| 1:u:122:GLU:OE1 | 1:u:126:ILE:HD11 | 2.17 | 0.44 |
| 1:v:168:ASN:OD1 | 1:v:169:LYS:N | 2.50 | 0.44 |
| 1:w:262:LEU:HD23 | 1:w:262:LEU:HA | 1.84 | 0.44 |
| 1:z:238:ASP:C | 1:z:238:ASP:OD2 | 2.60 | 0.44 |
| 1:B:158:MET:HB2 | 1:i:220:GLU:OE1 | 2.17 | 0.44 |
| 1:B:222:LEU:HG | 1:B:226:ILE:HD11 | 1.99 | 0.44 |
| 1:E:84:GLU:HA | 1:E:87:ASN:HD22 | 1.81 | 0.44 |
| 1:I:13:THR:HG22 | 1:I:17:TYR:HE1 | 1.82 | 0.44 |
| 1:N:318:ALA:CB | 1:O:125:ARG:HH22 | 2.31 | 0.44 |
| 1:O:55:ASN:O | 1:O:59:ARG:HG2 | 2.18 | 0.44 |
| 1:P:25:GLN:O | 1:P:29:MET:HG2 | 2.17 | 0.44 |
| 1:R:149:ILE:O | 1:R:149:ILE:HG13 | 2.17 | 0.44 |
| 1:R:201:ASP:OD2 | 1:R:205:GLN:HB2 | 2.18 | 0.44 |
| 1:k:158:MET:CE | 1:k:160:GLU:HB2 | 2.41 | 0.44 |
| 1:m:82:MET:O | 1:m:85:THR:OG1 | 2.25 | 0.44 |
| 1:o:168:ASN:OD1 | 1:o:169:LYS:N | 2.51 | 0.44 |
| 1:p:370:ASN:HA | 1:p:373:LEU:HD13 | 1.99 | 0.44 |
| 1:u:9:VAL:HA | 1:u:12:MET:SD | 2.57 | 0.44 |
| 1:x:25:GLN:OE1 | 1:x:26:GLN:N | 2.50 | 0.44 |
| 1:z:79:GLU:HA | 1:z:82:MET:CE | 2.44 | 0.44 |
| 1:z:88:ILE:O | 1:z:92:MET:HG3 | 2.17 | 0.44 |
| 1:z:234:LYS:HE2 | 1:z:234:LYS:HA | 1.98 | 0.44 |
| 1:3:168:ASN:HD21 | 1:3:170:MET:HE1 | 1.81 | 0.44 |
| 1:A:239:GLN:CD | 1:A:239:GLN:H | 2.25 | 0.44 |
| 1:C:2:ALA:O | 1:C:3:VAL:C | 2.61 | 0.44 |
| 1:D:16:ARG:O | 1:D:20:ASN:ND2 | 2.50 | 0.44 |
| 1:J:331:ALA:HB1 | 1:J:335:ARG:HH12 | 1.82 | 0.44 |
| 1:L:88:ILE:CG2 | 1:L:123:LEU:HD21 | 2.48 | 0.44 |
| 1:P:167:ASP:OD1 | 1:P:167:ASP:N | 2.50 | 0.44 |
| 1:Q:163:ASP:O | 1:Q:300:TYR:OH | 2.32 | 0.44 |
| 1:R:79:GLU:HA | 1:R:82:MET:HG3 | 2.00 | 0.44 |
| 1:R:345:THR:O | 1:R:349:THR:OG1 | 2.34 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:177:GLN:NE2 | 1:V:272:LYS:HE2 | 2.33 | 0.44 |
| 1:h:61:LEU:O | 1:h:65:VAL:HG23 | 2.17 | 0.44 |
| 1:k:53:ARG:O | 1:k:57:GLN:HG3 | 2.18 | 0.44 |
| 1:k:300:TYR:CE1 | 1:k:304:HIS:NE2 | 2.69 | 0.44 |
| 1:m:50:ILE:O | 1:m:54:LEU:HD12 | 2.17 | 0.44 |
| 1:m:125:ARG:HH11 | 1:m:129:THR:HG21 | 1.81 | 0.44 |
| 1:p:57:GLN:O | 1:p:61:LEU:HG | 2.18 | 0.44 |
| 1:p:238:ASP:OD2 | 1:p:242:LYS:HB2 | 2.18 | 0.44 |
| 1:s:44:ASP:OD1 | 1:s:46:ALA:N | 2.50 | 0.44 |
| 1:w:171:MET:HB3 | 1:w:276:VAL:HG23 | 1.99 | 0.44 |
| 1:x:97:LEU:HD23 | 1:x:97:LEU:HA | 1.68 | 0.44 |
| 1:3:64:ALA:HB1 | 1:3:149:ILE:C | 2.42 | 0.44 |
| 1:G:194:ASP:CG | 1:G:261:GLY:H | 2.25 | 0.44 |
| 1:H:16:ARG:HH12 | 1:o:327:GLU:CD | 2.26 | 0.44 |
| 1:H:116:VAL:HG21 | 1:H:281:VAL:HG11 | 1.97 | 0.44 |
| 1:H:139:ASN:C | 1:H:139:ASN:OD1 | 2.60 | 0.44 |
| 1:I:93:ARG:HE | 1:I:291:VAL:HG13 | 1.83 | 0.44 |
| 1:I:369:PRO:HD2 | 1:I:370:ASN:H | 1.82 | 0.44 |
| 1:J:270:GLU:CD | 1:J:271:GLY:H | 2.25 | 0.44 |
| 1:K:196:LYS:HD2 | 1:K:210:ASN:OD1 | 2.17 | 0.44 |
| 1:L:333:LYS:NZ | 1:L:337:LYS:HD2 | 2.33 | 0.44 |
| 1:M:161:LEU:HD23 | 1:M:161:LEU:HA | 1.88 | 0.44 |
| 1:O:30:GLU:OE1 | 1:O:30:GLU:C | 2.61 | 0.44 |
| 1:O:288:GLN:OE1 | 1:O:288:GLN:HA | 2.18 | 0.44 |
| 1:P:32:LEU:HD11 | 1:P:341:PHE:CD1 | 2.53 | 0.44 |
| 1:Q:89:LEU:HA | 1:Q:92:MET:HE3 | 1.98 | 0.44 |
| 1:Q:91:ARG:O | 1:Q:95:LEU:HG | 2.17 | 0.44 |
| 1:T:57:GLN:O | 1:T:61:LEU:HD23 | 2.18 | 0.44 |
| 1:T:69:ASN:O | 1:T:72:ILE:HG22 | 2.18 | 0.44 |
| 1:T:287:ALA:O | 1:T:291:VAL:HG23 | 2.16 | 0.44 |
| 1:U:68:ALA:O | 1:U:72:ILE:HG12 | 2.17 | 0.44 |
| 1:h:19:ASN:HA | 1:h:22:ASN:ND2 | 2.28 | 0.44 |
| 1:i:224:THR:HA | 1:i:227:ASN:HD22 | 1.83 | 0.44 |
| 1:m:262:LEU:O | 1:m:266:LEU:HG | 2.16 | 0.44 |
| 1:n:137:LEU:HD23 | 1:n:137:LEU:HA | 1.79 | 0.44 |
| 1:p:37:LYS:HG2 | 1:p:337:LYS:O | 2.18 | 0.44 |
| 1:q:321:ASN:O | 1:q:325:ILE:HD12 | 2.17 | 0.44 |
| 1:t:142:HIS:ND1 | 1:t:161:LEU:HD12 | 2.32 | 0.44 |
| 1:2:16:ARG:HG2 | 1:2:17:TYR:N | 2.32 | 0.44 |
| 1:A:120:ASN:HA | 1:A:123:LEU:HD12 | 1.99 | 0.44 |
| 1:A:159:LEU:HB2 | 1:A:311:PHE:CE1 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:243:LEU:HD13 | 1:A:266:LEU:HD13 | 2.00 | 0.44 |
| 1:C:361:ILE:HD11 | 1:D:32:LEU:HB2 | 1.99 | 0.44 |
| 1:D:270:GLU:O | 1:D:272:LYS:NZ | 2.42 | 0.44 |
| 1:E:31:ARG:O | 1:E:31:ARG:HD2 | 2.18 | 0.44 |
| 1:E:101:ASN:O | 1:E:109:ARG:NH2 | 2.50 | 0.44 |
| 1:E:174:VAL:HG22 | 1:E:273:LYS:HG2 | 2.00 | 0.44 |
| 1:F:158:MET:HE3 | 1:F:159:LEU:C | 2.43 | 0.44 |
| 1:G:120:ASN:C | 1:G:120:ASN:OD1 | 2.59 | 0.44 |
| 1:H:168:ASN:HB3 | 1:H:171:MET:HG2 | 1.98 | 0.44 |
| 1:J:38:ILE:HD12 | 1:J:43:ASP:HB2 | 1.98 | 0.44 |
| 1:L:115:GLU:O | 1:L:119:LEU:HG | 2.17 | 0.44 |
| 1:O:89:LEU:HA | 1:O:92:MET:HE3 | 1.99 | 0.44 |
| 1:O:320:SER:HA | 1:O:323:ASP:OD1 | 2.18 | 0.44 |
| 1:Q:192:LYS:HE3 | 1:Q:261:GLY:HA3 | 2.00 | 0.44 |
| 1:R:340:ASP:OD1 | 1:R:340:ASP:C | 2.61 | 0.44 |
| 1:T:91:ARG:O | 1:T:95:LEU:HG | 2.17 | 0.44 |
| 1:c:142:HIS:NE2 | 1:c:145:LYS:HG3 | 2.32 | 0.44 |
| 1:c:339:THR:HG22 | 1:c:344:GLU:OE1 | 2.17 | 0.44 |
| 1:i:53:ARG:HB2 | 1:i:53:ARG:NH1 | 2.33 | 0.44 |
| 1:i:83:ASN:HA | 1:i:305:ARG:HH12 | 1.82 | 0.44 |
| 1:k:175:SER:O | 1:k:271:GLY:HA2 | 2.18 | 0.44 |
| 1:n:300:TYR:CD1 | 1:n:300:TYR:C | 2.95 | 0.44 |
| 1:s:37:LYS:HG3 | 1:s:38:ILE:HD12 | 1.99 | 0.44 |
| 1:w:165:ARG:NE | 1:w:167:ASP:OD1 | 2.35 | 0.44 |
| 1:1:231:ASP:O | 1:1:251:LYS:NZ | 2.51 | 0.44 |
| 1:1:232:LEU:HD23 | 1:1:232:LEU:HA | 1.75 | 0.44 |
| 1:2:197:ILE:HB | 1:2:209:ILE:HB | 1.98 | 0.44 |
| 1:2:318:ALA:O | 1:2:322:LEU:HG | 2.18 | 0.44 |
| 1:3:52:ASN:O | 1:3:56:VAL:HG12 | 2.18 | 0.44 |
| 1:3:209:ILE:HD12 | 1:3:209:ILE:N | 2.33 | 0.44 |
| 1:A:290:SER:O | 1:A:293:ILE:HG22 | 2.17 | 0.44 |
| 1:B:52:ASN:O | 1:B:56:VAL:HG23 | 2.17 | 0.44 |
| 1:B:84:GLU:HA | 1:B:84:GLU:OE2 | 2.18 | 0.44 |
| 1:B:112:ILE:O | 1:B:116:VAL:HG23 | 2.18 | 0.44 |
| 1:E:195:LEU:HD22 | 1:E:211:ILE:HD13 | 1.99 | 0.44 |
| 1:E:240:ASP:HB3 | 1:E:242:LYS:HG3 | 2.00 | 0.44 |
| 1:G:295:ASP:OD1 | 1:G:295:ASP:N | 2.49 | 0.44 |
| 1:H:4:ASN:HB2 | 1:o:338:ASP:OD1 | 2.18 | 0.44 |
| 1:H:6:ASN:N | 1:H:6:ASN:ND2 | 2.65 | 0.44 |
| 1:I:174:VAL:HG23 | 1:I:249:ASN:OD1 | 2.18 | 0.44 |
| 1:J:221:GLU:OE1 | 1:J:221:GLU:N | 2.46 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:250:ASN:OD1 | 1:J:250:ASN:C | 2.61 | 0.44 |
| 1:J:287:ALA:O | 1:J:291:VAL:HG23 | 2.17 | 0.44 |
| 1:O:50:ILE:O | 1:O:54:LEU:HD22 | 2.17 | 0.44 |
| 1:Q:348:MET:O | 1:Q:352:GLN:OE1 | 2.36 | 0.44 |
| 1:S:55:ASN:HB2 | 1:S:333:LYS:HZ2 | 1.82 | 0.44 |
| 1:T:93:ARG:HG2 | 1:T:294:ILE:CG2 | 2.43 | 0.44 |
| 1:U:91:ARG:HG3 | 1:U:119:LEU:HD21 | 1.99 | 0.44 |
| 1:U:164:MET:HE2 | 1:U:164:MET:N | 2.31 | 0.44 |
| 1:c:177:GLN:NE2 | 1:c:178:ALA:H | 2.16 | 0.44 |
| 1:c:353:ILE:HD12 | 1:c:353:ILE:H | 1.82 | 0.44 |
| 1:h:155:GLU:CD | 1:i:129:THR:HG22 | 2.43 | 0.44 |
| 1:h:321:ASN:O | 1:h:325:ILE:HG13 | 2.18 | 0.44 |
| 1:i:63:VAL:O | 1:i:67:ASN:OD1 | 2.36 | 0.44 |
| 1:j:366:LYS:O | 1:j:369:PRO:HD2 | 2.17 | 0.44 |
| 1:m:176:TYR:HB2 | 1:m:245:ILE:HG22 | 1.99 | 0.44 |
| 1:n:37:LYS:NZ | 1:n:336:ILE:O | 2.40 | 0.44 |
| 1:n:137:LEU:C | 1:n:138:LEU:HD23 | 2.42 | 0.44 |
| 1:r:234:LYS:O | 1:r:245:ILE:HD12 | 2.18 | 0.44 |
| 1:r:311:PHE:O | 1:r:315:PHE:HD1 | 2.00 | 0.44 |
| 1:t:30:GLU:OE2 | 1:t:30:GLU:N | 2.51 | 0.44 |
| 1:u:225:TYR:O | 1:u:229:GLN:HG2 | 2.18 | 0.44 |
| 1:v:145:LYS:O | 1:v:159:LEU:N | 2.43 | 0.44 |
| 1:v:311:PHE:CE1 | 1:v:315:PHE:HE1 | 2.36 | 0.44 |
| 1:w:9:VAL:HA | 1:w:12:MET:CE | 2.48 | 0.44 |
| 1:x:49:GLN:HA | 1:x:52:ASN:HD22 | 1.82 | 0.44 |
| 1:x:322:LEU:HA | 1:x:325:ILE:HD12 | 2.00 | 0.44 |
| 1:2:88:ILE:HG22 | 1:2:92:MET:CE | 2.48 | 0.44 |
| 1:2:128:GLU:OE1 | 1:2:165:ARG:NH1 | 2.51 | 0.44 |
| 1:3:234:LYS:HD2 | 1:3:234:LYS:N | 2.32 | 0.44 |
| 1:E:39:ASN:OD1 | 1:E:39:ASN:N | 2.50 | 0.44 |
| 1:E:49:GLN:NE2 | 1:l:302:ASP:HB3 | 2.32 | 0.44 |
| 1:E:266:LEU:HD23 | 1:E:266:LEU:HA | 1.78 | 0.44 |
| 1:F:170:MET:HG3 | 1:F:300:TYR:CD1 | 2.53 | 0.44 |
| 1:H:10:SER:HA | 1:H:13:THR:HG22 | 1.99 | 0.44 |
| 1:I:243:LEU:HD23 | 1:I:245:ILE:HD11 | 2.00 | 0.44 |
| 1:M:109:ARG:HA | 1:M:112:ILE:HD12 | 1.99 | 0.44 |
| 1:S:304:HIS:HA | 1:S:307:GLU:OE1 | 2.18 | 0.44 |
| 1:S:332:SER:O | 1:S:336:ILE:HG13 | 2.18 | 0.44 |
| 1:U:159:LEU:HB2 | 1:U:311:PHE:CE1 | 2.53 | 0.44 |
| 1:j:257:GLU:N | 1:j:257:GLU:CD | 2.76 | 0.44 |
| 1:k:55:ASN:OD1 | 1:k:55:ASN:C | 2.60 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:l:334:SER:O | 1:l:335:ARG:C | 2.60 | 0.44 |
| 1:r:137:LEU:HD22 | 1:r:161:LEU:HD13 | 1.99 | 0.44 |
| 1:s:113:GLN:OE1 | 1:s:281:VAL:HG22 | 2.17 | 0.44 |
| 1:t:236:SER:HB3 | 1:t:288:GLN:OE1 | 2.17 | 0.44 |
| 1:u:184:LYS:HG3 | 1:u:184:LYS:O | 2.18 | 0.44 |
| 1:x:55:ASN:OD1 | 1:x:55:ASN:C | 2.60 | 0.44 |
| 1:z:266:LEU:HD13 | 1:z:268:LEU:HD21 | 2.00 | 0.44 |
| 1:1:34:SER:HA | 1:z:17:TYR:CE1 | 2.52 | 0.44 |
| 1:1:231:ASP:C | 1:1:231:ASP:OD1 | 2.60 | 0.44 |
| 1:A:209:ILE:HG22 | 1:A:211:ILE:HD11 | 2.00 | 0.44 |
| 1:B:53:ARG:NH2 | 1:u:108:GLU:OE1 | 2.47 | 0.44 |
| 1:C:50:ILE:CD1 | 1:k:108:GLU:HG2 | 2.48 | 0.44 |
| 1:E:9:VAL:HA | 1:E:12:MET:HG3 | 1.99 | 0.44 |
| 1:E:13:THR:HG22 | 1:l:327:GLU:OE2 | 2.18 | 0.44 |
| 1:E:25:GLN:O | 1:E:29:MET:HG2 | 2.18 | 0.44 |
| 1:F:128:GLU:OE1 | 1:F:165:ARG:NH1 | 2.51 | 0.44 |
| 1:G:63:VAL:HA | 1:G:66:ARG:HH12 | 1.81 | 0.44 |
| 1:H:66:ARG:HD2 | 1:H:66:ARG:N | 2.33 | 0.44 |
| 1:O:169:LYS:HA | 1:O:273:LYS:HZ1 | 1.83 | 0.44 |
| 1:Q:222:LEU:HD12 | 1:Q:222:LEU:O | 2.17 | 0.44 |
| 1:S:318:ALA:CB | 1:T:125:ARG:HH22 | 2.30 | 0.44 |
| 1:V:109:ARG:NE | 1:V:282:THR:O | 2.48 | 0.44 |
| 1:m:88:ILE:HG23 | 1:m:119:LEU:HD12 | 2.00 | 0.44 |
| 1:m:176:TYR:HB2 | 1:m:245:ILE:CG2 | 2.48 | 0.44 |
| 1:n:37:LYS:O | 1:n:38:ILE:HG13 | 2.18 | 0.44 |
| 1:p:225:TYR:O | 1:p:229:GLN:HG2 | 2.18 | 0.44 |
| 1:q:320:SER:HB2 | 1:r:84:GLU:OE1 | 2.17 | 0.44 |
| 1:r:25:GLN:OE1 | 1:r:25:GLN:C | 2.61 | 0.44 |
| 1:w:144:ALA:C | 1:w:145:LYS:HD2 | 2.42 | 0.44 |
| 1:x:201:ASP:OD1 | 1:x:205:GLN:HB3 | 2.18 | 0.44 |
| 1:x:273:LYS:N | 1:x:273:LYS:HD2 | 2.33 | 0.44 |
| 1:1:168:ASN:HB3 | 1:1:171:MET:HE3 | 2.00 | 0.43 |
| 1:3:295:ASP:O | 1:3:299:LYS:HG2 | 2.17 | 0.43 |
| 1:A:71:GLY:HA2 | 1:A:74:ILE:HD12 | 2.00 | 0.43 |
| 1:A:276:VAL:HA | 1:A:279:ILE:CD1 | 2.48 | 0.43 |
| 1:D:340:ASP:C | 1:D:340:ASP:OD1 | 2.61 | 0.43 |
| 1:E:113:GLN:OE1 | 1:E:281:VAL:HG22 | 2.18 | 0.43 |
| 1:F:367:GLN:N | 1:F:367:GLN:CD | 2.76 | 0.43 |
| 1:G:120:ASN:ND2 | 1:G:277:ASP:HA | 2.32 | 0.43 |
| 1:G:179:GLU:N | 1:G:179:GLU:CD | 2.76 | 0.43 |
| 1:G:272:LYS:HD3 | 1:G:273:LYS:N | 2.32 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:248:GLY:O | 1:J:252:VAL:HG12 | 2.18 | 0.43 |
| 1:K:367:GLN:HA | 1:K:370:ASN:OD1 | 2.18 | 0.43 |
| 1:L:170:MET:HA | 1:L:170:MET:HE3 | 1.99 | 0.43 |
| 1:O:178:ALA:HB3 | 1:O:243:LEU:H | 1.81 | 0.43 |
| 1:S:159:LEU:HB2 | 1:S:311:PHE:CE2 | 2.53 | 0.43 |
| 1:S:163:ASP:O | 1:S:168:ASN:ND2 | 2.51 | 0.43 |
| 1:U:160:GLU:OE2 | 1:U:161:LEU:N | 2.51 | 0.43 |
| 1:c:92:MET:HE1 | 1:c:116:VAL:HG22 | 1.99 | 0.43 |
| 1:i:56:VAL:HG22 | 1:t:90:GLN:OE1 | 2.18 | 0.43 |
| 1:j:53:ARG:NH1 | 1:k:133:GLY:O | 2.50 | 0.43 |
| 1:k:158:MET:HE2 | 1:v:184:LYS:HD3 | 1.99 | 0.43 |
| 1:l:83:ASN:HA | 1:l:305:ARG:HH12 | 1.83 | 0.43 |
| 1:n:162:LYS:HE3 | 1:n:300:TYR:CZ | 2.53 | 0.43 |
| 1:p:106:LYS:O | 1:p:110:VAL:HG23 | 2.18 | 0.43 |
| 1:q:70:ASP:O | 1:q:74:ILE:HG12 | 2.18 | 0.43 |
| 1:t:63:VAL:HA | 1:t:66:ARG:HG2 | 2.00 | 0.43 |
| 1:v:336:ILE:HD12 | 1:v:336:ILE:H | 1.83 | 0.43 |
| 1:w:47:GLY:HA2 | 1:w:50:ILE:HD12 | 1.99 | 0.43 |
| 1:x:300:TYR:CZ | 1:x:304:HIS:CE1 | 3.06 | 0.43 |
| 1:1:132:PHE:C | 1:1:132:PHE:CD1 | 2.96 | 0.43 |
| 1:A:185:ASP:OD1 | 1:A:185:ASP:N | 2.51 | 0.43 |
| 1:B:320:SER:HA | 1:B:323:ASP:OD1 | 2.18 | 0.43 |
| 1:C:72:ILE:HD12 | 1:C:72:ILE:HA | 1.83 | 0.43 |
| 1:C:153:ASN:ND2 | 1:j:291:VAL:HG13 | 2.33 | 0.43 |
| 1:D:220:GLU:H | 1:D:220:GLU:CD | 2.26 | 0.43 |
| 1:E:97:LEU:HD23 | 1:E:97:LEU:HA | 1.70 | 0.43 |
| 1:F:209:ILE:HG22 | 1:F:211:ILE:CD1 | 2.47 | 0.43 |
| 1:I:162:LYS:HD2 | 1:I:162:LYS:N | 2.34 | 0.43 |
| 1:L:53:ARG:NH1 | 1:M:133:GLY:O | 2.50 | 0.43 |
| 1:M:32:LEU:HD23 | 1:M:32:LEU:HA | 1.65 | 0.43 |
| 1:M:126:ILE:O | 1:M:130:THR:HG23 | 2.18 | 0.43 |
| 1:M:239:GLN:OE1 | 1:M:285:GLY:N | 2.50 | 0.43 |
| 1:N:234:LYS:O | 1:N:245:ILE:HA | 2.18 | 0.43 |
| 1:S:79:GLU:OE2 | 1:S:305:ARG:NE | 2.46 | 0.43 |
| 1:S:177:GLN:OE1 | 1:S:177:GLN:N | 2.51 | 0.43 |
| 1:c:173:GLY:H | 1:c:293:ILE:HG23 | 1.83 | 0.43 |
| 1:h:162:LYS:HE2 | 1:h:304:HIS:CE1 | 2.53 | 0.43 |
| 1:i:318:ALA:O | 1:i:322:LEU:HG | 2.18 | 0.43 |
| 1:k:16:ARG:NH1 | 1:v:323:ASP:OD2 | 2.41 | 0.43 |
| 1:l:28:SER:O | 1:l:31:ARG:HB3 | 2.17 | 0.43 |
| 1:l:142:HIS:CE1 | 1:l:161:LEU:HD12 | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:m:222:LEU:HG | 1:m:226:ILE:HD11 | 2.00 | 0.43 |
| 1:n:170:MET:HG3 | 1:n:300:TYR:CE2 | 2.52 | 0.43 |
| 1:o:9:VAL:O | 1:o:12:MET:HG3 | 2.17 | 0.43 |
| 1:o:108:GLU:O | 1:o:112:ILE:HG13 | 2.19 | 0.43 |
| 1:o:164:MET:HA | 1:o:164:MET:HE3 | 2.01 | 0.43 |
| 1:p:12:MET:HE2 | 1:p:12:MET:HB2 | 1.75 | 0.43 |
| 1:p:117:THR:O | 1:p:121:ASP:OD2 | 2.36 | 0.43 |
| 1:q:137:LEU:HB2 | 1:q:138:LEU:HD12 | 2.00 | 0.43 |
| 1:r:170:MET:HE1 | 1:r:250:ASN:HD22 | 1.83 | 0.43 |
| 1:t:289:GLU:O | 1:t:293:ILE:HG13 | 2.18 | 0.43 |
| 1:u:279:ILE:HG23 | 1:u:290:SER:HB3 | 2.00 | 0.43 |
| 1:v:32:LEU:CD2 | 1:v:344:GLU:HG2 | 2.48 | 0.43 |
| 1:v:44:ASP:CG | 1:v:47:GLY:H | 2.26 | 0.43 |
| 1:w:161:LEU:HD23 | 1:w:162:LYS:HZ3 | 1.82 | 0.43 |
| 1:1:170:MET:HE2 | 1:1:170:MET:N | 2.32 | 0.43 |
| 1:1:274:VAL:HG11 | 1:1:289:GLU:OE2 | 2.18 | 0.43 |
| 1:2:133:GLY:HA3 | 1:p:53:ARG:NH1 | 2.26 | 0.43 |
| 1:A:190:GLU:HG3 | 1:A:191:GLY:N | 2.33 | 0.43 |
| 1:B:94:ASP:OD2 | 1:B:94:ASP:N | 2.51 | 0.43 |
| 1:D:206:GLU:OE1 | 1:D:206:GLU:HA | 2.19 | 0.43 |
| 1:E:179:GLU:OE2 | 1:E:179:GLU:N | 2.41 | 0.43 |
| 1:G:6:ASN:O | 1:m:350:LYS:NZ | 2.41 | 0.43 |
| 1:G:79:GLU:HA | 1:G:82:MET:HE2 | 2.00 | 0.43 |
| 1:H:318:ALA:O | 1:H:322:LEU:HD13 | 2.17 | 0.43 |
| 1:I:157:VAL:CG2 | 1:I:314:ARG:HH12 | 2.31 | 0.43 |
| 1:J:188:VAL:HG22 | 1:J:222:LEU:HD12 | 2.00 | 0.43 |
| 1:J:321:ASN:OD1 | 1:J:325:ILE:HD11 | 2.17 | 0.43 |
| 1:J:336:ILE:HD12 | 1:J:336:ILE:H | 1.83 | 0.43 |
| 1:K:139:ASN:O | 1:K:141:THR:HG23 | 2.18 | 0.43 |
| 1:L:357:ALA:O | 1:L:361:ILE:HG12 | 2.19 | 0.43 |
| 1:N:321:ASN:OD1 | 1:O:126:ILE:HG23 | 2.17 | 0.43 |
| 1:N:357:ALA:O | 1:N:361:ILE:HG12 | 2.18 | 0.43 |
| 1:O:50:ILE:HG22 | 1:O:54:LEU:HD21 | 2.00 | 0.43 |
| 1:O:274:VAL:HG21 | 1:O:289:GLU:OE1 | 2.19 | 0.43 |
| 1:R:91:ARG:HH12 | 1:R:95:LEU:HD21 | 1.84 | 0.43 |
| 1:R:214:LYS:HE2 | 1:S:165:ARG:NH2 | 2.33 | 0.43 |
| 1:S:195:LEU:HB2 | 1:S:262:LEU:HD12 | 2.00 | 0.43 |
| 1:V:160:GLU:C | 1:V:161:LEU:HD23 | 2.43 | 0.43 |
| 1:h:313:ASN:ND2 | 1:i:115:GLU:OE2 | 2.51 | 0.43 |
| 1:l:345:THR:O | 1:l:349:THR:HG23 | 2.18 | 0.43 |
| 1:m:137:LEU:HB3 | 1:m:138:LEU:HD23 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:o:115:GLU:O | 1:o:119:LEU:HD13 | 2.19 | 0.43 |
| 1:r:84:GLU:HA | 1:r:84:GLU:OE2 | 2.18 | 0.43 |
| 1:w:37:LYS:HZ2 | 1:w:339:THR:HA | 1.83 | 0.43 |
| 1:1:168:ASN:OD1 | 1:1:170:MET:N | 2.45 | 0.43 |
| 1:1:353:ILE:HG13 | 1:1:353:ILE:H | 1.70 | 0.43 |
| 1:3:210:ASN:C | 1:3:211:ILE:HD13 | 2.43 | 0.43 |
| 1:B:165:ARG:HG2 | 1:B:165:ARG:HH11 | 1.83 | 0.43 |
| 1:B:178:ALA:O | 1:B:242:LYS:HD3 | 2.18 | 0.43 |
| 1:C:166:SER:OG | 1:C:277:ASP:OD1 | 2.25 | 0.43 |
| 1:C:214:LYS:HD3 | 1:C:214:LYS:N | 2.33 | 0.43 |
| 1:D:44:ASP:C | 1:D:44:ASP:OD1 | 2.61 | 0.43 |
| 1:D:361:ILE:HD13 | 1:D:361:ILE:N | 2.33 | 0.43 |
| 1:E:93:ARG:HA | 1:E:294:ILE:HD13 | 2.00 | 0.43 |
| 1:E:170:MET:HE2 | 1:E:170:MET:HA | 2.00 | 0.43 |
| 1:G:88:ILE:O | 1:G:92:MET:HG3 | 2.19 | 0.43 |
| 1:G:139:ASN:OD1 | 1:G:141:THR:HG23 | 2.17 | 0.43 |
| 1:J:211:ILE:HG13 | 1:J:226:ILE:CD1 | 2.49 | 0.43 |
| 1:L:4:ASN:OD1 | 1:L:4:ASN:C | 2.61 | 0.43 |
| 1:N:82:MET:N | 1:N:82:MET:SD | 2.91 | 0.43 |
| 1:N:322:LEU:HA | 1:N:325:ILE:HD12 | 1.99 | 0.43 |
| 1:O:226:ILE:HD12 | 1:O:226:ILE:HA | 1.82 | 0.43 |
| 1:V:327:GLU:OE1 | 1:V:327:GLU:HA | 2.18 | 0.43 |
| 1:c:123:LEU:HD11 | 1:c:166:SER:HB3 | 2.00 | 0.43 |
| 1:i:303:SER:O | 1:i:307:GLU:HG3 | 2.17 | 0.43 |
| 1:m:47:GLY:HA2 | 1:m:50:ILE:HD12 | 2.01 | 0.43 |
| 1:o:185:ASP:OD1 | 1:o:185:ASP:N | 2.51 | 0.43 |
| 1:p:93:ARG:HG3 | 1:p:294:ILE:CG2 | 2.46 | 0.43 |
| 1:p:260:GLY:O | 1:p:263:SER:HB3 | 2.18 | 0.43 |
| 1:q:369:PRO:HD2 | 1:q:370:ASN:N | 2.33 | 0.43 |
| 1:r:57:GLN:O | 1:r:61:LEU:HG | 2.19 | 0.43 |
| 1:r:78:ALA:O | 1:r:82:MET:HE3 | 2.17 | 0.43 |
| 1:r:147:PHE:CE1 | 1:r:159:LEU:HD23 | 2.54 | 0.43 |
| 1:r:193:ASN:C | 1:r:193:ASN:OD1 | 2.61 | 0.43 |
| 1:r:235:ALA:HB2 | 1:r:245:ILE:HD13 | 2.00 | 0.43 |
| 1:r:284:VAL:O | 1:r:288:GLN:HG2 | 2.18 | 0.43 |
| 1:r:319:ILE:HD12 | 1:r:319:ILE:H | 1.83 | 0.43 |
| 1:s:3:VAL:HG23 | 1:t:18:LEU:HD21 | 1.99 | 0.43 |
| 1:s:126:ILE:HG13 | 1:s:126:ILE:H | 1.69 | 0.43 |
| 1:s:272:LYS:C | 1:s:273:LYS:HD3 | 2.43 | 0.43 |
| 1:t:205:GLN:N | 1:t:205:GLN:OE1 | 2.50 | 0.43 |
| 1:v:180:SER:HA | 1:v:242:LYS:HE3 | 1.98 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:3:67:ASN:HA | 1:3:70:ASP:OD2 | 2.19 | 0.43 |
| 1:D:72:ILE:HD12 | 1:D:72:ILE:HA | 1.84 | 0.43 |
| 1:D:89:LEU:HD12 | 1:D:298:LEU:HD13 | 2.01 | 0.43 |
| 1:D:208:GLU:N | 1:D:208:GLU:OE2 | 2.51 | 0.43 |
| 1:D:357:ALA:O | 1:D:361:ILE:HG12 | 2.17 | 0.43 |
| 1:E:16:ARG:NH1 | 1:l:327:GLU:OE1 | 2.51 | 0.43 |
| 1:J:61:LEU:CD2 | 1:J:151:ALA:HB2 | 2.49 | 0.43 |
| 1:J:335:ARG:HG3 | 1:J:335:ARG:NH1 | 2.34 | 0.43 |
| 1:K:292:ALA:O | 1:K:295:ASP:OD1 | 2.35 | 0.43 |
| 1:M:239:GLN:CD | 1:M:239:GLN:H | 2.25 | 0.43 |
| 1:N:297:ALA:O | 1:N:301:VAL:HG12 | 2.19 | 0.43 |
| 1:P:177:GLN:H | 1:P:272:LYS:HZ3 | 1.67 | 0.43 |
| 1:Q:166:SER:HB2 | 1:Q:276:VAL:HB | 1.99 | 0.43 |
| 1:Q:185:ASP:OD2 | 1:Q:186:TRP:N | 2.51 | 0.43 |
| 1:Q:300:TYR:O | 1:Q:304:HIS:CE1 | 2.71 | 0.43 |
| 1:R:224:THR:HA | 1:R:227:ASN:HD22 | 1.83 | 0.43 |
| 1:h:319:ILE:HG13 | 1:h:319:ILE:H | 1.69 | 0.43 |
| 1:i:205:GLN:OE1 | 1:i:206:GLU:N | 2.47 | 0.43 |
| 1:m:142:HIS:CG | 1:m:143:GLY:N | 2.86 | 0.43 |
| 1:n:290:SER:O | 1:n:293:ILE:HG22 | 2.18 | 0.43 |
| 1:n:349:THR:O | 1:n:353:ILE:HG23 | 2.18 | 0.43 |
| 1:o:55:ASN:O | 1:o:59:ARG:HG2 | 2.19 | 0.43 |
| 1:p:197:ILE:HG12 | 1:p:209:ILE:HB | 1.99 | 0.43 |
| 1:q:248:GLY:O | 1:q:252:VAL:HG12 | 2.18 | 0.43 |
| 1:r:152:ASP:O | 1:r:155:GLU:HG3 | 2.18 | 0.43 |
| 1:t:112:ILE:O | 1:t:116:VAL:HG23 | 2.18 | 0.43 |
| 1:t:234:LYS:HE2 | 1:t:234:LYS:HA | 2.01 | 0.43 |
| 1:u:47:GLY:O | 1:u:51:SER:OG | 2.27 | 0.43 |
| 1:v:79:GLU:OE1 | 1:v:305:ARG:NH2 | 2.47 | 0.43 |
| 1:w:93:ARG:HA | 1:w:294:ILE:HD13 | 2.01 | 0.43 |
| 1:w:93:ARG:HB2 | 1:w:294:ILE:HG21 | 2.00 | 0.43 |
| 1:w:97:LEU:HD23 | 1:w:97:LEU:HA | 1.85 | 0.43 |
| 1:w:109:ARG:HB3 | 1:w:282:THR:HA | 2.00 | 0.43 |
| 1:2:317:HIS:CE1 | 1:3:87:ASN:HD21 | 2.36 | 0.43 |
| 1:3:170:MET:HE2 | 1:3:300:TYR:CE1 | 2.54 | 0.43 |
| 1:3:288:GLN:O | 1:3:291:VAL:HG12 | 2.19 | 0.43 |
| 1:A:84:GLU:O | 1:A:88:ILE:HG13 | 2.19 | 0.43 |
| 1:D:85:THR:O | 1:D:89:LEU:HG | 2.19 | 0.43 |
| 1:D:153:ASN:OD1 | 1:k:291:VAL:HG13 | 2.18 | 0.43 |
| 1:E:5:VAL:HG12 | 1:l:341:PHE:HE1 | 1.83 | 0.43 |
| 1:F:170:MET:HE1 | 1:F:250:ASN:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:338:ASP:OD2 | 1:F:338:ASP:N | 2.51 | 0.43 |
| 1:H:70:ASP:O | 1:H:74:ILE:HG12 | 2.18 | 0.43 |
| 1:I:95:LEU:HD11 | 1:I:115:GLU:HG2 | 2.00 | 0.43 |
| 1:M:105:SER:OG | 1:M:108:GLU:OE1 | 2.34 | 0.43 |
| 1:M:185:ASP:OD1 | 1:M:185:ASP:N | 2.51 | 0.43 |
| 1:P:168:ASN:HD21 | 1:P:170:MET:CE | 2.32 | 0.43 |
| 1:R:72:ILE:HD12 | 1:R:72:ILE:HA | 1.90 | 0.43 |
| 1:R:243:LEU:HD23 | 1:R:244:GLN:N | 2.34 | 0.43 |
| 1:S:290:SER:O | 1:S:294:ILE:HG22 | 2.18 | 0.43 |
| 1:T:30:GLU:CD | 1:T:39:ASN:HD22 | 2.25 | 0.43 |
| 1:T:88:ILE:HG13 | 1:T:88:ILE:H | 1.62 | 0.43 |
| 1:T:304:HIS:HA | 1:T:307:GLU:OE1 | 2.19 | 0.43 |
| 1:i:125:ARG:O | 1:i:129:THR:HG23 | 2.19 | 0.43 |
| 1:k:316:ASN:O | 1:k:319:ILE:HG22 | 2.18 | 0.43 |
| 1:l:78:ALA:O | 1:l:82:MET:HG3 | 2.17 | 0.43 |
| 1:m:25:GLN:HG2 | 1:m:29:MET:CE | 2.49 | 0.43 |
| 1:o:173:GLY:HA3 | 1:o:246:PHE:CE1 | 2.54 | 0.43 |
| 1:s:32:LEU:HA | 1:s:32:LEU:HD13 | 1.81 | 0.43 |
| 1:u:64:ALA:HB1 | 1:u:149:ILE:O | 2.19 | 0.43 |
| 1:v:194:ASP:HB2 | 1:v:196:LYS:NZ | 2.33 | 0.43 |
| 1:w:88:ILE:O | 1:w:92:MET:HG3 | 2.19 | 0.43 |
| 1:w:333:LYS:HE3 | 1:w:333:LYS:HB3 | 1.89 | 0.43 |
| 1:x:31:ARG:NH1 | 1:x:37:LYS:O | 2.50 | 0.43 |
| 1:z:7:THR:HG22 | 1:z:8:ASN:H | 1.83 | 0.43 |
| 1:3:191:GLY:O | 1:3:192:LYS:HD2 | 2.17 | 0.43 |
| 1:A:82:MET:O | 1:A:85:THR:OG1 | 2.31 | 0.43 |
| 1:D:193:ASN:ND2 | 1:D:213:ALA:O | 2.46 | 0.43 |
| 1:F:72:ILE:HA | 1:F:72:ILE:HD12 | 1.79 | 0.43 |
| 1:G:218:ASP:CG | 1:G:219:ILE:N | 2.77 | 0.43 |
| 1:J:366:LYS:O | 1:J:369:PRO:HD2 | 2.19 | 0.43 |
| 1:K:120:ASN:C | 1:K:120:ASN:OD1 | 2.62 | 0.43 |
| 1:K:330:ASN:O | 1:K:333:LYS:HG2 | 2.18 | 0.43 |
| 1:L:78:ALA:HB1 | 1:L:82:MET:HE3 | 1.99 | 0.43 |
| 1:N:145:LYS:O | 1:N:158:MET:HG2 | 2.19 | 0.43 |
| 1:N:287:ALA:HB3 | 1:N:288:GLN:NE2 | 2.33 | 0.43 |
| 1:N:312:GLN:HG3 | 1:N:313:ASN:N | 2.33 | 0.43 |
| 1:P:162:LYS:HG2 | 1:P:304:HIS:NE2 | 2.33 | 0.43 |
| 1:S:211:ILE:HG23 | 1:S:225:TYR:HE1 | 1.84 | 0.43 |
| 1:V:218:ASP:CG | 1:V:219:ILE:N | 2.76 | 0.43 |
| 1:c:3:VAL:HG13 | 1:c:3:VAL:O | 2.19 | 0.43 |
| 1:h:167:ASP:OD1 | 1:h:167:ASP:N | 2.50 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:h:218:ASP:HB3 | 1:h:221:GLU:HG3 | 2.00 | 0.43 |
| 1:i:273:LYS:HD2 | 1:i:274:VAL:N | 2.34 | 0.43 |
| 1:j:208:GLU:O | 1:j:209:ILE:HD13 | 2.18 | 0.43 |
| 1:n:25:GLN:OE1 | 1:n:29:MET:HE2 | 2.19 | 0.43 |
| 1:o:218:ASP:CG | 1:o:219:ILE:N | 2.76 | 0.43 |
| 1:q:318:ALA:O | 1:q:322:LEU:HG | 2.18 | 0.43 |
| 1:r:31:ARG:HH12 | 1:r:37:LYS:HB2 | 1.83 | 0.43 |
| 1:u:334:SER:HA | 1:u:338:ASP:OD1 | 2.19 | 0.43 |
| 1:w:161:LEU:HA | 1:w:162:LYS:HZ2 | 1.82 | 0.43 |
| 1:z:149:ILE:HG21 | 1:z:315:PHE:CE2 | 2.54 | 0.43 |
| 1:z:236:SER:OG | 1:z:244:GLN:HB2 | 2.19 | 0.43 |
| 1:1:121:ASP:OD2 | 1:z:314:ARG:NH2 | 2.35 | 0.43 |
| 1:3:89:LEU:HA | 1:3:92:MET:HE3 | 2.00 | 0.43 |
| 1:A:150:GLY:O | 1:A:151:ALA:C | 2.60 | 0.43 |
| 1:C:113:GLN:OE1 | 1:C:281:VAL:HG22 | 2.17 | 0.43 |
| 1:G:293:ILE:HG13 | 1:G:293:ILE:H | 1.64 | 0.43 |
| 1:H:88:ILE:HG13 | 1:H:88:ILE:H | 1.70 | 0.43 |
| 1:H:311:PHE:C | 1:H:311:PHE:CD2 | 2.97 | 0.43 |
| 1:I:163:ASP:O | 1:I:300:TYR:OH | 2.35 | 0.43 |
| 1:J:166:SER:OG | 1:J:277:ASP:OD1 | 2.34 | 0.43 |
| 1:L:190:GLU:O | 1:L:192:LYS:NZ | 2.41 | 0.43 |
| 1:M:22:ASN:HD22 | 1:M:22:ASN:N | 2.17 | 0.43 |
| 1:M:162:LYS:HE2 | 1:M:162:LYS:HB2 | 1.86 | 0.43 |
| 1:N:205:GLN:CD | 1:N:205:GLN:N | 2.77 | 0.43 |
| 1:N:366:LYS:O | 1:N:369:PRO:HD2 | 2.19 | 0.43 |
| 1:R:188:VAL:HG22 | 1:R:189:ALA:N | 2.33 | 0.43 |
| 1:S:192:LYS:HD3 | 1:S:261:GLY:HA3 | 2.00 | 0.43 |
| 1:c:138:LEU:HB3 | 1:c:164:MET:HG2 | 1.99 | 0.43 |
| 1:c:184:LYS:NZ | 1:c:218:ASP:OD2 | 2.51 | 0.43 |
| 1:c:373:LEU:O | 1:c:373:LEU:HD12 | 2.19 | 0.43 |
| 1:h:109:ARG:HH12 | 1:h:284:VAL:HG22 | 1.83 | 0.43 |
| 1:h:246:PHE:C | 1:h:246:PHE:CD2 | 2.96 | 0.43 |
| 1:j:364:GLN:HA | 1:j:367:GLN:HG2 | 2.00 | 0.43 |
| 1:n:362:LEU:HD12 | 1:n:362:LEU:HA | 1.84 | 0.43 |
| 1:o:52:ASN:O | 1:o:56:VAL:HG12 | 2.18 | 0.43 |
| 1:o:138:LEU:HD12 | 1:o:164:MET:HG2 | 2.00 | 0.43 |
| 1:o:158:MET:HE2 | 1:z:184:LYS:HG2 | 2.00 | 0.43 |
| 1:r:366:LYS:O | 1:r:369:PRO:HD2 | 2.19 | 0.43 |
| 1:t:295:ASP:HA | 1:t:298:LEU:HD12 | 2.01 | 0.43 |
| 1:u:279:ILE:HG21 | 1:u:290:SER:HB3 | 2.01 | 0.43 |
| 1:w:366:LYS:O | 1:w:369:PRO:HD2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:x:340:ASP:C | 1:x:340:ASP:OD2 | 2.61 | 0.43 |
| 1:l:82:MET:HE2 | 1:l:82:MET:HB3 | 1.95 | 0.43 |
| 1:A:119:LEU:HD23 | 1:A:119:LEU:HA | 1.82 | 0.43 |
| 1:E:72:ILE:HD12 | 1:E:72:ILE:HA | 1.82 | 0.43 |
| 1:F:66:ARG:HA | 1:F:69:ASN:ND2 | 2.33 | 0.43 |
| 1:H:92:MET:HE2 | 1:H:92:MET:HB3 | 1.86 | 0.43 |
| 1:I:125:ARG:HG2 | 1:I:125:ARG:NH1 | 2.33 | 0.43 |
| 1:I:270:GLU:OE2 | 1:I:271:GLY:N | 2.51 | 0.43 |
| 1:J:27:THR:HG22 | 1:J:31:ARG:HD2 | 2.00 | 0.43 |
| 1:J:171:MET:N | 1:J:171:MET:SD | 2.92 | 0.43 |
| 1:M:168:ASN:OD1 | 1:M:170:MET:HE2 | 2.18 | 0.43 |
| 1:O:160:GLU:OE1 | 1:O:162:LYS:HD3 | 2.19 | 0.43 |
| 1:R:79:GLU:OE2 | 1:R:305:ARG:NE | 2.52 | 0.43 |
| 1:T:316:ASN:HA | 1:T:319:ILE:HD12 | 2.00 | 0.43 |
| 1:V:57:GLN:O | 1:V:61:LEU:HG | 2.19 | 0.43 |
| 1:h:28:SER:HA | 1:h:344:GLU:OE1 | 2.19 | 0.43 |
| 1:i:273:LYS:HZ3 | 1:i:275:THR:CG2 | 2.17 | 0.43 |
| 1:k:64:ALA:HB1 | 1:k:149:ILE:O | 2.18 | 0.43 |
| 1:k:165:ARG:NH2 | 1:u:214:LYS:HE3 | 2.34 | 0.43 |
| 1:k:187:ASN:C | 1:k:187:ASN:OD1 | 2.61 | 0.43 |
| 1:p:222:LEU:O | 1:p:226:ILE:HG13 | 2.19 | 0.43 |
| 1:r:66:ARG:CZ | 1:r:66:ARG:HB2 | 2.48 | 0.43 |
| 1:u:49:GLN:O | 1:u:53:ARG:HG3 | 2.19 | 0.43 |
| 1:w:338:ASP:OD1 | 1:w:338:ASP:N | 2.52 | 0.43 |
| 1:x:257:GLU:N | 1:x:257:GLU:CD | 2.77 | 0.43 |
| 1:x:295:ASP:O | 1:x:299:LYS:HD3 | 2.18 | 0.43 |
| 1:x:330:ASN:ND2 | 1:x:330:ASN:H | 2.16 | 0.43 |
| 1:z:246:PHE:HD2 | 1:z:292:ALA:HB3 | 1.84 | 0.43 |
| 1:1:109:ARG:HA | 1:1:112:ILE:HG22 | 1.99 | 0.43 |
| 1:1:125:ARG:O | 1:1:129:THR:HG22 | 2.18 | 0.43 |
| 1:1:138:LEU:HD13 | 1:1:164:MET:HG3 | 1.99 | 0.43 |
| 1:2:159:LEU:HD22 | 1:2:311:PHE:CE2 | 2.53 | 0.43 |
| 1:3:229:GLN:HA | 1:3:229:GLN:HE21 | 1.84 | 0.43 |
| 1:B:196:LYS:HB3 | 1:B:208:GLU:OE2 | 2.18 | 0.43 |
| 1:C:298:LEU:O | 1:C:302:ASP:OD1 | 2.37 | 0.43 |
| 1:D:196:LYS:O | 1:D:197:ILE:HD13 | 2.19 | 0.43 |
| 1:E:192:LYS:O | 1:E:192:LYS:HG3 | 2.17 | 0.43 |
| 1:F:233:VAL:CG2 | 1:F:245:ILE:HD11 | 2.49 | 0.43 |
| 1:F:301:VAL:O | 1:F:305:ARG:HG2 | 2.19 | 0.43 |
| 1:H:166:SER:HB2 | 1:H:276:VAL:HG23 | 2.00 | 0.43 |
| 1:M:199:LEU:HD12 | 1:M:200:THR:C | 2.44 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:50:ILE:HG22 | 1:N:54:LEU:CD1 | 2.49 | 0.43 |
| 1:O:163:ASP:OD1 | 1:O:164:MET:N | 2.51 | 0.43 |
| 1:O:193:ASN:HA | 1:O:262:LEU:HD21 | 2.00 | 0.43 |
| 1:P:248:GLY:H | 1:P:251:LYS:HE2 | 1.82 | 0.43 |
| 1:S:89:LEU:O | 1:S:294:ILE:HD11 | 2.19 | 0.43 |
| 1:V:194:ASP:OD2 | 1:V:196:LYS:NZ | 2.52 | 0.43 |
| 1:c:130:THR:HG21 | 1:c:138:LEU:HG | 2.00 | 0.43 |
| 1:c:318:ALA:O | 1:c:322:LEU:HG | 2.19 | 0.43 |
| 1:l:192:LYS:O | 1:l:262:LEU:HD13 | 2.18 | 0.43 |
| 1:n:265:GLU:OE2 | 1:n:265:GLU:HA | 2.19 | 0.43 |
| 1:o:181:GLY:HA2 | 1:o:242:LYS:HG2 | 2.01 | 0.43 |
| 1:p:221:GLU:O | 1:p:224:THR:OG1 | 2.32 | 0.43 |
| 1:p:222:LEU:HD23 | 1:p:226:ILE:HD11 | 2.01 | 0.43 |
| 1:q:109:ARG:HB3 | 1:q:282:THR:HA | 2.01 | 0.43 |
| 1:q:312:GLN:O | 1:q:316:ASN:ND2 | 2.51 | 0.43 |
| 1:r:91:ARG:HA | 1:r:94:ASP:OD1 | 2.19 | 0.43 |
| 1:s:67:ASN:HA | 1:s:70:ASP:OD2 | 2.19 | 0.43 |
| 1:v:195:LEU:C | 1:v:196:LYS:HD2 | 2.44 | 0.43 |
| 1:x:32:LEU:HD13 | 1:x:32:LEU:HA | 1.91 | 0.43 |
| 1:1:82:MET:HE2 | 1:1:301:VAL:HG13 | 2.01 | 0.42 |
| 1:1:350:LYS:O | 1:1:354:LEU:HG | 2.19 | 0.42 |
| 1:2:31:ARG:HD2 | 1:2:344:GLU:OE1 | 2.19 | 0.42 |
| 1:2:111:ALA:O | 1:2:114:GLU:N | 2.52 | 0.42 |
| 1:2:349:THR:HA | 1:2:352:GLN:NE2 | 2.33 | 0.42 |
| 1:3:300:TYR:O | 1:3:304:HIS:CD2 | 2.72 | 0.42 |
| 1:A:321:ASN:ND2 | 1:B:126:ILE:HD12 | 2.33 | 0.42 |
| 1:E:328:ASN:OD1 | 1:F:76:GLN:HG3 | 2.19 | 0.42 |
| 1:G:172:GLY:O | 1:G:249:ASN:HB3 | 2.20 | 0.42 |
| 1:H:141:THR:H | 1:H:141:THR:HG1 | 1.66 | 0.42 |
| 1:I:93:ARG:NE | 1:I:291:VAL:HG13 | 2.33 | 0.42 |
| 1:I:148:GLN:NE2 | 1:I:150:GLY:O | 2.44 | 0.42 |
| 1:J:145:LYS:HA | 1:J:145:LYS:HD3 | 1.80 | 0.42 |
| 1:L:92:MET:HB2 | 1:L:294:ILE:CD1 | 2.49 | 0.42 |
| 1:L:116:VAL:O | 1:L:120:ASN:OD1 | 2.36 | 0.42 |
| 1:L:368:ALA:HB3 | 1:L:369:PRO:HD3 | 2.01 | 0.42 |
| 1:M:273:LYS:HD2 | 1:M:273:LYS:N | 2.34 | 0.42 |
| 1:N:70:ASP:O | 1:N:74:ILE:HG12 | 2.19 | 0.42 |
| 1:N:293:ILE:HD12 | 1:N:293:ILE:HA | 1.93 | 0.42 |
| 1:O:44:ASP:C | 1:O:44:ASP:OD1 | 2.62 | 0.42 |
| 1:O:152:ASP:OD1 | 1:O:153:ASN:N | 2.43 | 0.42 |
| 1:T:37:LYS:HG2 | 1:T:337:LYS:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:64:ALA:HB1 | 1:U:149:ILE:O | 2.19 | 0.42 |
| 1:V:160:GLU:O | 1:V:161:LEU:HD23 | 2.18 | 0.42 |
| 1:c:375:LEU:HD23 | 1:c:375:LEU:HA | 1.77 | 0.42 |
| 1:h:344:GLU:HA | 1:h:344:GLU:OE2 | 2.19 | 0.42 |
| 1:i:26:GLN:HA | 1:i:29:MET:HE3 | 2.01 | 0.42 |
| 1:i:92:MET:HE2 | 1:i:116:VAL:HG13 | 2.00 | 0.42 |
| 1:i:333:LYS:HE2 | 1:i:333:LYS:HB2 | 1.88 | 0.42 |
| 1:k:125:ARG:NH1 | 1:k:129:THR:HG21 | 2.33 | 0.42 |
| 1:l:29:MET:SD | 1:l:344:GLU:HA | 2.59 | 0.42 |
| 1:l:29:MET:HE3 | 1:l:347:ALA:HB3 | 2.00 | 0.42 |
| 1:o:196:LYS:HB3 | 1:o:259:SER:OG | 2.18 | 0.42 |
| 1:p:250:ASN:ND2 | 1:p:250:ASN:C | 2.75 | 0.42 |
| 1:q:173:GLY:HA3 | 1:q:246:PHE:CZ | 2.53 | 0.42 |
| 1:r:77:THR:HG21 | 1:r:132:PHE:HD2 | 1.84 | 0.42 |
| 1:r:83:ASN:HA | 1:r:305:ARG:NH1 | 2.34 | 0.42 |
| 1:s:295:ASP:OD2 | 1:s:295:ASP:C | 2.62 | 0.42 |
| 1:v:46:ALA:O | 1:v:50:ILE:HG13 | 2.19 | 0.42 |
| 1:x:225:TYR:O | 1:x:229:GLN:HG2 | 2.19 | 0.42 |
| 1:z:44:ASP:OD1 | 1:z:44:ASP:C | 2.62 | 0.42 |
| 1:1:5:VAL:HG12 | 1:1:6:ASN:CG | 2.45 | 0.42 |
| 1:3:5:VAL:HG22 | 1:3:372:ALA:HB1 | 2.00 | 0.42 |
| 1:3:233:VAL:CG2 | 1:3:245:ILE:HG22 | 2.49 | 0.42 |
| 1:C:138:LEU:HD12 | 1:C:164:MET:CG | 2.49 | 0.42 |
| 1:E:4:ASN:C | 1:E:4:ASN:OD1 | 2.62 | 0.42 |
| 1:E:170:MET:HE1 | 1:E:249:ASN:O | 2.19 | 0.42 |
| 1:I:153:ASN:HB2 | 1:p:234:LYS:HE2 | 2.01 | 0.42 |
| 1:O:162:LYS:HG2 | 1:O:304:HIS:CE1 | 2.54 | 0.42 |
| 1:O:311:PHE:CZ | 1:O:315:PHE:HE1 | 2.38 | 0.42 |
| 1:Q:70:ASP:N | 1:Q:70:ASP:OD1 | 2.50 | 0.42 |
| 1:S:190:GLU:HA | 1:S:193:ASN:ND2 | 2.34 | 0.42 |
| 1:S:366:LYS:O | 1:S:369:PRO:HD2 | 2.18 | 0.42 |
| 1:j:113:GLN:OE1 | 1:j:281:VAL:HG22 | 2.19 | 0.42 |
| 1:j:169:LYS:HE3 | 1:j:249:ASN:HB3 | 2.01 | 0.42 |
| 1:k:196:LYS:HE3 | 1:k:210:ASN:HB2 | 2.01 | 0.42 |
| 1:m:290:SER:O | 1:m:294:ILE:HG12 | 2.18 | 0.42 |
| 1:o:122:GLU:OE2 | 1:o:122:GLU:HA | 2.19 | 0.42 |
| 1:u:73:SER:HA | 1:u:76:GLN:HG3 | 2.01 | 0.42 |
| 1:1:336:ILE:HG22 | 1:1:337:LYS:NZ | 2.34 | 0.42 |
| 1:2:124:ASN:O | 1:2:128:GLU:HG2 | 2.20 | 0.42 |
| 1:2:125:ARG:HG2 | 1:2:125:ARG:NH1 | 2.34 | 0.42 |
| 1:2:149:ILE:HG21 | 1:2:315:PHE:CZ | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:3:85:THR:HA | 1:3:88:ILE:HD12 | 2.01 | 0.42 |
| 1:3:147:PHE:HE1 | 1:3:159:LEU:HD23 | 1.83 | 0.42 |
| 1:3:239:GLN:CD | 1:3:239:GLN:H | 2.27 | 0.42 |
| 1:A:193:ASN:HA | 1:A:262:LEU:HD21 | 2.00 | 0.42 |
| 1:B:44:ASP:OD1 | 1:B:44:ASP:C | 2.62 | 0.42 |
| 1:B:159:LEU:HD12 | 1:B:160:GLU:N | 2.33 | 0.42 |
| 1:E:220:GLU:O | 1:E:224:THR:HG22 | 2.19 | 0.42 |
| 1:F:15:GLN:HE22 | 1:l:343:LYS:HD2 | 1.84 | 0.42 |
| 1:G:171:MET:HB3 | 1:G:276:VAL:HG23 | 2.00 | 0.42 |
| 1:J:288:GLN:HE22 | 1:U:148:GLN:HE21 | 1.67 | 0.42 |
| 1:K:321:ASN:ND2 | 1:h:126:ILE:HG12 | 2.35 | 0.42 |
| 1:L:193:ASN:OD1 | 1:L:193:ASN:N | 2.44 | 0.42 |
| 1:M:75:ALA:HB1 | 1:M:308:LEU:HD12 | 2.01 | 0.42 |
| 1:M:162:LYS:HE3 | 1:M:170:MET:HE3 | 2.01 | 0.42 |
| 1:M:333:LYS:C | 1:M:333:LYS:HD2 | 2.45 | 0.42 |
| 1:N:64:ALA:HB1 | 1:N:149:ILE:O | 2.18 | 0.42 |
| 1:N:203:TYR:CD2 | 1:N:205:GLN:NE2 | 2.84 | 0.42 |
| 1:O:93:ARG:HE | 1:O:93:ARG:HB3 | 1.49 | 0.42 |
| 1:O:106:LYS:HB2 | 1:O:106:LYS:NZ | 2.34 | 0.42 |
| 1:O:147:PHE:HE2 | 1:O:159:LEU:HD23 | 1.84 | 0.42 |
| 1:P:3:VAL:HG13 | 1:P:3:VAL:O | 2.20 | 0.42 |
| 1:Q:218:ASP:OD1 | 1:Q:219:ILE:N | 2.52 | 0.42 |
| 1:R:232:LEU:HD13 | 1:R:251:LYS:HZ1 | 1.83 | 0.42 |
| 1:U:97:LEU:HD23 | 1:U:291:VAL:HG21 | 2.01 | 0.42 |
| 1:i:159:LEU:HD13 | 1:i:311:PHE:CE2 | 2.55 | 0.42 |
| 1:k:222:LEU:HG | 1:k:226:ILE:HD11 | 2.00 | 0.42 |
| 1:l:50:ILE:HG13 | 1:l:50:ILE:H | 1.66 | 0.42 |
| 1:l:214:LYS:HG3 | 1:l:217:ASP:OD1 | 2.19 | 0.42 |
| 1:n:12:MET:H | 1:n:12:MET:HG3 | 1.58 | 0.42 |
| 1:n:240:ASP:OD1 | 1:n:240:ASP:C | 2.62 | 0.42 |
| 1:s:354:LEU:HA | 1:s:354:LEU:HD23 | 1.76 | 0.42 |
| 1:w:346:THR:O | 1:w:348:MET:N | 2.52 | 0.42 |
| 1:x:124:ASN:O | 1:x:128:GLU:HG2 | 2.20 | 0.42 |
| 1:z:111:ALA:O | 1:z:115:GLU:OE1 | 2.36 | 0.42 |
| 1:1:319:ILE:HA | 1:1:322:LEU:HG | 2.02 | 0.42 |
| 1:1:357:ALA:O | 1:1:361:ILE:HG13 | 2.19 | 0.42 |
| 1:A:115:GLU:OE2 | 1:V:313:ASN:ND2 | 2.51 | 0.42 |
| 1:A:366:LYS:O | 1:A:369:PRO:HD2 | 2.19 | 0.42 |
| 1:B:67:ASN:OD1 | 1:i:101:ASN:ND2 | 2.52 | 0.42 |
| 1:B:162:LYS:HE2 | 1:B:304:HIS:CE1 | 2.54 | 0.42 |
| 1:C:106:LYS:O | 1:C:110:VAL:HG23 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:266:LEU:HD23 | 1:C:266:LEU:HA | 1.88 | 0.42 |
| 1:I:5:VAL:HG12 | 1:I:6:ASN:N | 2.34 | 0.42 |
| 1:I:50:ILE:HD13 | 1:I:50:ILE:HA | 1.88 | 0.42 |
| 1:K:136:LYS:HA | 1:K:136:LYS:HD3 | 1.87 | 0.42 |
| 1:K:321:ASN:OD1 | 1:K:321:ASN:C | 2.62 | 0.42 |
| 1:L:173:GLY:HA3 | 1:L:246:PHE:HE2 | 1.84 | 0.42 |
| 1:M:28:SER:HB3 | 1:M:348:MET:HB2 | 2.01 | 0.42 |
| 1:P:208:GLU:OE1 | 1:P:210:ASN:ND2 | 2.52 | 0.42 |
| 1:Q:89:LEU:HA | 1:Q:92:MET:CE | 2.49 | 0.42 |
| 1:R:69:ASN:O | 1:R:72:ILE:HG22 | 2.19 | 0.42 |
| 1:T:142:HIS:CG | 1:T:143:GLY:H | 2.37 | 0.42 |
| 1:T:236:SER:OG | 1:T:244:GLN:HB2 | 2.19 | 0.42 |
| 1:h:199:LEU:HB3 | 1:h:256:VAL:HG22 | 2.01 | 0.42 |
| 1:i:13:THR:HA | 1:i:16:ARG:HG3 | 2.02 | 0.42 |
| 1:i:340:ASP:OD1 | 1:i:340:ASP:C | 2.62 | 0.42 |
| 1:j:189:ALA:HB3 | 1:j:192:LYS:HB2 | 2.01 | 0.42 |
| 1:n:276:VAL:O | 1:n:279:ILE:HG23 | 2.19 | 0.42 |
| 1:o:91:ARG:HH12 | 1:o:95:LEU:HD21 | 1.84 | 0.42 |
| 1:q:113:GLN:OE1 | 1:q:281:VAL:HG22 | 2.19 | 0.42 |
| 1:r:66:ARG:HB2 | 1:r:66:ARG:NH1 | 2.34 | 0.42 |
| 1:t:222:LEU:O | 1:t:226:ILE:HG13 | 2.20 | 0.42 |
| 1:u:142:HIS:CG | 1:u:161:LEU:HD12 | 2.54 | 0.42 |
| 1:x:31:ARG:HG2 | 1:x:37:LYS:HA | 2.01 | 0.42 |
| 1:x:162:LYS:HD3 | 1:x:162:LYS:N | 2.34 | 0.42 |
| 1:1:80:GLY:CA | 1:z:324:ASN:HD21 | 2.33 | 0.42 |
| 1:A:335:ARG:NH1 | 1:B:73:SER:OG | 2.51 | 0.42 |
| 1:B:147:PHE:O | 1:B:156:ALA:HB1 | 2.20 | 0.42 |
| 1:C:192:LYS:HE3 | 1:C:192:LYS:HA | 2.02 | 0.42 |
| 1:E:36:PHE:CD1 | 1:E:337:LYS:HG2 | 2.55 | 0.42 |
| 1:E:319:ILE:HG13 | 1:E:319:ILE:H | 1.61 | 0.42 |
| 1:E:321:ASN:HB2 | 1:F:84:GLU:HG3 | 2.02 | 0.42 |
| 1:F:344:GLU:OE1 | 1:F:344:GLU:HA | 2.19 | 0.42 |
| 1:I:106:LYS:O | 1:I:110:VAL:HG23 | 2.19 | 0.42 |
| 1:I:208:GLU:O | 1:I:209:ILE:HD13 | 2.19 | 0.42 |
| 1:I:245:ILE:N | 1:I:245:ILE:HD12 | 2.34 | 0.42 |
| 1:K:88:ILE:HG21 | 1:K:123:LEU:HG | 2.00 | 0.42 |
| 1:K:340:ASP:OD1 | 1:K:340:ASP:C | 2.62 | 0.42 |
| 1:M:72:ILE:HG13 | 1:M:72:ILE:H | 1.65 | 0.42 |
| 1:N:300:TYR:CZ | 1:N:304:HIS:CE1 | 3.08 | 0.42 |
| 1:O:8:ASN:ND2 | 1:O:365:ALA:O | 2.50 | 0.42 |
| 1:O:367:GLN:OE1 | 1:O:367:GLN:HA | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:162:LYS:HD2 | 1:T:163:ASP:N | 2.25 | 0.42 |
| 1:U:105:SER:N | 1:U:108:GLU:OE2 | 2.53 | 0.42 |
| 1:U:239:GLN:H | 1:U:239:GLN:CD | 2.26 | 0.42 |
| 1:V:38:ILE:CD1 | 1:V:43:ASP:HB2 | 2.49 | 0.42 |
| 1:V:245:ILE:HD12 | 1:V:245:ILE:HA | 1.97 | 0.42 |
| 1:h:108:GLU:O | 1:h:112:ILE:HG13 | 2.19 | 0.42 |
| 1:k:257:GLU:CD | 1:k:257:GLU:N | 2.77 | 0.42 |
| 1:l:179:GLU:OE1 | 1:l:242:LYS:NZ | 2.49 | 0.42 |
| 1:l:238:ASP:OD2 | 1:l:238:ASP:C | 2.62 | 0.42 |
| 1:m:72:ILE:HG13 | 1:m:72:ILE:H | 1.62 | 0.42 |
| 1:m:272:LYS:C | 1:m:273:LYS:HD3 | 2.45 | 0.42 |
| 1:p:15:GLN:HE22 | 1:z:343:LYS:HZ2 | 1.67 | 0.42 |
| 1:r:18:LEU:HD23 | 1:r:358:SER:HB2 | 2.01 | 0.42 |
| 1:t:173:GLY:HA2 | 1:t:249:ASN:OD1 | 2.18 | 0.42 |
| 1:t:218:ASP:OD1 | 1:t:219:ILE:HG22 | 2.20 | 0.42 |
| 1:v:143:GLY:HA3 | 1:v:145:LYS:NZ | 2.34 | 0.42 |
| 1:x:28:SER:OG | 1:x:29:MET:SD | 2.77 | 0.42 |
| 1:3:342:ALA:HB3 | 1:s:15:GLN:NE2 | 2.34 | 0.42 |
| 1:A:30:GLU:OE1 | 1:A:30:GLU:C | 2.62 | 0.42 |
| 1:A:299:LYS:HE2 | 1:A:299:LYS:HB2 | 1.73 | 0.42 |
| 1:C:97:LEU:HD23 | 1:C:97:LEU:HA | 1.73 | 0.42 |
| 1:D:173:GLY:HA3 | 1:D:246:PHE:CZ | 2.54 | 0.42 |
| 1:G:169:LYS:HB2 | 1:G:170:MET:HE2 | 2.00 | 0.42 |
| 1:J:120:ASN:OD1 | 1:J:120:ASN:C | 2.62 | 0.42 |
| 1:L:333:LYS:HZ2 | 1:L:337:LYS:HD2 | 1.83 | 0.42 |
| 1:Q:104:ASN:O | 1:Q:109:ARG:NH2 | 2.36 | 0.42 |
| 1:R:188:VAL:HG11 | 1:R:216:GLY:N | 2.33 | 0.42 |
| 1:T:37:LYS:NZ | 1:T:336:ILE:O | 2.33 | 0.42 |
| 1:T:276:VAL:O | 1:T:279:ILE:HG12 | 2.19 | 0.42 |
| 1:V:196:LYS:HG2 | 1:V:210:ASN:OD1 | 2.20 | 0.42 |
| 1:c:105:SER:OG | 1:c:106:LYS:N | 2.51 | 0.42 |
| 1:h:59:ARG:NH2 | 1:s:91:ARG:HD2 | 2.34 | 0.42 |
| 1:h:224:THR:HA | 1:h:227:ASN:OD1 | 2.19 | 0.42 |
| 1:j:46:ALA:O | 1:j:50:ILE:HG13 | 2.19 | 0.42 |
| 1:j:113:GLN:HA | 1:j:116:VAL:CG1 | 2.50 | 0.42 |
| 1:m:160:GLU:HG2 | 1:m:162:LYS:NZ | 2.34 | 0.42 |
| 1:m:196:LYS:HE2 | 1:m:210:ASN:HD21 | 1.84 | 0.42 |
| 1:m:333:LYS:HA | 1:m:336:ILE:HD12 | 2.00 | 0.42 |
| 1:o:108:GLU:OE1 | 1:o:108:GLU:N | 2.32 | 0.42 |
| 1:p:125:ARG:NH1 | 1:p:125:ARG:HG2 | 2.33 | 0.42 |
| 1:p:192:LYS:NZ | 1:p:265:GLU:OE1 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:s:153:ASN:OD1 | 1:s:153:ASN:C | 2.62 | 0.42 |
| 1:s:368:ALA:HB3 | 1:s:369:PRO:HD3 | 2.02 | 0.42 |
| 1:u:174:VAL:HG23 | 1:u:249:ASN:OD1 | 2.20 | 0.42 |
| 1:w:22:ASN:OD1 | 1:w:22:ASN:N | 2.53 | 0.42 |
| 1:x:108:GLU:O | 1:x:112:ILE:HG13 | 2.20 | 0.42 |
| 1:x:205:GLN:C | 1:x:205:GLN:OE1 | 2.63 | 0.42 |
| 1:x:302:ASP:N | 1:x:302:ASP:OD1 | 2.51 | 0.42 |
| 1:z:115:GLU:O | 1:z:119:LEU:HG | 2.19 | 0.42 |
| 1:1:324:ASN:HA | 1:1:327:GLU:OE2 | 2.19 | 0.42 |
| 1:2:93:ARG:HE | 1:2:291:VAL:CG1 | 2.32 | 0.42 |
| 1:2:170:MET:HE2 | 1:2:170:MET:N | 2.35 | 0.42 |
| 1:A:89:LEU:HB3 | 1:A:298:LEU:HD21 | 2.02 | 0.42 |
| 1:A:308:LEU:HD23 | 1:A:308:LEU:HA | 1.85 | 0.42 |
| 1:B:108:GLU:H | 1:B:108:GLU:CD | 2.27 | 0.42 |
| 1:C:267:GLY:C | 1:C:268:LEU:HD23 | 2.45 | 0.42 |
| 1:C:273:LYS:HD3 | 1:C:273:LYS:N | 2.35 | 0.42 |
| 1:D:88:ILE:HG23 | 1:D:119:LEU:CD1 | 2.46 | 0.42 |
| 1:G:361:ILE:HD12 | 1:G:361:ILE:HA | 1.83 | 0.42 |
| 1:J:63:VAL:HG13 | 1:J:66:ARG:HH12 | 1.85 | 0.42 |
| 1:L:51:SER:HB2 | 1:L:333:LYS:NZ | 2.34 | 0.42 |
| 1:L:72:ILE:HD12 | 1:L:72:ILE:HA | 1.81 | 0.42 |
| 1:N:50:ILE:HG22 | 1:N:54:LEU:HD12 | 2.02 | 0.42 |
| 1:P:158:MET:HE2 | 1:P:158:MET:HB2 | 1.86 | 0.42 |
| 1:R:90:GLN:HB3 | 1:c:59:ARG:NH2 | 2.11 | 0.42 |
| 1:S:187:ASN:ND2 | 1:S:216:GLY:O | 2.48 | 0.42 |
| 1:c:217:ASP:OD1 | 1:c:217:ASP:N | 2.52 | 0.42 |
| 1:k:54:LEU:HD12 | 1:k:329:VAL:HG13 | 2.02 | 0.42 |
| 1:k:178:ALA:HA | 1:k:268:LEU:HD23 | 2.02 | 0.42 |
| 1:k:208:GLU:O | 1:k:209:ILE:HD13 | 2.19 | 0.42 |
| 1:k:276:VAL:O | 1:k:279:ILE:HG23 | 2.19 | 0.42 |
| 1:n:136:LYS:HD3 | 1:n:136:LYS:HA | 1.92 | 0.42 |
| 1:n:232:LEU:HA | 1:n:251:LYS:NZ | 2.34 | 0.42 |
| 1:p:95:LEU:HD12 | 1:p:116:VAL:HG22 | 2.02 | 0.42 |
| 1:s:123:LEU:HA | 1:s:126:ILE:HD12 | 2.02 | 0.42 |
| 1:u:339:THR:OG1 | 1:u:340:ASP:N | 2.51 | 0.42 |
| 1:w:320:SER:O | 1:w:323:ASP:OD1 | 2.38 | 0.42 |
| 1:x:251:LYS:NZ | 1:x:251:LYS:HB2 | 2.35 | 0.42 |
| 1:z:218:ASP:CG | 1:z:219:ILE:N | 2.77 | 0.42 |
| 1:z:271:GLY:O | 1:z:273:LYS:NZ | 2.45 | 0.42 |
| 1:D:94:ASP:OD1 | 1:D:94:ASP:N | 2.53 | 0.42 |
| 1:D:292:ALA:HB2 | 1:O:153:ASN:HD21 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:53:ARG:NH1 | 1:E:53:ARG:HB2 | 2.35 | 0.42 |
| 1:G:205:GLN:HB3 | 1:G:207:GLN:HE22 | 1.85 | 0.42 |
| 1:H:49:GLN:NE2 | 1:o:302:ASP:HB3 | 2.33 | 0.42 |
| 1:I:239:GLN:HG2 | 1:I:240:ASP:OD1 | 2.20 | 0.42 |
| 1:J:223:ALA:O | 1:J:226:ILE:HG22 | 2.20 | 0.42 |
| 1:K:91:ARG:O | 1:K:95:LEU:HG | 2.19 | 0.42 |
| 1:L:162:LYS:HB2 | 1:L:164:MET:HE1 | 2.02 | 0.42 |
| 1:N:104:ASN:OD1 | 1:N:105:SER:N | 2.52 | 0.42 |
| 1:O:177:GLN:C | 1:O:177:GLN:CD | 2.88 | 0.42 |
| 1:O:195:LEU:HB2 | 1:O:262:LEU:HD12 | 2.00 | 0.42 |
| 1:R:131:SER:HB3 | 1:R:136:LYS:HE3 | 2.01 | 0.42 |
| 1:R:176:TYR:OH | 1:R:255:GLU:OE1 | 2.27 | 0.42 |
| 1:R:226:ILE:HG13 | 1:R:226:ILE:H | 1.75 | 0.42 |
| 1:S:222:LEU:O | 1:S:226:ILE:HG13 | 2.20 | 0.42 |
| 1:U:93:ARG:HB2 | 1:U:294:ILE:HG21 | 2.02 | 0.42 |
| 1:U:167:ASP:HB3 | 1:U:277:ASP:OD2 | 2.20 | 0.42 |
| 1:U:301:VAL:HA | 1:U:304:HIS:CD2 | 2.55 | 0.42 |
| 1:V:118:ALA:HA | 1:V:121:ASP:OD1 | 2.20 | 0.42 |
| 1:V:279:ILE:HG21 | 1:V:293:ILE:HG21 | 2.01 | 0.42 |
| 1:i:240:ASP:OD2 | 1:i:242:LYS:HG3 | 2.20 | 0.42 |
| 1:i:321:ASN:HD21 | 1:u:126:ILE:HG23 | 1.84 | 0.42 |
| 1:j:159:LEU:HD23 | 1:j:160:GLU:N | 2.35 | 0.42 |
| 1:l:72:ILE:O | 1:l:76:GLN:HG3 | 2.20 | 0.42 |
| 1:p:171:MET:HE2 | 1:p:300:TYR:CD2 | 2.54 | 0.42 |
| 1:r:147:PHE:HE1 | 1:r:159:LEU:HD23 | 1.85 | 0.42 |
| 1:s:38:ILE:O | 1:s:337:LYS:NZ | 2.52 | 0.42 |
| 1:s:287:ALA:HA | 1:s:290:SER:OG | 2.20 | 0.42 |
| 1:s:300:TYR:CD1 | 1:s:300:TYR:C | 2.96 | 0.42 |
| 1:u:105:SER:OG | 1:u:106:LYS:N | 2.52 | 0.42 |
| 1:u:158:MET:SD | 1:u:158:MET:C | 3.03 | 0.42 |
| 1:v:19:ASN:OD1 | 1:v:20:ASN:ND2 | 2.53 | 0.42 |
| 1:x:109:ARG:HB3 | 1:x:282:THR:HA | 2.00 | 0.42 |
| 1:z:173:GLY:HA2 | 1:z:249:ASN:OD1 | 2.19 | 0.42 |
| 1:1:95:LEU:HG | 1:1:95:LEU:H | 1.69 | 0.42 |
| 1:1:210:ASN:O | 1:1:211:ILE:HD13 | 2.20 | 0.42 |
| 1:1:294:ILE:O | 1:1:298:LEU:HG | 2.20 | 0.42 |
| 1:2:17:TYR:CD1 | 1:3:33:SER:HB3 | 2.54 | 0.42 |
| 1:2:78:ALA:O | 1:2:82:MET:HG3 | 2.19 | 0.42 |
| 1:2:170:MET:HG3 | 1:2:300:TYR:OH | 2.20 | 0.42 |
| 1:B:125:ARG:HD2 | 1:B:125:ARG:C | 2.45 | 0.42 |
| 1:B:196:LYS:HB3 | 1:B:196:LYS:HE3 | 1.79 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:19:ASN:OD1 | 1:M:2:ALA:N | 2.52 | 0.42 |
| 1:D:50:ILE:HD11 | 1:w:108:GLU:OE1 | 2.20 | 0.42 |
| 1:E:209:ILE:HG22 | 1:E:211:ILE:HD11 | 2.02 | 0.42 |
| 1:G:202:SER:HB3 | 1:G:251:LYS:C | 2.45 | 0.42 |
| 1:H:142:HIS:NE2 | 1:H:145:LYS:HE2 | 2.35 | 0.42 |
| 1:J:9:VAL:O | 1:J:12:MET:HG3 | 2.20 | 0.42 |
| 1:L:192:LYS:HD3 | 1:L:192:LYS:N | 2.35 | 0.42 |
| 1:M:320:SER:O | 1:M:324:ASN:ND2 | 2.49 | 0.42 |
| 1:P:50:ILE:N | 1:P:50:ILE:HD13 | 2.35 | 0.42 |
| 1:P:314:ARG:HG3 | 1:Q:122:GLU:OE1 | 2.20 | 0.42 |
| 1:Q:161:LEU:HD23 | 1:Q:161:LEU:HA | 1.86 | 0.42 |
| 1:Q:333:LYS:HA | 1:Q:336:ILE:HD12 | 2.02 | 0.42 |
| 1:R:175:SER:O | 1:R:271:GLY:HA2 | 2.20 | 0.42 |
| 1:i:12:MET:O | 1:i:16:ARG:HG3 | 2.20 | 0.42 |
| 1:i:182:LYS:HD2 | 1:i:186:TRP:CD1 | 2.55 | 0.42 |
| 1:j:240:ASP:OD1 | 1:j:240:ASP:N | 2.49 | 0.42 |
| 1:k:66:ARG:CZ | 1:k:66:ARG:HB3 | 2.49 | 0.42 |
| 1:l:161:LEU:C | 1:l:162:LYS:HD3 | 2.45 | 0.42 |
| 1:l:193:ASN:OD1 | 1:l:193:ASN:N | 2.53 | 0.42 |
| 1:m:304:HIS:ND1 | 1:m:304:HIS:N | 2.67 | 0.42 |
| 1:s:170:MET:HB2 | 1:s:300:TYR:CE2 | 2.54 | 0.42 |
| 1:s:236:SER:O | 1:s:244:GLN:N | 2.49 | 0.42 |
| 1:v:42:LYS:HE2 | 1:v:42:LYS:HB2 | 1.82 | 0.42 |
| 1:v:122:GLU:OE2 | 1:v:125:ARG:NH2 | 2.51 | 0.42 |
| 1:v:292:ALA:HA | 1:v:295:ASP:OD2 | 2.20 | 0.42 |
| 1:x:231:ASP:OD2 | 1:x:231:ASP:N | 2.53 | 0.42 |
| 1:z:7:THR:HG22 | 1:z:8:ASN:N | 2.34 | 0.42 |
| 1:z:194:ASP:OD2 | 1:z:261:GLY:N | 2.42 | 0.42 |
| 1:z:337:LYS:HZ2 | 1:z:337:LYS:HG2 | 1.71 | 0.42 |
| 1:1:199:LEU:HB3 | 1:1:256:VAL:HG22 | 2.01 | 0.42 |
| 1:2:81:ALA:O | 1:2:84:GLU:HG3 | 2.19 | 0.42 |
| 1:2:321:ASN:ND2 | 1:3:126:ILE:HG23 | 2.35 | 0.42 |
| 1:3:108:GLU:O | 1:3:112:ILE:HG12 | 2.20 | 0.42 |
| 1:D:210:ASN:O | 1:D:211:ILE:HD13 | 2.20 | 0.42 |
| 1:F:262:LEU:O | 1:F:266:LEU:HG | 2.19 | 0.42 |
| 1:G:372:ALA:O | 1:G:375:LEU:HG | 2.20 | 0.42 |
| 1:H:192:LYS:HD2 | 1:H:192:LYS:HA | 1.86 | 0.42 |
| 1:I:276:VAL:O | 1:I:279:ILE:HG12 | 2.19 | 0.42 |
| 1:J:367:GLN:OE1 | 1:J:367:GLN:HA | 2.20 | 0.42 |
| 1:K:142:HIS:CE1 | 1:K:161:LEU:HD13 | 2.55 | 0.42 |
| 1:L:319:ILE:HA | 1:L:322:LEU:HD12 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:70:ASP:O | 1:T:74:ILE:HG12 | 2.20 | 0.42 |
| 1:T:138:LEU:HD12 | 1:T:164:MET:CG | 2.46 | 0.42 |
| 1:T:368:ALA:O | 1:T:371:SER:OG | 2.37 | 0.42 |
| 1:U:61:LEU:HD23 | 1:U:151:ALA:HB2 | 2.02 | 0.42 |
| 1:i:308:LEU:O | 1:i:312:GLN:HG3 | 2.20 | 0.42 |
| 1:j:30:GLU:OE2 | 1:j:39:ASN:ND2 | 2.45 | 0.42 |
| 1:j:244:GLN:C | 1:j:245:ILE:HD12 | 2.44 | 0.42 |
| 1:j:361:ILE:HG13 | 1:j:361:ILE:H | 1.69 | 0.42 |
| 1:n:315:PHE:O | 1:n:319:ILE:HG13 | 2.20 | 0.42 |
| 1:n:350:LYS:O | 1:n:353:ILE:HG13 | 2.20 | 0.42 |
| 1:o:78:ALA:O | 1:o:82:MET:HG3 | 2.20 | 0.42 |
| 1:s:124:ASN:O | 1:s:128:GLU:HG2 | 2.20 | 0.42 |
| 1:v:125:ARG:NH1 | 1:v:129:THR:HG21 | 2.35 | 0.42 |
| 1:w:210:ASN:O | 1:w:211:ILE:HD13 | 2.20 | 0.42 |
| 1:z:262:LEU:HA | 1:z:265:GLU:HB3 | 2.02 | 0.42 |
| 1:1:113:GLN:OE1 | 1:1:281:VAL:HG22 | 2.19 | 0.41 |
| 1:1:123:LEU:HA | 1:1:123:LEU:HD23 | 1.84 | 0.41 |
| 1:1:218:ASP:HB3 | 1:1:221:GLU:OE2 | 2.20 | 0.41 |
| 1:1:272:LYS:HD3 | 1:1:273:LYS:N | 2.35 | 0.41 |
| 1:1:293:ILE:HG13 | 1:1:293:ILE:H | 1.67 | 0.41 |
| 1:2:222:LEU:O | 1:2:226:ILE:HG13 | 2.20 | 0.41 |
| 1:2:244:GLN:NE2 | 1:2:289:GLU:OE2 | 2.52 | 0.41 |
| 1:2:352:GLN:O | 1:2:356:GLN:NE2 | 2.52 | 0.41 |
| 1:3:105:SER:O | 1:3:109:ARG:HG3 | 2.20 | 0.41 |
| 1:A:300:TYR:CD2 | 1:A:300:TYR:C | 2.97 | 0.41 |
| 1:B:314:ARG:HG3 | 1:j:122:GLU:HB2 | 2.00 | 0.41 |
| 1:C:84:GLU:OE1 | 1:C:84:GLU:HA | 2.19 | 0.41 |
| 1:E:185:ASP:OD1 | 1:E:185:ASP:N | 2.53 | 0.41 |
| 1:E:202:SER:HA | 1:E:253:GLU:HB2 | 2.02 | 0.41 |
| 1:E:226:ILE:HD12 | 1:E:226:ILE:HA | 1.84 | 0.41 |
| 1:E:239:GLN:H | 1:E:239:GLN:CD | 2.27 | 0.41 |
| 1:E:321:ASN:O | 1:E:325:ILE:HG13 | 2.20 | 0.41 |
| 1:F:218:ASP:OD2 | 1:F:218:ASP:C | 2.64 | 0.41 |
| 1:G:187:ASN:OD1 | 1:G:188:VAL:N | 2.53 | 0.41 |
| 1:H:163:ASP:OD2 | 1:H:165:ARG:NH2 | 2.53 | 0.41 |
| 1:I:59:ARG:O | 1:I:62:ASP:OD1 | 2.38 | 0.41 |
| 1:J:63:VAL:HG22 | 1:J:66:ARG:NH2 | 2.35 | 0.41 |
| 1:L:170:MET:HB2 | 1:L:300:TYR:CD2 | 2.55 | 0.41 |
| 1:L:270:GLU:OE1 | 1:L:271:GLY:N | 2.52 | 0.41 |
| 1:N:199:LEU:HD21 | 1:N:232:LEU:HD22 | 2.02 | 0.41 |
| 1:O:168:ASN:OD1 | 1:O:169:LYS:HG2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:114:GLU:OE1 | 1:Q:114:GLU:HA | 2.20 | 0.41 |
| 1:Q:272:LYS:HE3 | 1:Q:273:LYS:H | 1.85 | 0.41 |
| 1:T:178:ALA:HB3 | 1:T:242:LYS:HB3 | 2.02 | 0.41 |
| 1:h:239:GLN:HE22 | 1:h:283:SER:HB2 | 1.85 | 0.41 |
| 1:k:322:LEU:HA | 1:k:325:ILE:HD12 | 2.02 | 0.41 |
| 1:p:93:ARG:NH1 | 1:p:295:ASP:OD1 | 2.52 | 0.41 |
| 1:r:175:SER:O | 1:r:271:GLY:HA2 | 2.20 | 0.41 |
| 1:t:236:SER:HB2 | 1:t:244:GLN:CG | 2.49 | 0.41 |
| 1:v:9:VAL:O | 1:v:12:MET:HE3 | 2.19 | 0.41 |
| 1:v:159:LEU:HD22 | 1:v:311:PHE:CZ | 2.55 | 0.41 |
| 1:v:299:LYS:HD2 | 1:v:299:LYS:O | 2.20 | 0.41 |
| 1:z:128:GLU:O | 1:z:136:LYS:NZ | 2.36 | 0.41 |
| 1:2:36:PHE:CD1 | 1:2:337:LYS:HE3 | 2.55 | 0.41 |
| 1:2:37:LYS:HG2 | 1:2:338:ASP:C | 2.44 | 0.41 |
| 1:2:287:ALA:O | 1:2:291:VAL:HG23 | 2.20 | 0.41 |
| 1:A:262:LEU:O | 1:A:266:LEU:HG | 2.19 | 0.41 |
| 1:B:84:GLU:O | 1:B:88:ILE:HG13 | 2.20 | 0.41 |
| 1:B:199:LEU:HD21 | 1:B:232:LEU:HD23 | 2.01 | 0.41 |
| 1:E:59:ARG:HD2 | 1:l:94:ASP:OD2 | 2.21 | 0.41 |
| 1:E:106:LYS:O | 1:E:110:VAL:HG23 | 2.20 | 0.41 |
| 1:E:184:LYS:HE2 | 1:E:184:LYS:HA | 2.02 | 0.41 |
| 1:G:31:ARG:NH2 | 1:G:37:LYS:O | 2.46 | 0.41 |
| 1:G:287:ALA:O | 1:G:291:VAL:HG12 | 2.19 | 0.41 |
| 1:I:153:ASN:ND2 | 1:p:292:ALA:HB2 | 2.36 | 0.41 |
| 1:I:300:TYR:O | 1:I:303:SER:OG | 2.30 | 0.41 |
| 1:L:295:ASP:O | 1:L:299:LYS:HD2 | 2.20 | 0.41 |
| 1:O:311:PHE:CZ | 1:O:315:PHE:CE1 | 3.08 | 0.41 |
| 1:R:131:SER:HB3 | 1:R:136:LYS:CE | 2.50 | 0.41 |
| 1:R:192:LYS:N | 1:R:192:LYS:HD3 | 2.35 | 0.41 |
| 1:T:50:ILE:O | 1:T:54:LEU:HG | 2.19 | 0.41 |
| 1:T:210:ASN:O | 1:T:211:ILE:HD13 | 2.20 | 0.41 |
| 1:T:226:ILE:HG13 | 1:T:226:ILE:H | 1.71 | 0.41 |
| 1:i:279:ILE:HB | 1:i:290:SER:OG | 2.20 | 0.41 |
| 1:i:362:LEU:HD12 | 1:i:362:LEU:O | 2.20 | 0.41 |
| 1:l:4:ASN:OD1 | 1:l:5:VAL:N | 2.53 | 0.41 |
| 1:n:210:ASN:C | 1:n:211:ILE:HD12 | 2.45 | 0.41 |
| 1:o:367:GLN:OE1 | 1:o:370:ASN:HB3 | 2.20 | 0.41 |
| 1:p:5:VAL:O | 1:p:6:ASN:OD1 | 2.38 | 0.41 |
| 1:B:217:ASP:OD2 | 1:B:217:ASP:N | 2.53 | 0.41 |
| 1:C:44:ASP:OD1 | 1:C:44:ASP:C | 2.63 | 0.41 |
| 1:C:214:LYS:HE3 | 1:O:165:ARG:HH21 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:15:GLN:HE21 | 1:j:342:ALA:HB1 | 1.86 | 0.41 |
| 1:F:105:SER:H | 1:F:108:GLU:CD | 2.27 | 0.41 |
| 1:I:218:ASP:OD1 | 1:I:219:ILE:N | 2.47 | 0.41 |
| 1:K:86:THR:O | 1:K:90:GLN:HG3 | 2.20 | 0.41 |
| 1:L:126:ILE:HG13 | 1:L:126:ILE:H | 1.72 | 0.41 |
| 1:L:313:ASN:OD1 | 1:L:317:HIS:HD2 | 2.04 | 0.41 |
| 1:N:333:LYS:NZ | 1:N:337:LYS:HG3 | 2.35 | 0.41 |
| 1:N:375:LEU:HD12 | 1:N:375:LEU:HA | 1.74 | 0.41 |
| 1:P:28:SER:C | 1:P:29:MET:HE2 | 2.45 | 0.41 |
| 1:Q:176:TYR:CE1 | 1:Q:256:VAL:HB | 2.55 | 0.41 |
| 1:R:240:ASP:OD1 | 1:R:240:ASP:N | 2.53 | 0.41 |
| 1:S:291:VAL:HA | 1:S:294:ILE:HG22 | 2.02 | 0.41 |
| 1:T:302:ASP:OD1 | 1:T:302:ASP:N | 2.53 | 0.41 |
| 1:U:72:ILE:HG23 | 1:U:312:GLN:HG2 | 2.02 | 0.41 |
| 1:c:31:ARG:NH1 | 1:c:37:LYS:HB2 | 2.35 | 0.41 |
| 1:h:295:ASP:OD1 | 1:h:296:ALA:N | 2.53 | 0.41 |
| 1:l:32:LEU:HD12 | 1:l:344:GLU:HB2 | 2.01 | 0.41 |
| 1:l:208:GLU:O | 1:l:209:ILE:HD13 | 2.20 | 0.41 |
| 1:m:97:LEU:HD23 | 1:m:97:LEU:HA | 1.84 | 0.41 |
| 1:m:108:GLU:H | 1:m:108:GLU:CD | 2.25 | 0.41 |
| 1:n:170:MET:HB3 | 1:n:300:TYR:CD2 | 2.55 | 0.41 |
| 1:n:179:GLU:C | 1:n:242:LYS:HE2 | 2.45 | 0.41 |
| 1:o:62:ASP:OD1 | 1:o:62:ASP:N | 2.52 | 0.41 |
| 1:o:84:GLU:HG3 | 1:o:88:ILE:HD11 | 2.02 | 0.41 |
| 1:p:25:GLN:HB3 | 1:p:351:SER:OG | 2.19 | 0.41 |
| 1:p:169:LYS:HD2 | 1:p:169:LYS:C | 2.45 | 0.41 |
| 1:t:138:LEU:HB3 | 1:t:164:MET:HG3 | 2.02 | 0.41 |
| 1:v:183:GLY:C | 1:v:185:ASP:H | 2.28 | 0.41 |
| 1:x:63:VAL:HG13 | 1:x:66:ARG:HH12 | 1.85 | 0.41 |
| 1:z:29:MET:HE2 | 1:z:29:MET:HB2 | 1.83 | 0.41 |
| 1:z:279:ILE:HD12 | 1:z:279:ILE:HA | 1.77 | 0.41 |
| 1:2:327:GLU:OE1 | 1:q:16:ARG:NH2 | 2.49 | 0.41 |
| 1:3:334:SER:HA | 1:3:338:ASP:OD2 | 2.20 | 0.41 |
| 1:A:29:MET:HG3 | 1:A:348:MET:HE1 | 2.02 | 0.41 |
| 1:B:192:LYS:O | 1:B:262:LEU:HG | 2.20 | 0.41 |
| 1:E:353:ILE:HD11 | 1:Q:370:ASN:ND2 | 2.36 | 0.41 |
| 1:G:262:LEU:O | 1:G:266:LEU:HG | 2.20 | 0.41 |
| 1:H:52:ASN:O | 1:H:56:VAL:HG23 | 2.19 | 0.41 |
| 1:H:153:ASN:ND2 | 1:o:292:ALA:HB2 | 2.34 | 0.41 |
| 1:H:350:LYS:O | 1:H:354:LEU:HD12 | 2.21 | 0.41 |
| 1:I:163:ASP:O | 1:I:164:MET:HE2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:98:GLN:HE21 | 1:J:98:GLN:C | 2.24 | 0.41 |
| 1:N:287:ALA:O | 1:N:291:VAL:HG23 | 2.20 | 0.41 |
| 1:O:171:MET:N | 1:O:171:MET:SD | 2.93 | 0.41 |
| 1:R:258:PHE:CD2 | 1:R:268:LEU:HD11 | 2.55 | 0.41 |
| 1:S:66:ARG:HH21 | 1:S:70:ASP:CG | 2.29 | 0.41 |
| 1:T:255:GLU:OE2 | 1:T:255:GLU:HA | 2.19 | 0.41 |
| 1:U:168:ASN:O | 1:U:171:MET:HB2 | 2.20 | 0.41 |
| 1:i:257:GLU:CD | 1:i:257:GLU:N | 2.78 | 0.41 |
| 1:i:276:VAL:HA | 1:i:279:ILE:HG23 | 2.01 | 0.41 |
| 1:k:38:ILE:HD11 | 1:k:336:ILE:HG22 | 2.02 | 0.41 |
| 1:k:44:ASP:OD1 | 1:k:44:ASP:C | 2.63 | 0.41 |
| 1:l:185:ASP:OD1 | 1:l:185:ASP:N | 2.54 | 0.41 |
| 1:l:332:SER:O | 1:l:333:LYS:C | 2.63 | 0.41 |
| 1:n:234:LYS:HB3 | 1:n:234:LYS:HE2 | 1.81 | 0.41 |
| 1:o:218:ASP:CG | 1:o:219:ILE:H | 2.29 | 0.41 |
| 1:p:155:GLU:H | 1:p:155:GLU:HG3 | 1.74 | 0.41 |
| 1:p:302:ASP:OD1 | 1:p:302:ASP:N | 2.50 | 0.41 |
| 1:p:367:GLN:OE1 | 1:p:367:GLN:HA | 2.20 | 0.41 |
| 1:s:3:VAL:HG22 | 1:t:22:ASN:ND2 | 2.36 | 0.41 |
| 1:s:44:ASP:CG | 1:s:47:GLY:H | 2.29 | 0.41 |
| 1:s:314:ARG:HH21 | 1:t:122:GLU:N | 2.17 | 0.41 |
| 1:z:243:LEU:HD23 | 1:z:244:GLN:N | 2.34 | 0.41 |
| 1:2:82:MET:HE2 | 1:2:82:MET:HB3 | 1.83 | 0.41 |
| 1:2:84:GLU:CD | 1:2:126:ILE:HD13 | 2.46 | 0.41 |
| 1:3:59:ARG:HA | 1:3:62:ASP:OD1 | 2.20 | 0.41 |
| 1:B:303:SER:O | 1:B:307:GLU:HG3 | 2.20 | 0.41 |
| 1:F:340:ASP:OD2 | 1:Q:2:ALA:HA | 2.19 | 0.41 |
| 1:G:138:LEU:HD12 | 1:G:164:MET:CG | 2.50 | 0.41 |
| 1:G:334:SER:HA | 1:G:338:ASP:OD1 | 2.20 | 0.41 |
| 1:K:279:ILE:HG21 | 1:K:293:ILE:HG21 | 2.01 | 0.41 |
| 1:L:79:GLU:CD | 1:L:305:ARG:HH21 | 2.29 | 0.41 |
| 1:L:196:LYS:NZ | 1:L:208:GLU:OE1 | 2.53 | 0.41 |
| 1:L:328:ASN:OD1 | 1:M:76:GLN:HB3 | 2.20 | 0.41 |
| 1:L:375:LEU:HD11 | 1:M:362:LEU:HD22 | 2.03 | 0.41 |
| 1:M:214:LYS:HD3 | 1:M:214:LYS:C | 2.45 | 0.41 |
| 1:O:53:ARG:NH1 | 1:O:53:ARG:HB2 | 2.35 | 0.41 |
| 1:O:311:PHE:CE1 | 1:O:315:PHE:HE1 | 2.39 | 0.41 |
| 1:P:26:GLN:O | 1:P:30:GLU:HG2 | 2.21 | 0.41 |
| 1:P:37:LYS:NZ | 1:P:336:ILE:O | 2.54 | 0.41 |
| 1:P:126:ILE:O | 1:P:130:THR:OG1 | 2.25 | 0.41 |
| 1:P:168:ASN:O | 1:P:171:MET:HG2 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:125:ARG:HH11 | 1:S:125:ARG:HG2 | 1.85 | 0.41 |
| 1:U:253:GLU:C | 1:U:253:GLU:CD | 2.88 | 0.41 |
| 1:V:106:LYS:NZ | 1:V:282:THR:HB | 2.36 | 0.41 |
| 1:c:175:SER:HA | 1:c:245:ILE:O | 2.21 | 0.41 |
| 1:j:174:VAL:HG13 | 1:j:273:LYS:HE2 | 2.03 | 0.41 |
| 1:k:18:LEU:O | 1:k:22:ASN:OD1 | 2.39 | 0.41 |
| 1:l:201:ASP:C | 1:l:201:ASP:OD2 | 2.63 | 0.41 |
| 1:l:217:ASP:HB3 | 1:l:221:GLU:HG3 | 2.02 | 0.41 |
| 1:n:236:SER:HB2 | 1:n:244:GLN:HG3 | 2.02 | 0.41 |
| 1:n:361:ILE:HD11 | 1:z:29:MET:CG | 2.50 | 0.41 |
| 1:p:289:GLU:O | 1:p:293:ILE:HG22 | 2.20 | 0.41 |
| 1:p:323:ASP:OD1 | 1:p:323:ASP:C | 2.62 | 0.41 |
| 1:r:179:GLU:OE2 | 1:r:269:GLY:HA3 | 2.21 | 0.41 |
| 1:r:240:ASP:HB2 | 1:r:242:LYS:HG3 | 2.02 | 0.41 |
| 1:s:132:PHE:CD1 | 1:s:132:PHE:C | 2.98 | 0.41 |
| 1:t:299:LYS:HZ2 | 1:t:303:SER:HB2 | 1.85 | 0.41 |
| 1:x:311:PHE:CE2 | 1:x:315:PHE:CE1 | 3.08 | 0.41 |
| 1:1:42:LYS:HA | 1:1:42:LYS:HD3 | 1.78 | 0.41 |
| 1:2:97:LEU:HD23 | 1:2:97:LEU:HA | 1.72 | 0.41 |
| 1:A:78:ALA:O | 1:A:82:MET:HG3 | 2.20 | 0.41 |
| 1:A:168:ASN:OD1 | 1:A:168:ASN:C | 2.63 | 0.41 |
| 1:B:67:ASN:OD1 | 1:i:101:ASN:HB2 | 2.20 | 0.41 |
| 1:E:178:ALA:O | 1:E:242:LYS:HB3 | 2.21 | 0.41 |
| 1:F:223:ALA:HA | 1:F:226:ILE:HD12 | 2.02 | 0.41 |
| 1:G:155:GLU:OE1 | 1:o:129:THR:HG22 | 2.21 | 0.41 |
| 1:H:31:ARG:HG2 | 1:H:37:LYS:HA | 2.02 | 0.41 |
| 1:H:250:ASN:OD1 | 1:H:250:ASN:C | 2.63 | 0.41 |
| 1:I:91:ARG:CZ | 1:I:95:LEU:HD21 | 2.51 | 0.41 |
| 1:J:44:ASP:OD1 | 1:J:44:ASP:C | 2.64 | 0.41 |
| 1:L:82:MET:H | 1:L:82:MET:HG3 | 1.72 | 0.41 |
| 1:M:50:ILE:HG22 | 1:M:54:LEU:HD11 | 2.03 | 0.41 |
| 1:N:214:LYS:NZ | 1:N:217:ASP:OD1 | 2.42 | 0.41 |
| 1:O:189:ALA:HB1 | 1:O:192:LYS:CE | 2.49 | 0.41 |
| 1:Q:22:ASN:N | 1:Q:22:ASN:ND2 | 2.67 | 0.41 |
| 1:Q:88:ILE:O | 1:Q:91:ARG:HB3 | 2.21 | 0.41 |
| 1:R:201:ASP:OD2 | 1:R:207:GLN:NE2 | 2.54 | 0.41 |
| 1:T:321:ASN:O | 1:T:325:ILE:HG12 | 2.20 | 0.41 |
| 1:U:159:LEU:HB2 | 1:U:311:PHE:HE1 | 1.85 | 0.41 |
| 1:U:175:SER:O | 1:U:271:GLY:HA2 | 2.21 | 0.41 |
| 1:h:20:ASN:O | 1:h:23:SER:OG | 2.36 | 0.41 |
| 1:i:281:VAL:O | 1:i:281:VAL:HG22 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:j:108:GLU:OE2 | 1:j:108:GLU:N | 2.45 | 0.41 |
| 1:j:164:MET:HE2 | 1:j:164:MET:HA | 2.02 | 0.41 |
| 1:j:218:ASP:C | 1:j:218:ASP:OD1 | 2.64 | 0.41 |
| 1:m:125:ARG:NH1 | 1:m:125:ARG:HG2 | 2.36 | 0.41 |
| 1:n:17:TYR:CE1 | 1:z:34:SER:HA | 2.56 | 0.41 |
| 1:n:304:HIS:HA | 1:n:307:GLU:OE2 | 2.19 | 0.41 |
| 1:p:137:LEU:C | 1:p:138:LEU:HD23 | 2.45 | 0.41 |
| 1:p:210:ASN:C | 1:p:210:ASN:OD1 | 2.63 | 0.41 |
| 1:s:231:ASP:OD2 | 1:s:231:ASP:N | 2.53 | 0.41 |
| 1:s:246:PHE:CD2 | 1:s:246:PHE:C | 2.99 | 0.41 |
| 1:t:109:ARG:HA | 1:t:112:ILE:HD12 | 2.02 | 0.41 |
| 1:t:125:ARG:HG2 | 1:t:125:ARG:NH1 | 2.36 | 0.41 |
| 1:x:82:MET:HE2 | 1:x:82:MET:HB2 | 1.85 | 0.41 |
| 1:z:39:ASN:OD1 | 1:z:39:ASN:C | 2.63 | 0.41 |
| 1:z:84:GLU:OE1 | 1:z:84:GLU:HA | 2.20 | 0.41 |
| 1:z:293:ILE:HG13 | 1:z:293:ILE:H | 1.62 | 0.41 |
| 1:1:116:VAL:HA | 1:1:119:LEU:HD12 | 2.01 | 0.41 |
| 1:2:58:SER:HA | 1:2:61:LEU:HD12 | 2.01 | 0.41 |
| 1:A:149:ILE:CG2 | 1:B:125:ARG:HH12 | 2.34 | 0.41 |
| 1:A:157:VAL:HG11 | 1:A:314:ARG:HH11 | 1.85 | 0.41 |
| 1:E:303:SER:O | 1:E:307:GLU:OE2 | 2.38 | 0.41 |
| 1:F:57:GLN:O | 1:F:61:LEU:HG | 2.21 | 0.41 |
| 1:F:275:THR:OG1 | 1:F:276:VAL:N | 2.53 | 0.41 |
| 1:H:199:LEU:HB3 | 1:H:256:VAL:HG13 | 2.03 | 0.41 |
| 1:I:68:ALA:O | 1:I:72:ILE:HG13 | 2.21 | 0.41 |
| 1:I:210:ASN:C | 1:I:210:ASN:OD1 | 2.63 | 0.41 |
| 1:K:347:ALA:HA | 1:K:350:LYS:NZ | 2.36 | 0.41 |
| 1:M:95:LEU:HD23 | 1:M:95:LEU:HA | 1.82 | 0.41 |
| 1:O:29:MET:HE2 | 1:O:29:MET:HB3 | 1.97 | 0.41 |
| 1:Q:159:LEU:HD12 | 1:Q:160:GLU:H | 1.85 | 0.41 |
| 1:Q:361:ILE:N | 1:Q:361:ILE:HD13 | 2.35 | 0.41 |
| 1:S:294:ILE:HG21 | 1:S:294:ILE:HD13 | 1.83 | 0.41 |
| 1:S:318:ALA:O | 1:S:322:LEU:HD23 | 2.21 | 0.41 |
| 1:T:239:GLN:H | 1:T:239:GLN:CD | 2.29 | 0.41 |
| 1:V:175:SER:O | 1:V:271:GLY:HA2 | 2.21 | 0.41 |
| 1:V:184:LYS:HD2 | 1:V:184:LYS:C | 2.45 | 0.41 |
| 1:j:319:ILE:HG13 | 1:j:319:ILE:H | 1.69 | 0.41 |
| 1:l:367:GLN:O | 1:l:370:ASN:HB3 | 2.21 | 0.41 |
| 1:n:61:LEU:HB3 | 1:n:322:LEU:HD12 | 2.03 | 0.41 |
| 1:t:109:ARG:HB3 | 1:t:282:THR:HA | 2.02 | 0.41 |
| 1:t:239:GLN:CD | 1:t:239:GLN:H | 2.28 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:w:257:GLU:N | 1:w:257:GLU:OE2 | 2.53 | 0.41 |
| 1:2:37:LYS:HG2 | 1:2:338:ASP:O | 2.21 | 0.41 |
| 1:A:136:LYS:HA | 1:A:136:LYS:HD3 | 1.67 | 0.41 |
| 1:A:166:SER:O | 1:A:276:VAL:HG22 | 2.20 | 0.41 |
| 1:A:169:LYS:C | 1:A:169:LYS:HD3 | 2.46 | 0.41 |
| 1:A:171:MET:O | 1:A:293:ILE:HD11 | 2.20 | 0.41 |
| 1:A:195:LEU:O | 1:A:196:LYS:HD3 | 2.21 | 0.41 |
| 1:B:88:ILE:O | 1:B:92:MET:HG3 | 2.20 | 0.41 |
| 1:D:162:LYS:CG | 1:D:304:HIS:HD2 | 2.34 | 0.41 |
| 1:F:112:ILE:O | 1:F:116:VAL:HG23 | 2.21 | 0.41 |
| 1:G:82:MET:HE2 | 1:G:82:MET:HB2 | 1.91 | 0.41 |
| 1:G:91:ARG:HA | 1:G:91:ARG:HD2 | 1.70 | 0.41 |
| 1:M:37:LYS:HG2 | 1:M:337:LYS:O | 2.20 | 0.41 |
| 1:N:270:GLU:CD | 1:N:271:GLY:N | 2.79 | 0.41 |
| 1:N:336:ILE:HD12 | 1:N:336:ILE:H | 1.85 | 0.41 |
| 1:R:218:ASP:OD2 | 1:R:219:ILE:N | 2.53 | 0.41 |
| 1:R:286:GLY:HA2 | 1:R:289:GLU:OE2 | 2.21 | 0.41 |
| 1:c:248:GLY:O | 1:c:252:VAL:N | 2.47 | 0.41 |
| 1:c:299:LYS:HE3 | 1:c:299:LYS:CA | 2.48 | 0.41 |
| 1:j:4:ASN:ND2 | 1:u:334:SER:HG | 2.15 | 0.41 |
| 1:j:312:GLN:O | 1:j:316:ASN:ND2 | 2.48 | 0.41 |
| 1:l:210:ASN:O | 1:l:211:ILE:HD13 | 2.21 | 0.41 |
| 1:m:125:ARG:HH11 | 1:m:125:ARG:HG2 | 1.85 | 0.41 |
| 1:q:176:TYR:OH | 1:q:255:GLU:HG2 | 2.20 | 0.41 |
| 1:r:173:GLY:HA3 | 1:r:246:PHE:CE2 | 2.56 | 0.41 |
| 1:s:9:VAL:O | 1:s:12:MET:HG2 | 2.20 | 0.41 |
| 1:s:319:ILE:HD13 | 1:s:322:LEU:HD12 | 2.01 | 0.41 |
| 1:t:82:MET:HG3 | 1:t:82:MET:H | 1.63 | 0.41 |
| 1:t:147:PHE:CD1 | 1:t:147:PHE:N | 2.88 | 0.41 |
| 1:t:272:LYS:NZ | 1:t:272:LYS:HB2 | 2.36 | 0.41 |
| 1:u:37:LYS:O | 1:u:37:LYS:HG3 | 2.20 | 0.41 |
| 1:u:262:LEU:HD23 | 1:u:262:LEU:HA | 1.92 | 0.41 |
| 1:v:221:GLU:H | 1:v:221:GLU:HG3 | 1.72 | 0.41 |
| 1:v:353:ILE:HG13 | 1:v:353:ILE:H | 1.76 | 0.41 |
| 1:w:26:GLN:HG3 | 1:w:30:GLU:OE2 | 2.20 | 0.41 |
| 1:w:59:ARG:O | 1:w:63:VAL:HG23 | 2.21 | 0.41 |
| 1:w:196:LYS:HZ1 | 1:w:196:LYS:HB3 | 1.85 | 0.41 |
| 1:x:106:LYS:NZ | 1:x:282:THR:O | 2.54 | 0.41 |
| 1:1:109:ARG:O | 1:1:112:ILE:HG22 | 2.21 | 0.41 |
| 1:1:363:ALA:O | 1:1:367:GLN:NE2 | 2.52 | 0.41 |
| 1:2:195:LEU:HB2 | 1:2:262:LEU:HB2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:300:TYR:CE2 | 1:2:304:HIS:NE2 | 2.88 | 0.41 |
| 1:2:356:GLN:N | 1:2:356:GLN:CD | 2.79 | 0.41 |
| 1:3:37:LYS:HD3 | 1:3:339:THR:HA | 2.03 | 0.41 |
| 1:3:234:LYS:HA | 1:3:234:LYS:HE3 | 2.03 | 0.41 |
| 1:3:340:ASP:HB3 | 1:3:343:LYS:NZ | 2.36 | 0.41 |
| 1:A:104:ASN:O | 1:A:109:ARG:NH2 | 2.45 | 0.41 |
| 1:B:177:GLN:HG2 | 1:B:178:ALA:O | 2.21 | 0.41 |
| 1:C:334:SER:HB2 | 1:N:7:THR:HG21 | 2.03 | 0.41 |
| 1:C:340:ASP:OD2 | 1:C:340:ASP:C | 2.63 | 0.41 |
| 1:D:51:SER:HA | 1:D:54:LEU:HD12 | 2.03 | 0.41 |
| 1:D:170:MET:HE3 | 1:D:250:ASN:CB | 2.51 | 0.41 |
| 1:D:192:LYS:O | 1:D:262:LEU:HG | 2.21 | 0.41 |
| 1:E:122:GLU:OE2 | 1:E:125:ARG:NE | 2.54 | 0.41 |
| 1:F:84:GLU:HA | 1:F:87:ASN:OD1 | 2.21 | 0.41 |
| 1:F:85:THR:O | 1:F:89:LEU:HD22 | 2.21 | 0.41 |
| 1:F:261:GLY:C | 1:F:264:GLY:H | 2.28 | 0.41 |
| 1:G:169:LYS:HB2 | 1:G:170:MET:CE | 2.50 | 0.41 |
| 1:G:297:ALA:O | 1:G:301:VAL:HG23 | 2.21 | 0.41 |
| 1:I:338:ASP:OD2 | 1:T:4:ASN:HB3 | 2.21 | 0.41 |
| 1:K:218:ASP:O | 1:K:222:LEU:N | 2.45 | 0.41 |
| 1:L:173:GLY:HA3 | 1:L:246:PHE:CE2 | 2.56 | 0.41 |
| 1:M:165:ARG:HH11 | 1:M:165:ARG:HG2 | 1.86 | 0.41 |
| 1:M:260:GLY:O | 1:M:263:SER:HB3 | 2.21 | 0.41 |
| 1:N:143:GLY:O | 1:N:145:LYS:HG2 | 2.21 | 0.41 |
| 1:N:273:LYS:HD3 | 1:N:274:VAL:N | 2.36 | 0.41 |
| 1:N:318:ALA:HA | 1:O:125:ARG:HH22 | 1.86 | 0.41 |
| 1:O:193:ASN:OD1 | 1:O:193:ASN:N | 2.49 | 0.41 |
| 1:P:159:LEU:HD12 | 1:P:160:GLU:H | 1.84 | 0.41 |
| 1:Q:293:ILE:HD12 | 1:Q:293:ILE:HA | 1.94 | 0.41 |
| 1:R:236:SER:OG | 1:c:153:ASN:ND2 | 2.54 | 0.41 |
| 1:R:366:LYS:O | 1:R:369:PRO:HD2 | 2.21 | 0.41 |
| 1:S:290:SER:O | 1:S:293:ILE:HG22 | 2.21 | 0.41 |
| 1:T:30:GLU:OE1 | 1:T:39:ASN:ND2 | 2.49 | 0.41 |
| 1:T:141:THR:O | 1:T:141:THR:OG1 | 2.35 | 0.41 |
| 1:T:298:LEU:O | 1:T:301:VAL:HG22 | 2.21 | 0.41 |
| 1:U:288:GLN:O | 1:U:288:GLN:NE2 | 2.39 | 0.41 |
| 1:U:343:LYS:HB2 | 1:U:344:GLU:OE2 | 2.20 | 0.41 |
| 1:V:257:GLU:C | 1:V:257:GLU:OE2 | 2.64 | 0.41 |
| 1:V:272:LYS:HD3 | 1:V:272:LYS:N | 2.36 | 0.41 |
| 1:c:115:GLU:O | 1:c:119:LEU:HG | 2.21 | 0.41 |
| 1:c:139:ASN:C | 1:c:141:THR:N | 2.77 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:c:183:GLY:C | 1:c:185:ASP:H | 2.29 | 0.41 |
| 1:h:227:ASN:ND2 | 1:h:235:ALA:H | 2.19 | 0.41 |
| 1:j:9:VAL:HA | 1:j:12:MET:CE | 2.51 | 0.41 |
| 1:k:196:LYS:O | 1:k:197:ILE:HD13 | 2.20 | 0.41 |
| 1:l:314:ARG:NE | 1:m:122:GLU:OE2 | 2.43 | 0.41 |
| 1:m:92:MET:HE2 | 1:m:92:MET:HB3 | 1.77 | 0.41 |
| 1:n:297:ALA:O | 1:n:301:VAL:HG12 | 2.21 | 0.41 |
| 1:n:361:ILE:HA | 1:n:361:ILE:HD12 | 1.83 | 0.41 |
| 1:p:92:MET:HE2 | 1:p:92:MET:HB3 | 1.93 | 0.41 |
| 1:r:91:ARG:HH11 | 1:r:91:ARG:HG3 | 1.84 | 0.41 |
| 1:r:170:MET:HE3 | 1:r:300:TYR:HB2 | 2.02 | 0.41 |
| 1:s:307:GLU:OE2 | 1:s:308:LEU:HD23 | 2.21 | 0.41 |
| 1:u:257:GLU:N | 1:u:257:GLU:CD | 2.79 | 0.41 |
| 1:u:335:ARG:NH2 | 1:v:73:SER:OG | 2.54 | 0.41 |
| 1:v:287:ALA:O | 1:v:291:VAL:HG23 | 2.21 | 0.41 |
| 1:v:299:LYS:O | 1:v:299:LYS:NZ | 2.50 | 0.41 |
| 1:v:311:PHE:O | 1:v:315:PHE:HD1 | 2.04 | 0.41 |
| 1:w:19:ASN:HA | 1:w:22:ASN:OD1 | 2.21 | 0.41 |
| 1:w:142:HIS:ND1 | 1:w:161:LEU:HB2 | 2.36 | 0.41 |
| 1:w:157:VAL:HG12 | 1:w:158:MET:H | 1.86 | 0.41 |
| 1:x:345:THR:O | 1:x:348:MET:HE3 | 2.21 | 0.41 |
| 1:3:128:GLU:OE2 | 1:3:165:ARG:NH1 | 2.54 | 0.41 |
| 1:B:349:THR:O | 1:B:353:ILE:HD12 | 2.21 | 0.41 |
| 1:E:59:ARG:HH12 | 1:l:90:GLN:HB3 | 1.86 | 0.41 |
| 1:E:193:ASN:OD1 | 1:E:193:ASN:N | 2.54 | 0.41 |
| 1:E:201:ASP:OD2 | 1:E:203:TYR:HB2 | 2.21 | 0.41 |
| 1:E:245:ILE:HD12 | 1:E:245:ILE:HA | 1.87 | 0.41 |
| 1:H:159:LEU:HD13 | 1:H:311:PHE:CD1 | 2.56 | 0.41 |
| 1:H:231:ASP:OD1 | 1:H:231:ASP:C | 2.64 | 0.41 |
| 1:H:338:ASP:OD2 | 1:H:338:ASP:C | 2.64 | 0.41 |
| 1:I:86:THR:O | 1:I:90:GLN:HG3 | 2.21 | 0.41 |
| 1:I:113:GLN:OE1 | 1:I:281:VAL:HG22 | 2.21 | 0.41 |
| 1:M:120:ASN:OD1 | 1:M:120:ASN:C | 2.64 | 0.41 |
| 1:N:34:SER:OG | 1:N:39:ASN:ND2 | 2.52 | 0.41 |
| 1:O:363:ALA:O | 1:O:367:GLN:HG2 | 2.20 | 0.41 |
| 1:Q:123:LEU:HA | 1:Q:126:ILE:HD12 | 2.02 | 0.41 |
| 1:Q:225:TYR:O | 1:Q:229:GLN:NE2 | 2.47 | 0.41 |
| 1:R:12:MET:O | 1:R:16:ARG:HG3 | 2.21 | 0.41 |
| 1:R:188:VAL:HG22 | 1:R:189:ALA:H | 1.84 | 0.41 |
| 1:R:375:LEU:HD23 | 1:R:375:LEU:HA | 1.84 | 0.41 |
| 1:T:272:LYS:NZ | 1:T:272:LYS:HB3 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:91:ARG:HD3 | 1:U:91:ARG:C | 2.46 | 0.41 |
| 1:c:178:ALA:HB1 | 1:c:266:LEU:O | 2.21 | 0.41 |
| 1:i:37:LYS:NZ | 1:i:338:ASP:O | 2.47 | 0.41 |
| 1:i:196:LYS:HE2 | 1:i:196:LYS:HB2 | 1.86 | 0.41 |
| 1:j:146:SER:HA | 1:j:158:MET:HA | 2.02 | 0.41 |
| 1:j:245:ILE:HD12 | 1:j:245:ILE:N | 2.36 | 0.41 |
| 1:j:250:ASN:OD1 | 1:j:250:ASN:C | 2.63 | 0.41 |
| 1:l:4:ASN:OD1 | 1:l:4:ASN:C | 2.64 | 0.41 |
| 1:o:232:LEU:CA | 1:o:251:LYS:HZ1 | 2.29 | 0.41 |
| 1:s:171:MET:HB3 | 1:s:276:VAL:HG13 | 2.02 | 0.41 |
| 1:v:37:LYS:N | 1:v:339:THR:HB | 2.36 | 0.41 |
| 1:v:72:ILE:HD12 | 1:v:72:ILE:HA | 1.87 | 0.41 |
| 1:w:39:ASN:OD1 | 1:w:39:ASN:C | 2.64 | 0.41 |
| 1:w:125:ARG:HD2 | 1:w:129:THR:CG2 | 2.51 | 0.41 |
| 1:w:191:GLY:O | 1:w:192:LYS:HD2 | 2.21 | 0.41 |
| 1:w:293:ILE:HG13 | 1:w:293:ILE:H | 1.59 | 0.41 |
| 1:w:302:ASP:N | 1:w:302:ASP:OD1 | 2.53 | 0.41 |
| 1:z:279:ILE:HD11 | 1:z:290:SER:HA | 2.02 | 0.41 |
| 1:A:330:ASN:HD22 | 1:L:12:MET:HE1 | 1.86 | 0.40 |
| 1:B:184:LYS:CE | 1:M:144:ALA:HB2 | 2.50 | 0.40 |
| 1:C:345:THR:OG1 | 1:O:366:LYS:HE3 | 2.20 | 0.40 |
| 1:D:79:GLU:CD | 1:D:305:ARG:HH21 | 2.28 | 0.40 |
| 1:D:183:GLY:C | 1:D:185:ASP:H | 2.28 | 0.40 |
| 1:E:335:ARG:HB2 | 1:E:335:ARG:NH1 | 2.36 | 0.40 |
| 1:F:70:ASP:O | 1:F:74:ILE:HG13 | 2.21 | 0.40 |
| 1:F:225:TYR:O | 1:F:229:GLN:HG2 | 2.21 | 0.40 |
| 1:G:108:GLU:OE2 | 1:G:108:GLU:N | 2.44 | 0.40 |
| 1:H:142:HIS:CG | 1:H:143:GLY:N | 2.88 | 0.40 |
| 1:L:201:ASP:CG | 1:L:207:GLN:HE21 | 2.29 | 0.40 |
| 1:N:11:ALA:O | 1:N:15:GLN:HG3 | 2.21 | 0.40 |
| 1:N:111:ALA:O | 1:N:115:GLU:OE2 | 2.38 | 0.40 |
| 1:Q:88:ILE:HG22 | 1:Q:92:MET:CE | 2.51 | 0.40 |
| 1:S:155:GLU:OE1 | 1:T:129:THR:HG22 | 2.21 | 0.40 |
| 1:S:195:LEU:HG | 1:S:197:ILE:HD11 | 2.02 | 0.40 |
| 1:c:26:GLN:OE1 | 1:c:26:GLN:HA | 2.21 | 0.40 |
| 1:j:31:ARG:HG2 | 1:j:31:ARG:H | 1.68 | 0.40 |
| 1:j:343:LYS:H | 1:j:343:LYS:HG3 | 1.71 | 0.40 |
| 1:k:84:GLU:HA | 1:k:87:ASN:ND2 | 2.36 | 0.40 |
| 1:m:149:ILE:O | 1:m:149:ILE:HG13 | 2.21 | 0.40 |
| 1:m:170:MET:HE2 | 1:m:300:TYR:CE1 | 2.55 | 0.40 |
| 1:o:58:SER:HA | 1:o:61:LEU:HD12 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:o:199:LEU:CB | 1:o:256:VAL:HG22 | 2.49 | 0.40 |
| 1:p:101:ASN:OD1 | 1:p:103:SER:N | 2.50 | 0.40 |
| 1:s:321:ASN:OD1 | 1:s:325:ILE:HD11 | 2.20 | 0.40 |
| 1:t:92:MET:HE3 | 1:t:92:MET:HB2 | 1.96 | 0.40 |
| 1:t:335:ARG:HG3 | 1:t:336:ILE:HD13 | 2.03 | 0.40 |
| 1:w:328:ASN:HD22 | 1:x:76:GLN:HG3 | 1.85 | 0.40 |
| 1:z:91:ARG:O | 1:z:91:ARG:HD3 | 2.20 | 0.40 |
| 1:1:219:ILE:CD1 | 1:1:243:LEU:HD12 | 2.51 | 0.40 |
| 1:3:34:SER:HB2 | 1:3:36:PHE:HD2 | 1.86 | 0.40 |
| 1:C:300:TYR:CE2 | 1:C:304:HIS:NE2 | 2.85 | 0.40 |
| 1:E:173:GLY:HA2 | 1:E:249:ASN:OD1 | 2.21 | 0.40 |
| 1:E:290:SER:O | 1:E:294:ILE:HG13 | 2.21 | 0.40 |
| 1:I:125:ARG:HG2 | 1:I:125:ARG:HH11 | 1.86 | 0.40 |
| 1:K:186:TRP:HZ3 | 1:K:219:ILE:HD11 | 1.85 | 0.40 |
| 1:L:31:ARG:HD3 | 1:L:344:GLU:OE2 | 2.22 | 0.40 |
| 1:N:300:TYR:CE1 | 1:N:304:HIS:HE1 | 2.39 | 0.40 |
| 1:O:289:GLU:C | 1:O:289:GLU:OE2 | 2.64 | 0.40 |
| 1:P:70:ASP:O | 1:P:74:ILE:HD12 | 2.21 | 0.40 |
| 1:P:239:GLN:H | 1:P:239:GLN:CD | 2.29 | 0.40 |
| 1:P:312:GLN:HG3 | 1:P:313:ASN:N | 2.35 | 0.40 |
| 1:P:366:LYS:HB3 | 1:P:366:LYS:HE2 | 1.91 | 0.40 |
| 1:R:53:ARG:O | 1:R:56:VAL:HG22 | 2.20 | 0.40 |
| 1:R:205:GLN:C | 1:R:207:GLN:HE22 | 2.29 | 0.40 |
| 1:V:82:MET:CE | 1:V:164:MET:HE3 | 2.51 | 0.40 |
| 1:c:132:PHE:CD1 | 1:c:132:PHE:C | 2.99 | 0.40 |
| 1:c:211:ILE:CD1 | 1:c:226:ILE:HD12 | 2.50 | 0.40 |
| 1:h:249:ASN:HA | 1:h:252:VAL:O | 2.21 | 0.40 |
| 1:k:2:ALA:HB1 | 1:v:340:ASP:HB3 | 2.03 | 0.40 |
| 1:l:316:ASN:O | 1:l:319:ILE:HG22 | 2.21 | 0.40 |
| 1:n:17:TYR:HE1 | 1:z:34:SER:HA | 1.85 | 0.40 |
| 1:p:52:ASN:O | 1:p:56:VAL:HG22 | 2.21 | 0.40 |
| 1:s:158:MET:SD | 1:s:159:LEU:N | 2.94 | 0.40 |
| 1:s:239:GLN:OE1 | 1:s:284:VAL:HB | 2.22 | 0.40 |
| 1:t:63:VAL:O | 1:t:67:ASN:OD1 | 2.40 | 0.40 |
| 1:t:89:LEU:HA | 1:t:92:MET:HE3 | 2.04 | 0.40 |
| 1:x:49:GLN:HA | 1:x:52:ASN:ND2 | 2.36 | 0.40 |
| 1:x:368:ALA:HB3 | 1:x:369:PRO:HD3 | 2.03 | 0.40 |
| 1:1:61:LEU:HG | 1:1:61:LEU:H | 1.77 | 0.40 |
| 1:1:67:ASN:HA | 1:1:70:ASP:OD1 | 2.21 | 0.40 |
| 1:C:170:MET:HB3 | 1:C:300:TYR:CE1 | 2.56 | 0.40 |
| 1:F:307:GLU:OE2 | 1:F:307:GLU:N | 2.52 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:225:TYR:O | 1:G:229:GLN:HG2 | 2.21 | 0.40 |
| 1:I:232:LEU:HA | 1:I:251:LYS:NZ | 2.37 | 0.40 |
| 1:I:331:ALA:O | 1:I:335:ARG:HG3 | 2.21 | 0.40 |
| 1:J:50:ILE:O | 1:J:54:LEU:HG | 2.22 | 0.40 |
| 1:J:58:SER:HA | 1:J:61:LEU:HG | 2.04 | 0.40 |
| 1:L:89:LEU:O | 1:L:294:ILE:HD11 | 2.20 | 0.40 |
| 1:M:250:ASN:ND2 | 1:M:299:LYS:HD2 | 2.36 | 0.40 |
| 1:N:50:ILE:HD13 | 1:N:50:ILE:N | 2.37 | 0.40 |
| 1:Q:226:ILE:HA | 1:Q:226:ILE:HD12 | 1.81 | 0.40 |
| 1:R:224:THR:HA | 1:R:227:ASN:ND2 | 2.37 | 0.40 |
| 1:S:196:LYS:HD3 | 1:S:210:ASN:HA | 2.02 | 0.40 |
| 1:c:162:LYS:HE3 | 1:c:304:HIS:ND1 | 2.36 | 0.40 |
| 1:h:295:ASP:O | 1:h:299:LYS:HG2 | 2.22 | 0.40 |
| 1:h:311:PHE:C | 1:h:311:PHE:CD1 | 2.99 | 0.40 |
| 1:l:149:ILE:HG21 | 1:l:315:PHE:CE2 | 2.56 | 0.40 |
| 1:l:311:PHE:HE1 | 1:l:315:PHE:HE1 | 1.69 | 0.40 |
| 1:m:57:GLN:O | 1:m:61:LEU:HG | 2.22 | 0.40 |
| 1:o:190:GLU:CD | 1:o:191:GLY:N | 2.79 | 0.40 |
| 1:r:31:ARG:NH2 | 1:r:37:LYS:O | 2.54 | 0.40 |
| 1:r:243:LEU:HD23 | 1:r:244:GLN:N | 2.36 | 0.40 |
| 1:r:245:ILE:HD12 | 1:r:245:ILE:HA | 1.87 | 0.40 |
| 1:s:29:MET:O | 1:s:33:SER:OG | 2.34 | 0.40 |
| 1:s:49:GLN:OE1 | 1:s:53:ARG:HD2 | 2.21 | 0.40 |
| 1:t:194:ASP:CG | 1:t:261:GLY:H | 2.30 | 0.40 |
| 1:t:320:SER:O | 1:t:323:ASP:OD1 | 2.40 | 0.40 |
| 1:w:239:GLN:H | 1:w:239:GLN:CD | 2.30 | 0.40 |
| 1:x:63:VAL:HA | 1:x:66:ARG:NH1 | 2.35 | 0.40 |
| 1:1:126:ILE:HA | 1:1:129:THR:HG22 | 2.03 | 0.40 |
| 1:A:270:GLU:OE1 | 1:A:271:GLY:N | 2.52 | 0.40 |
| 1:A:279:ILE:HG21 | 1:A:290:SER:HB3 | 2.04 | 0.40 |
| 1:D:161:LEU:HA | 1:D:162:LYS:HZ2 | 1.87 | 0.40 |
| 1:E:50:ILE:HG13 | 1:E:50:ILE:H | 1.69 | 0.40 |
| 1:G:84:GLU:OE2 | 1:G:84:GLU:HA | 2.22 | 0.40 |
| 1:G:299:LYS:HE3 | 1:G:299:LYS:HB2 | 1.85 | 0.40 |
| 1:I:37:LYS:HG2 | 1:I:337:LYS:O | 2.22 | 0.40 |
| 1:K:16:ARG:HA | 1:K:19:ASN:ND2 | 2.36 | 0.40 |
| 1:L:370:ASN:OD1 | 1:L:370:ASN:C | 2.65 | 0.40 |
| 1:N:366:LYS:HB3 | 1:N:366:LYS:HE2 | 1.83 | 0.40 |
| 1:Q:83:ASN:HA | 1:Q:305:ARG:NH1 | 2.37 | 0.40 |
| 1:R:27:THR:O | 1:R:31:ARG:HG3 | 2.22 | 0.40 |
| 1:R:92:MET:HE3 | 1:R:116:VAL:HG13 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:257:GLU:OE2 | 1:R:258:PHE:N | 2.54 | 0.40 |
| 1:c:240:ASP:O | 1:c:240:ASP:OD2 | 2.40 | 0.40 |
| 1:j:219:ILE:HG13 | 1:j:237:VAL:HG21 | 2.02 | 0.40 |
| 1:j:353:ILE:N | 1:j:353:ILE:HD13 | 2.36 | 0.40 |
| 1:o:366:LYS:O | 1:o:369:PRO:HD2 | 2.20 | 0.40 |
| 1:q:353:ILE:HD13 | 1:q:353:ILE:N | 2.37 | 0.40 |
| 1:u:177:GLN:HE22 | 1:u:272:LYS:HE2 | 1.86 | 0.40 |
| 1:u:272:LYS:HE2 | 1:u:272:LYS:HB2 | 1.93 | 0.40 |
| 1:x:356:GLN:N | 1:x:356:GLN:CD | 2.80 | 0.40 |
| 1:l:29:MET:O | 1:l:33:SER:OG | 2.36 | 0.40 |
| 1:2:139:ASN:OD1 | 1:2:141:THR:HG23 | 2.22 | 0.40 |
| 1:B:239:GLN:H | 1:B:239:GLN:CD | 2.29 | 0.40 |
| 1:C:27:THR:HG22 | 1:C:31:ARG:HH21 | 1.86 | 0.40 |
| 1:G:196:LYS:HG3 | 1:G:259:SER:OG | 2.22 | 0.40 |
| 1:H:239:GLN:CD | 1:H:239:GLN:H | 2.30 | 0.40 |
| 1:J:15:GLN:O | 1:J:19:ASN:ND2 | 2.38 | 0.40 |
| 1:K:88:ILE:HG23 | 1:K:119:LEU:CD2 | 2.42 | 0.40 |
| 1:L:191:GLY:C | 1:L:192:LYS:HD3 | 2.46 | 0.40 |
| 1:L:240:ASP:OD1 | 1:L:240:ASP:N | 2.54 | 0.40 |
| 1:S:112:ILE:O | 1:S:116:VAL:HG23 | 2.22 | 0.40 |
| 1:T:8:ASN:O | 1:T:12:MET:HE2 | 2.22 | 0.40 |
| 1:U:109:ARG:NH2 | 1:U:283:SER:HA | 2.36 | 0.40 |
| 1:c:93:ARG:HB2 | 1:c:294:ILE:HG21 | 2.03 | 0.40 |
| 1:h:67:ASN:HA | 1:h:70:ASP:OD1 | 2.21 | 0.40 |
| 1:h:319:ILE:O | 1:h:323:ASP:OD1 | 2.39 | 0.40 |
| 1:k:99:SER:HB3 | 1:k:112:ILE:HD13 | 2.04 | 0.40 |
| 1:k:125:ARG:O | 1:k:129:THR:OG1 | 2.21 | 0.40 |
| 1:m:84:GLU:HA | 1:m:87:ASN:HD22 | 1.80 | 0.40 |
| 1:m:233:VAL:O | 1:m:234:LYS:HD2 | 2.21 | 0.40 |
| 1:o:319:ILE:H | 1:o:319:ILE:HG13 | 1.77 | 0.40 |
| 1:p:89:LEU:HD21 | 1:p:123:LEU:HD11 | 2.03 | 0.40 |
| 1:q:142:HIS:CD2 | 1:q:161:LEU:HD12 | 2.57 | 0.40 |
| 1:q:219:ILE:H | 1:q:219:ILE:HG12 | 1.71 | 0.40 |
| 1:q:300:TYR:CG | 1:q:304:HIS:HE1 | 2.39 | 0.40 |
| 1:w:131:SER:HB3 | 1:w:136:LYS:HD3 | 2.03 | 0.40 |
| 1:z:299:LYS:HD2 | 1:z:299:LYS:O | 2.22 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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 | 1 | 374/377 (99%) | 364 (97%) | 10 (3%) | 0 | 100 | 100 |
| 1 | 2 | 374/377 (99%) | 364 (97%) | 10 (3%) | 0 | 100 | 100 |
| 1 | 3 | 374/377 (99%) | 363 (97%) | 11 (3%) | 0 | 100 | 100 |
| 1 | A | 374/377 (99%) | 368 (98%) | 6 (2%) | 0 | 100 | 100 |
| 1 | B | 374/377 (99%) | 366 (98%) | 8 (2%) | 0 | 100 | 100 |
| 1 | C | 374/377 (99%) | 366 (98%) | 8 (2%) | 0 | 100 | 100 |
| 1 | D | 374/377 (99%) | 368 (98%) | 6 (2%) | 0 | 100 | 100 |
| 1 | E | 374/377 (99%) | 364 (97%) | 10 (3%) | 0 | 100 | 100 |
| 1 | F | 374/377 (99%) | 371 (99%) | 3 (1%) | 0 | 100 | 100 |
| 1 | G | 374/377 (99%) | 367 (98%) | 7 (2%) | 0 | 100 | 100 |
| 1 | H | 374/377 (99%) | 362 (97%) | 12 (3%) | 0 | 100 | 100 |
| 1 | I | 374/377 (99%) | 360 (96%) | 14 (4%) | 0 | 100 | 100 |
| 1 | J | 374/377 (99%) | 371 (99%) | 3 (1%) | 0 | 100 | 100 |
| 1 | K | 374/377 (99%) | 364 (97%) | 10 (3%) | 0 | 100 | 100 |
| 1 | L | 374/377 (99%) | 372 (100%) | 2 (0%) | 0 | 100 | 100 |
| 1 | M | 374/377 (99%) | 366 (98%) | 8 (2%) | 0 | 100 | 100 |
| 1 | N | 374/377 (99%) | 367 (98%) | 7 (2%) | 0 | 100 | 100 |
| 1 | O | 374/377 (99%) | 366 (98%) | 8 (2%) | 0 | 100 | 100 |
| 1 | P | 374/377 (99%) | 357 (96%) | 17 (4%) | 0 | 100 | 100 |
| 1 | Q | 374/377 (99%) | 370 (99%) | 4 (1%) | 0 | 100 | 100 |
| 1 | R | 374/377 (99%) | 363 (97%) | 11 (3%) | 0 | 100 | 100 |
| 1 | S | 374/377 (99%) | 368 (98%) | 6 (2%) | 0 | 100 | 100 |
| 1 | T | 374/377 (99%) | 366 (98%) | 8 (2%) | 0 | 100 | 100 |
| 1 | U | 374/377 (99%) | 367 (98%) | 7 (2%) | 0 | 100 | 100 |
| 1 | V | 374/377 (99%) | 366 (98%) | 8 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1 | c | 374/377 (99%) | 364 (97%) | 10 (3%) | 0 | 100 | 100 |
| 1 | h | 374/377 (99%) | 366 (98%) | 8 (2%) | 0 | 100 | 100 |
| 1 | i | 374/377 (99%) | 363 (97%) | 11 (3%) | 0 | 100 | 100 |
| 1 | j | 374/377 (99%) | 366 (98%) | 8 (2%) | 0 | 100 | 100 |
| 1 | k | 374/377 (99%) | 367 (98%) | 7 (2%) | 0 | 100 | 100 |
| 1 | l | 374/377 (99%) | 366 (98%) | 8 (2%) | 0 | 100 | 100 |
| 1 | m | 374/377 (99%) | 371 (99%) | 3 (1%) | 0 | 100 | 100 |
| 1 | n | 374/377 (99%) | 368 (98%) | 6 (2%) | 0 | 100 | 100 |
| 1 | o | 374/377 (99%) | 365 (98%) | 9 (2%) | 0 | 100 | 100 |
| 1 | p | 374/377 (99%) | 364 (97%) | 10 (3%) | 0 | 100 | 100 |
| 1 | q | 374/377 (99%) | 366 (98%) | 8 (2%) | 0 | 100 | 100 |
| 1 | r | 374/377 (99%) | 362 (97%) | 12 (3%) | 0 | 100 | 100 |
| 1 | s | 374/377 (99%) | 366 (98%) | 8 (2%) | 0 | 100 | 100 |
| 1 | t | 374/377 (99%) | 365 (98%) | 9 (2%) | 0 | 100 | 100 |
| 1 | u | 374/377 (99%) | 369 (99%) | 5 (1%) | 0 | 100 | 100 |
| 1 | v | 374/377 (99%) | 364 (97%) | 10 (3%) | 0 | 100 | 100 |
| 1 | w | 374/377 (99%) | 364 (97%) | 10 (3%) | 0 | 100 | 100 |
| 1 | x | 374/377 (99%) | 368 (98%) | 6 (2%) | 0 | 100 | 100 |
| 1 | z | 374/377 (99%) | 365 (98%) | 9 (2%) | 0 | 100 | 100 |
| All | All | 16456/16588 (99%) | 16095 (98%) | 361 (2%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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 | 1 | 300/301 (100%) | 296 (99%) | 4 (1%) | 61 | 72 |
| 1 | 2 | 300/301 (100%) | 299 (100%) | 1 (0%) | 86 | 83 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | 3 | 300/301 (100%) | 293 (98%) | 7 (2%) | 44 | 64 |
| 1 | A | 300/301 (100%) | 298 (99%) | 2 (1%) | 76 | 78 |
| 1 | B | 300/301 (100%) | 300 (100%) | 0 | 100 | 100 |
| 1 | C | 300/301 (100%) | 294 (98%) | 6 (2%) | 48 | 66 |
| 1 | D | 300/301 (100%) | 296 (99%) | 4 (1%) | 61 | 72 |
| 1 | E | 300/301 (100%) | 296 (99%) | 4 (1%) | 61 | 72 |
| 1 | F | 300/301 (100%) | 289 (96%) | 11 (4%) | 30 | 56 |
| 1 | G | 300/301 (100%) | 299 (100%) | 1 (0%) | 86 | 83 |
| 1 | H | 300/301 (100%) | 295 (98%) | 5 (2%) | 53 | 69 |
| 1 | I | 300/301 (100%) | 297 (99%) | 3 (1%) | 68 | 75 |
| 1 | J | 300/301 (100%) | 294 (98%) | 6 (2%) | 48 | 66 |
| 1 | K | 300/301 (100%) | 294 (98%) | 6 (2%) | 48 | 66 |
| 1 | L | 300/301 (100%) | 296 (99%) | 4 (1%) | 61 | 72 |
| 1 | M | 300/301 (100%) | 297 (99%) | 3 (1%) | 68 | 75 |
| 1 | N | 300/301 (100%) | 295 (98%) | 5 (2%) | 53 | 69 |
| 1 | O | 300/301 (100%) | 299 (100%) | 1 (0%) | 86 | 83 |
| 1 | P | 300/301 (100%) | 296 (99%) | 4 (1%) | 61 | 72 |
| 1 | Q | 300/301 (100%) | 294 (98%) | 6 (2%) | 48 | 66 |
| 1 | R | 300/301 (100%) | 295 (98%) | 5 (2%) | 53 | 69 |
| 1 | S | 300/301 (100%) | 298 (99%) | 2 (1%) | 76 | 78 |
| 1 | T | 300/301 (100%) | 296 (99%) | 4 (1%) | 61 | 72 |
| 1 | U | 300/301 (100%) | 297 (99%) | 3 (1%) | 68 | 75 |
| 1 | V | 300/301 (100%) | 294 (98%) | 6 (2%) | 48 | 66 |
| 1 | c | 300/301 (100%) | 297 (99%) | 3 (1%) | 68 | 75 |
| 1 | h | 300/301 (100%) | 295 (98%) | 5 (2%) | 53 | 69 |
| 1 | i | 300/301 (100%) | 299 (100%) | 1 (0%) | 86 | 83 |
| 1 | j | 300/301 (100%) | 298 (99%) | 2 (1%) | 76 | 78 |
| 1 | k | 300/301 (100%) | 293 (98%) | 7 (2%) | 44 | 64 |
| 1 | l | 300/301 (100%) | 289 (96%) | 11 (4%) | 30 | 56 |
| 1 | m | 300/301 (100%) | 297 (99%) | 3 (1%) | 68 | 75 |
| 1 | n | 300/301 (100%) | 296 (99%) | 4 (1%) | 61 | 72 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|--------------------|-------------|----------|-------------|----|
| 1 | o | 300/301 (100%) | 295 (98%) | 5 (2%) | 53 | 69 |
| 1 | p | 300/301 (100%) | 296 (99%) | 4 (1%) | 61 | 72 |
| 1 | q | 300/301 (100%) | 299 (100%) | 1 (0%) | 86 | 83 |
| 1 | r | 300/301 (100%) | 294 (98%) | 6 (2%) | 48 | 66 |
| 1 | s | 300/301 (100%) | 294 (98%) | 6 (2%) | 48 | 66 |
| 1 | t | 300/301 (100%) | 295 (98%) | 5 (2%) | 53 | 69 |
| 1 | u | 300/301 (100%) | 295 (98%) | 5 (2%) | 53 | 69 |
| 1 | v | 300/301 (100%) | 295 (98%) | 5 (2%) | 53 | 69 |
| 1 | w | 300/301 (100%) | 297 (99%) | 3 (1%) | 68 | 75 |
| 1 | x | 300/301 (100%) | 295 (98%) | 5 (2%) | 53 | 69 |
| 1 | z | 300/301 (100%) | 292 (97%) | 8 (3%) | 39 | 61 |
| All | All | 13200/13244 (100%) | 13008 (98%) | 192 (2%) | 55 | 70 |

All (192) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1 | 12 | MET |
| 1 | 1 | 55 | ASN |
| 1 | 1 | 57 | GLN |
| 1 | 1 | 250 | ASN |
| 1 | 2 | 38 | ILE |
| 1 | 3 | 49 | GLN |
| 1 | 3 | 76 | GLN |
| 1 | 3 | 177 | GLN |
| 1 | 3 | 197 | ILE |
| 1 | 3 | 219 | ILE |
| 1 | 3 | 245 | ILE |
| 1 | 3 | 344 | GLU |
| 1 | A | 54 | LEU |
| 1 | A | 193 | ASN |
| 1 | C | 6 | ASN |
| 1 | C | 104 | ASN |
| 1 | C | 169 | LYS |
| 1 | C | 217 | ASP |
| 1 | C | 253 | GLU |
| 1 | C | 338 | ASP |
| 1 | D | 12 | MET |
| 1 | D | 49 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 220 | GLU |
| 1 | D | 298 | LEU |
| 1 | E | 8 | ASN |
| 1 | E | 38 | ILE |
| 1 | E | 198 | ASN |
| 1 | E | 242 | LYS |
| 1 | F | 38 | ILE |
| 1 | F | 62 | ASP |
| 1 | F | 89 | LEU |
| 1 | F | 162 | LYS |
| 1 | F | 164 | MET |
| 1 | F | 177 | GLN |
| 1 | F | 198 | ASN |
| 1 | F | 210 | ASN |
| 1 | F | 249 | ASN |
| 1 | F | 338 | ASP |
| 1 | F | 340 | ASP |
| 1 | G | 277 | ASP |
| 1 | H | 6 | ASN |
| 1 | H | 53 | ARG |
| 1 | H | 76 | GLN |
| 1 | H | 97 | LEU |
| 1 | H | 255 | GLU |
| 1 | I | 19 | ASN |
| 1 | I | 106 | LYS |
| 1 | I | 364 | GLN |
| 1 | J | 4 | ASN |
| 1 | J | 38 | ILE |
| 1 | J | 251 | LYS |
| 1 | J | 304 | HIS |
| 1 | J | 316 | ASN |
| 1 | J | 333 | LYS |
| 1 | K | 15 | GLN |
| 1 | K | 38 | ILE |
| 1 | K | 126 | ILE |
| 1 | K | 251 | LYS |
| 1 | K | 256 | VAL |
| 1 | K | 343 | LYS |
| 1 | L | 6 | ASN |
| 1 | L | 87 | ASN |
| 1 | L | 171 | MET |
| 1 | L | 367 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 197 | ILE |
| 1 | M | 240 | ASP |
| 1 | M | 375 | LEU |
| 1 | N | 4 | ASN |
| 1 | N | 12 | MET |
| 1 | N | 13 | THR |
| 1 | N | 177 | GLN |
| 1 | N | 197 | ILE |
| 1 | O | 279 | ILE |
| 1 | P | 94 | ASP |
| 1 | P | 171 | MET |
| 1 | P | 229 | GLN |
| 1 | P | 243 | LEU |
| 1 | Q | 12 | MET |
| 1 | Q | 104 | ASN |
| 1 | Q | 123 | LEU |
| 1 | Q | 153 | ASN |
| 1 | Q | 209 | ILE |
| 1 | Q | 344 | GLU |
| 1 | R | 97 | LEU |
| 1 | R | 152 | ASP |
| 1 | R | 158 | MET |
| 1 | R | 192 | LYS |
| 1 | R | 238 | ASP |
| 1 | S | 4 | ASN |
| 1 | S | 97 | LEU |
| 1 | T | 104 | ASN |
| 1 | T | 120 | ASN |
| 1 | T | 328 | ASN |
| 1 | T | 364 | GLN |
| 1 | U | 38 | ILE |
| 1 | U | 74 | ILE |
| 1 | U | 210 | ASN |
| 1 | V | 38 | ILE |
| 1 | V | 82 | MET |
| 1 | V | 119 | LEU |
| 1 | V | 138 | LEU |
| 1 | V | 177 | GLN |
| 1 | V | 262 | LEU |
| 1 | c | 226 | ILE |
| 1 | c | 233 | VAL |
| 1 | c | 268 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | h | 6 | ASN |
| 1 | h | 126 | ILE |
| 1 | h | 158 | MET |
| 1 | h | 229 | GLN |
| 1 | h | 231 | ASP |
| 1 | i | 49 | GLN |
| 1 | j | 273 | LYS |
| 1 | j | 375 | LEU |
| 1 | k | 3 | VAL |
| 1 | k | 12 | MET |
| 1 | k | 126 | ILE |
| 1 | k | 219 | ILE |
| 1 | k | 333 | LYS |
| 1 | k | 338 | ASP |
| 1 | k | 367 | GLN |
| 1 | l | 22 | ASN |
| 1 | l | 32 | LEU |
| 1 | l | 39 | ASN |
| 1 | l | 145 | LYS |
| 1 | l | 197 | ILE |
| 1 | l | 208 | GLU |
| 1 | l | 210 | ASN |
| 1 | l | 239 | GLN |
| 1 | l | 288 | GLN |
| 1 | l | 338 | ASP |
| 1 | l | 339 | THR |
| 1 | m | 198 | ASN |
| 1 | m | 299 | LYS |
| 1 | m | 344 | GLU |
| 1 | n | 158 | MET |
| 1 | n | 197 | ILE |
| 1 | n | 338 | ASP |
| 1 | n | 339 | THR |
| 1 | o | 123 | LEU |
| 1 | o | 205 | GLN |
| 1 | o | 294 | ILE |
| 1 | o | 375 | LEU |
| 1 | o | 376 | LEU |
| 1 | p | 26 | GLN |
| 1 | p | 126 | ILE |
| 1 | p | 239 | GLN |
| 1 | p | 250 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | q | 197 | ILE |
| 1 | r | 15 | GLN |
| 1 | r | 126 | ILE |
| 1 | r | 155 | GLU |
| 1 | r | 229 | GLN |
| 1 | r | 253 | GLU |
| 1 | r | 350 | LYS |
| 1 | s | 26 | GLN |
| 1 | s | 185 | ASP |
| 1 | s | 193 | ASN |
| 1 | s | 231 | ASP |
| 1 | s | 326 | ASN |
| 1 | s | 337 | LYS |
| 1 | t | 85 | THR |
| 1 | t | 155 | GLU |
| 1 | t | 220 | GLU |
| 1 | t | 250 | ASN |
| 1 | t | 312 | GLN |
| 1 | u | 32 | LEU |
| 1 | u | 90 | GLN |
| 1 | u | 164 | MET |
| 1 | u | 210 | ASN |
| 1 | u | 289 | GLU |
| 1 | v | 36 | PHE |
| 1 | v | 39 | ASN |
| 1 | v | 141 | THR |
| 1 | v | 343 | LYS |
| 1 | v | 344 | GLU |
| 1 | w | 217 | ASP |
| 1 | w | 220 | GLU |
| 1 | w | 339 | THR |
| 1 | x | 89 | LEU |
| 1 | x | 249 | ASN |
| 1 | x | 330 | ASN |
| 1 | x | 344 | GLU |
| 1 | x | 353 | ILE |
| 1 | z | 16 | ARG |
| 1 | z | 32 | LEU |
| 1 | z | 38 | ILE |
| 1 | z | 123 | LEU |
| 1 | z | 210 | ASN |
| 1 | z | 218 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | z | 277 | ASP |
| 1 | z | 279 | ILE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (242) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1 | 52 | ASN |
| 1 | 1 | 87 | ASN |
| 1 | 1 | 98 | GLN |
| 1 | 1 | 148 | GLN |
| 1 | 1 | 187 | ASN |
| 1 | 1 | 312 | GLN |
| 1 | 1 | 324 | ASN |
| 1 | 2 | 55 | ASN |
| 1 | 2 | 120 | ASN |
| 1 | 2 | 205 | GLN |
| 1 | 2 | 244 | GLN |
| 1 | 2 | 317 | HIS |
| 1 | 2 | 328 | ASN |
| 1 | 2 | 352 | GLN |
| 1 | 3 | 22 | ASN |
| 1 | 3 | 83 | ASN |
| 1 | 3 | 87 | ASN |
| 1 | 3 | 210 | ASN |
| 1 | 3 | 330 | ASN |
| 1 | A | 20 | ASN |
| 1 | A | 124 | ASN |
| 1 | A | 142 | HIS |
| 1 | A | 198 | ASN |
| 1 | A | 324 | ASN |
| 1 | A | 330 | ASN |
| 1 | B | 49 | GLN |
| 1 | B | 83 | ASN |
| 1 | C | 120 | ASN |
| 1 | C | 205 | GLN |
| 1 | C | 210 | ASN |
| 1 | C | 239 | GLN |
| 1 | C | 317 | HIS |
| 1 | C | 352 | GLN |
| 1 | C | 356 | GLN |
| 1 | C | 367 | GLN |
| 1 | D | 57 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 76 | GLN |
| 1 | D | 90 | GLN |
| 1 | D | 120 | ASN |
| 1 | D | 153 | ASN |
| 1 | D | 239 | GLN |
| 1 | D | 324 | ASN |
| 1 | E | 22 | ASN |
| 1 | E | 49 | GLN |
| 1 | E | 87 | ASN |
| 1 | E | 177 | GLN |
| 1 | E | 205 | GLN |
| 1 | E | 288 | GLN |
| 1 | E | 330 | ASN |
| 1 | F | 15 | GLN |
| 1 | F | 69 | ASN |
| 1 | F | 104 | ASN |
| 1 | F | 148 | GLN |
| 1 | F | 153 | ASN |
| 1 | F | 193 | ASN |
| 1 | F | 244 | GLN |
| 1 | F | 288 | GLN |
| 1 | G | 142 | HIS |
| 1 | G | 148 | GLN |
| 1 | H | 6 | ASN |
| 1 | H | 39 | ASN |
| 1 | H | 239 | GLN |
| 1 | I | 87 | ASN |
| 1 | I | 124 | ASN |
| 1 | I | 239 | GLN |
| 1 | I | 250 | ASN |
| 1 | J | 98 | GLN |
| 1 | J | 120 | ASN |
| 1 | J | 124 | ASN |
| 1 | J | 187 | ASN |
| 1 | J | 205 | GLN |
| 1 | J | 288 | GLN |
| 1 | J | 330 | ASN |
| 1 | K | 76 | GLN |
| 1 | K | 207 | GLN |
| 1 | K | 304 | HIS |
| 1 | K | 316 | ASN |
| 1 | L | 104 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 207 | GLN |
| 1 | L | 249 | ASN |
| 1 | L | 304 | HIS |
| 1 | L | 317 | HIS |
| 1 | M | 22 | ASN |
| 1 | M | 55 | ASN |
| 1 | M | 135 | ASN |
| 1 | M | 229 | GLN |
| 1 | M | 244 | GLN |
| 1 | M | 367 | GLN |
| 1 | N | 4 | ASN |
| 1 | N | 229 | GLN |
| 1 | N | 249 | ASN |
| 1 | N | 304 | HIS |
| 1 | N | 328 | ASN |
| 1 | N | 356 | GLN |
| 1 | O | 120 | ASN |
| 1 | O | 142 | HIS |
| 1 | O | 304 | HIS |
| 1 | O | 312 | GLN |
| 1 | P | 20 | ASN |
| 1 | P | 25 | GLN |
| 1 | P | 177 | GLN |
| 1 | P | 187 | ASN |
| 1 | P | 205 | GLN |
| 1 | P | 207 | GLN |
| 1 | P | 229 | GLN |
| 1 | P | 244 | GLN |
| 1 | P | 316 | ASN |
| 1 | P | 330 | ASN |
| 1 | Q | 6 | ASN |
| 1 | Q | 55 | ASN |
| 1 | Q | 142 | HIS |
| 1 | Q | 153 | ASN |
| 1 | Q | 207 | GLN |
| 1 | Q | 304 | HIS |
| 1 | Q | 367 | GLN |
| 1 | Q | 370 | ASN |
| 1 | R | 19 | ASN |
| 1 | R | 207 | GLN |
| 1 | R | 227 | ASN |
| 1 | S | 25 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | S | 49 | GLN |
| 1 | S | 120 | ASN |
| 1 | S | 328 | ASN |
| 1 | S | 352 | GLN |
| 1 | T | 57 | GLN |
| 1 | T | 104 | ASN |
| 1 | T | 120 | ASN |
| 1 | T | 352 | GLN |
| 1 | U | 83 | ASN |
| 1 | U | 205 | GLN |
| 1 | U | 210 | ASN |
| 1 | U | 244 | GLN |
| 1 | U | 250 | ASN |
| 1 | U | 304 | HIS |
| 1 | U | 330 | ASN |
| 1 | V | 120 | ASN |
| 1 | V | 148 | GLN |
| 1 | V | 177 | GLN |
| 1 | V | 312 | GLN |
| 1 | V | 316 | ASN |
| 1 | c | 101 | ASN |
| 1 | c | 104 | ASN |
| 1 | c | 177 | GLN |
| 1 | c | 187 | ASN |
| 1 | c | 205 | GLN |
| 1 | c | 250 | ASN |
| 1 | c | 352 | GLN |
| 1 | h | 22 | ASN |
| 1 | h | 120 | ASN |
| 1 | h | 124 | ASN |
| 1 | h | 135 | ASN |
| 1 | h | 153 | ASN |
| 1 | h | 205 | GLN |
| 1 | h | 326 | ASN |
| 1 | i | 19 | ASN |
| 1 | i | 67 | ASN |
| 1 | i | 90 | GLN |
| 1 | i | 120 | ASN |
| 1 | i | 124 | ASN |
| 1 | i | 227 | ASN |
| 1 | i | 370 | ASN |
| 1 | j | 4 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | j | 25 | GLN |
| 1 | j | 49 | GLN |
| 1 | j | 55 | ASN |
| 1 | j | 104 | ASN |
| 1 | j | 124 | ASN |
| 1 | j | 142 | HIS |
| 1 | j | 244 | GLN |
| 1 | k | 120 | ASN |
| 1 | k | 142 | HIS |
| 1 | l | 19 | ASN |
| 1 | l | 83 | ASN |
| 1 | l | 104 | ASN |
| 1 | l | 288 | GLN |
| 1 | l | 330 | ASN |
| 1 | m | 87 | ASN |
| 1 | m | 168 | ASN |
| 1 | m | 187 | ASN |
| 1 | m | 210 | ASN |
| 1 | m | 244 | GLN |
| 1 | n | 22 | ASN |
| 1 | n | 321 | ASN |
| 1 | n | 324 | ASN |
| 1 | o | 25 | GLN |
| 1 | o | 55 | ASN |
| 1 | o | 239 | GLN |
| 1 | o | 312 | GLN |
| 1 | p | 15 | GLN |
| 1 | p | 19 | ASN |
| 1 | p | 124 | ASN |
| 1 | p | 239 | GLN |
| 1 | p | 312 | GLN |
| 1 | p | 321 | ASN |
| 1 | p | 326 | ASN |
| 1 | p | 330 | ASN |
| 1 | q | 19 | ASN |
| 1 | q | 57 | GLN |
| 1 | q | 124 | ASN |
| 1 | q | 148 | GLN |
| 1 | q | 316 | ASN |
| 1 | r | 198 | ASN |
| 1 | r | 239 | GLN |
| 1 | r | 249 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | r | 352 | GLN |
| 1 | s | 120 | ASN |
| 1 | s | 142 | HIS |
| 1 | s | 205 | GLN |
| 1 | s | 229 | GLN |
| 1 | t | 6 | ASN |
| 1 | t | 22 | ASN |
| 1 | t | 124 | ASN |
| 1 | t | 135 | ASN |
| 1 | t | 148 | GLN |
| 1 | t | 193 | ASN |
| 1 | t | 250 | ASN |
| 1 | t | 356 | GLN |
| 1 | u | 15 | GLN |
| 1 | u | 90 | GLN |
| 1 | u | 352 | GLN |
| 1 | u | 356 | GLN |
| 1 | v | 20 | ASN |
| 1 | v | 177 | GLN |
| 1 | v | 244 | GLN |
| 1 | v | 316 | ASN |
| 1 | v | 330 | ASN |
| 1 | w | 87 | ASN |
| 1 | w | 120 | ASN |
| 1 | w | 124 | ASN |
| 1 | w | 135 | ASN |
| 1 | w | 207 | GLN |
| 1 | w | 288 | GLN |
| 1 | w | 304 | HIS |
| 1 | w | 328 | ASN |
| 1 | w | 330 | ASN |
| 1 | w | 367 | GLN |
| 1 | x | 52 | ASN |
| 1 | x | 229 | GLN |
| 1 | x | 330 | ASN |
| 1 | z | 19 | ASN |
| 1 | z | 113 | GLN |
| 1 | z | 205 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

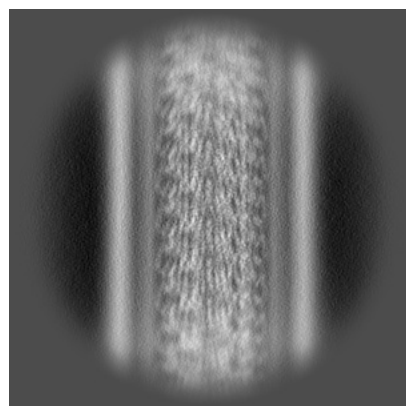
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53917. These allow visual inspection of the internal detail of the map and identification of artifacts.

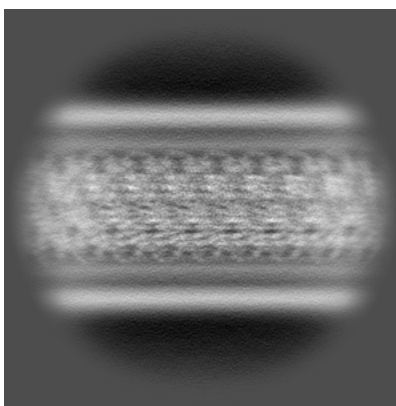
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

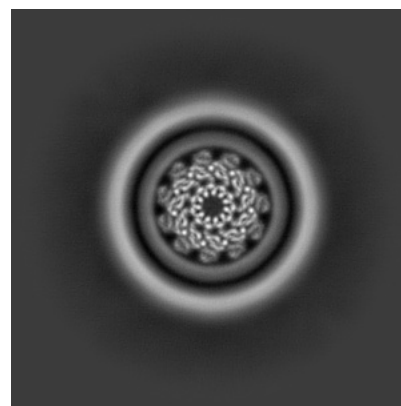
6.1.1 Primary map



X

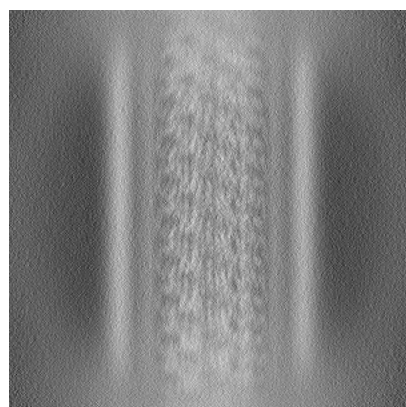


Y

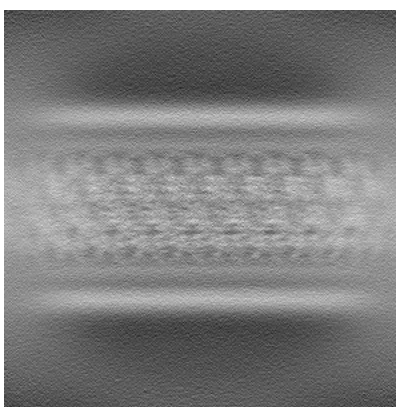


Z

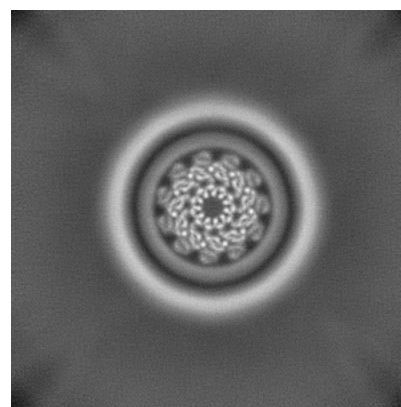
6.1.2 Raw map



X



Y

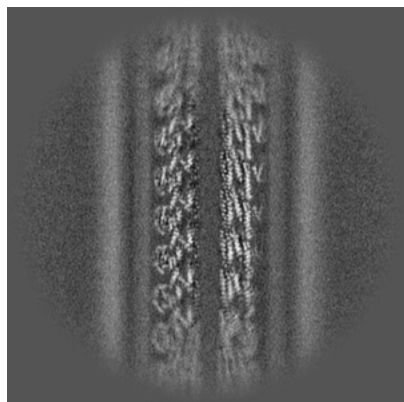


Z

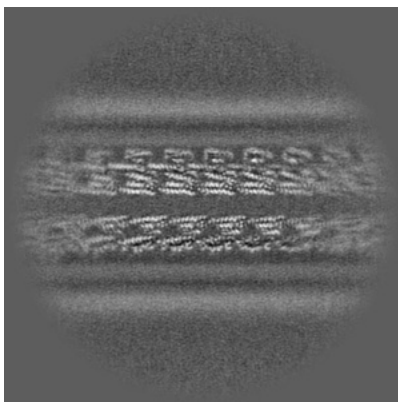
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

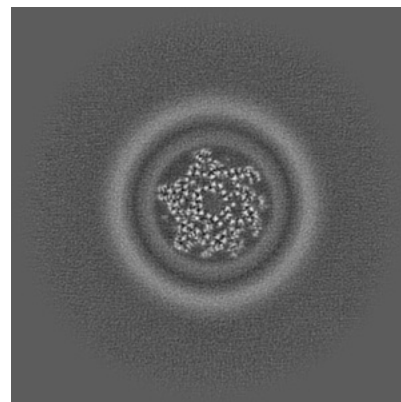
6.2.1 Primary map



X Index: 250

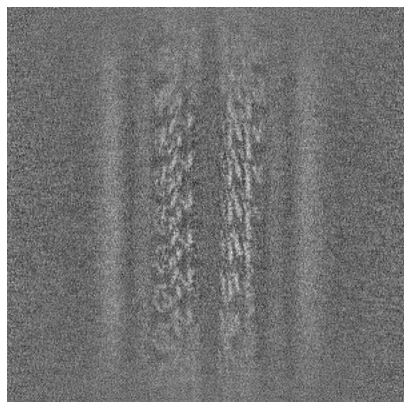


Y Index: 250

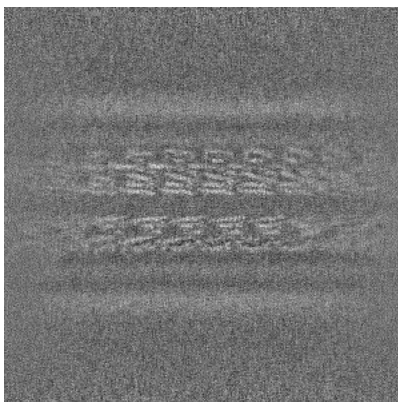


Z Index: 250

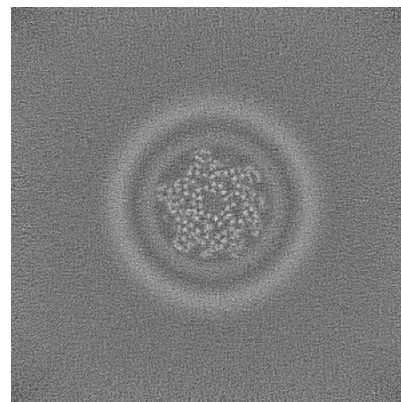
6.2.2 Raw map



X Index: 250



Y Index: 250

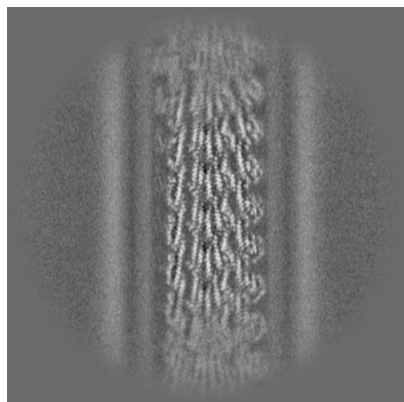


Z Index: 250

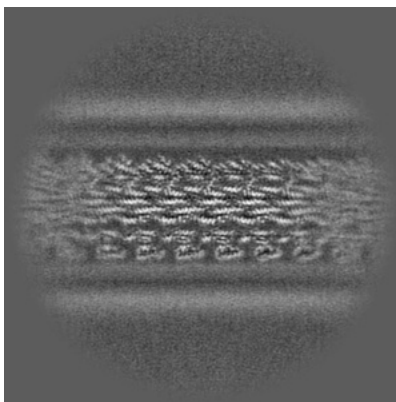
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

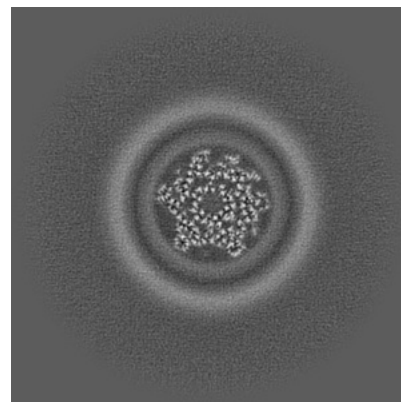
6.3.1 Primary map



X Index: 234

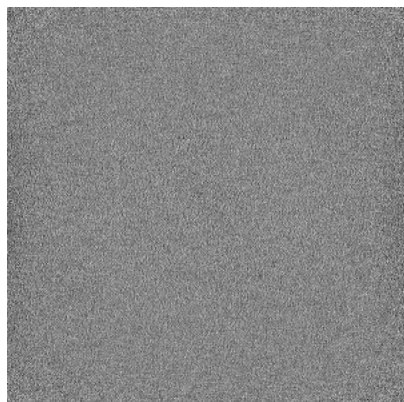


Y Index: 236

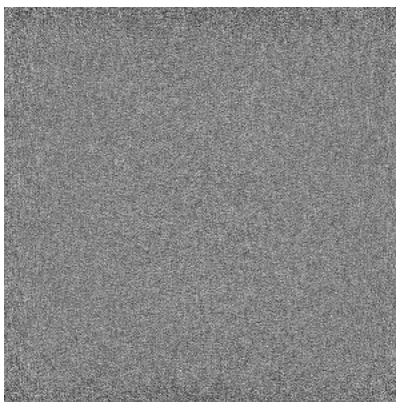


Z Index: 256

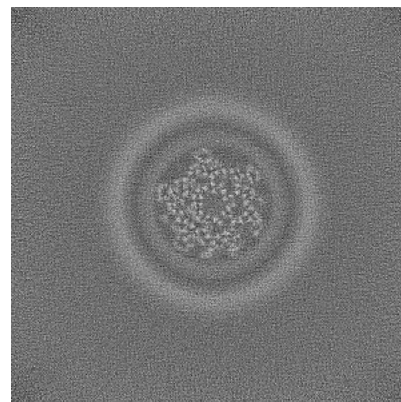
6.3.2 Raw map



X Index: 0



Y Index: 0

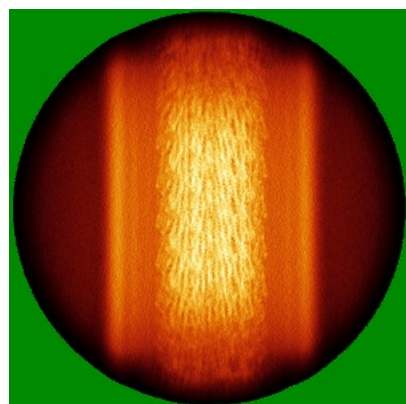


Z Index: 248

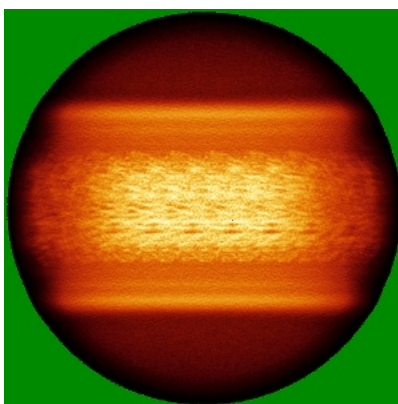
The images above show the largest variance slices of the map in three orthogonal directions.

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

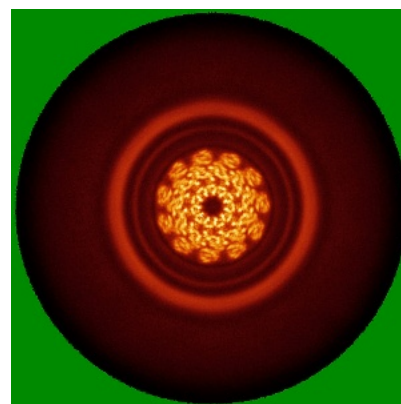
6.4.1 Primary map



X

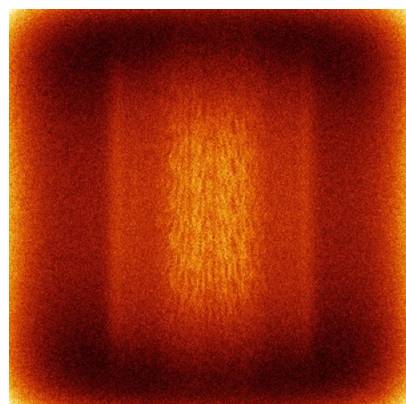


Y

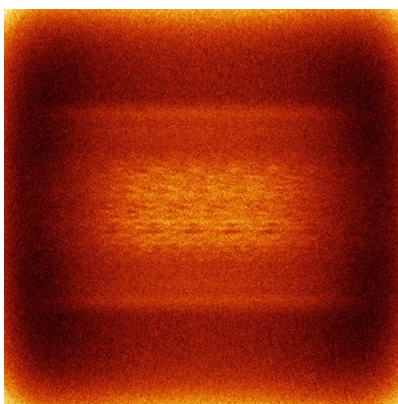


Z

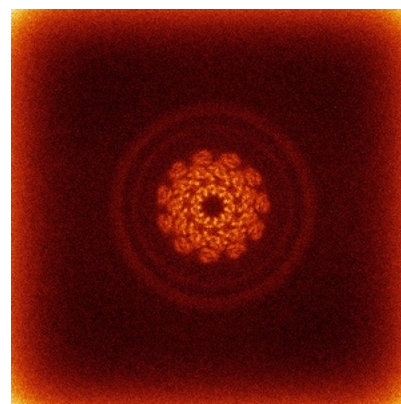
6.4.2 Raw map



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.

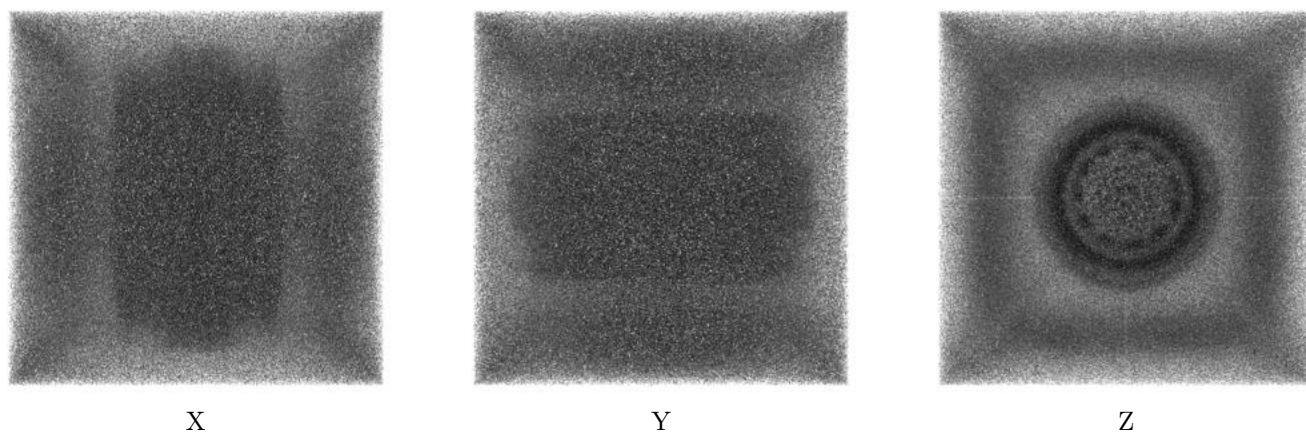
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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



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.

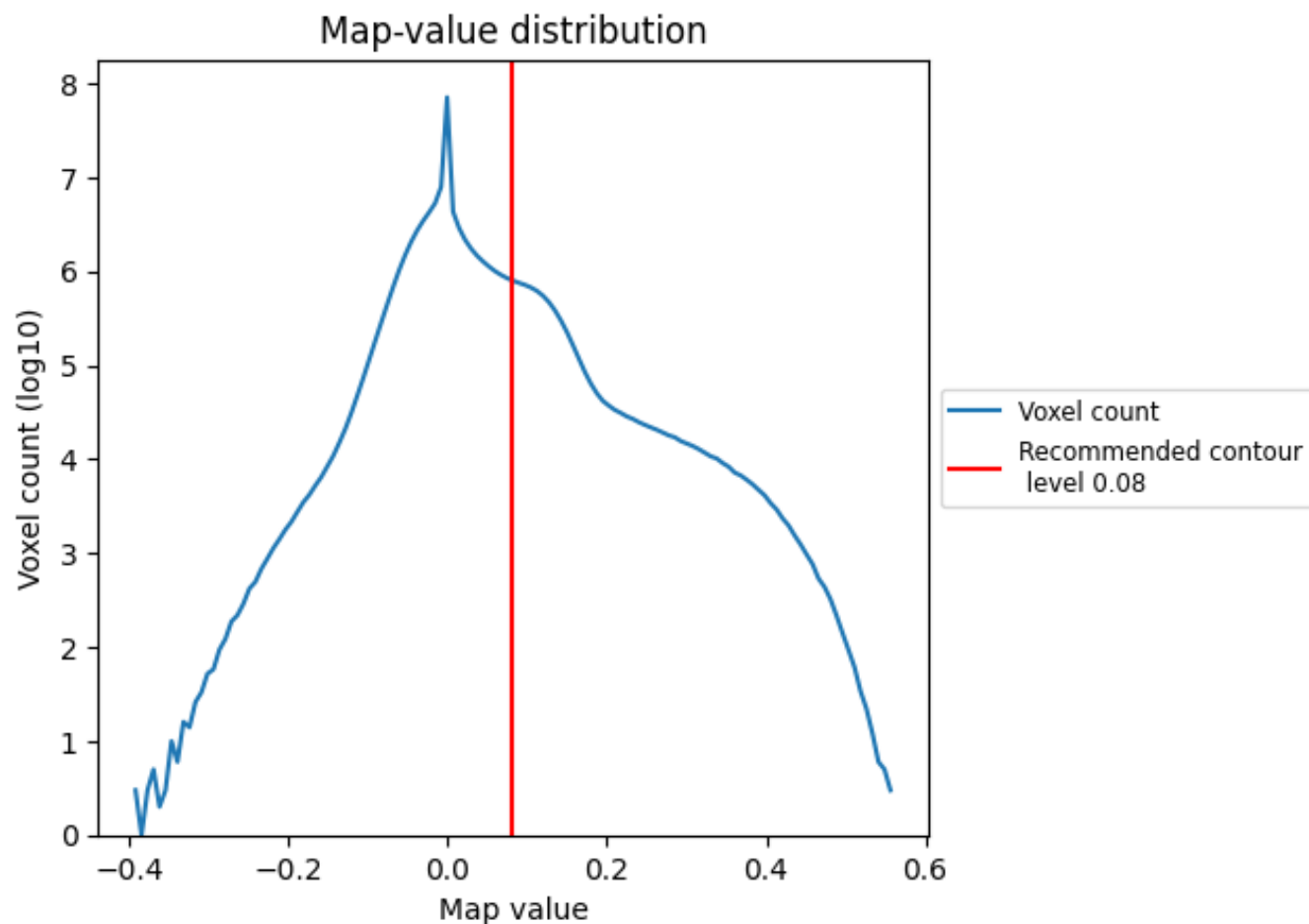
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

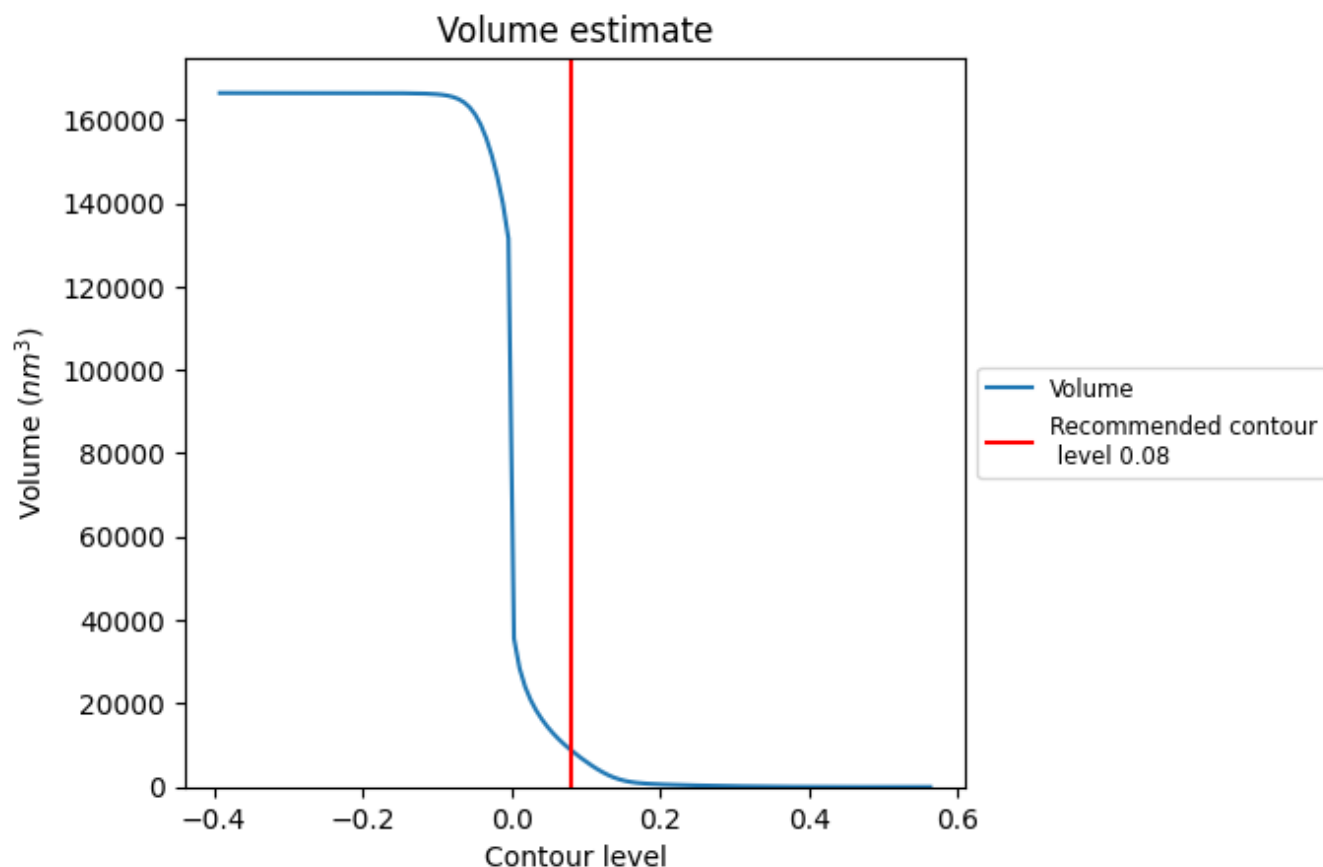
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

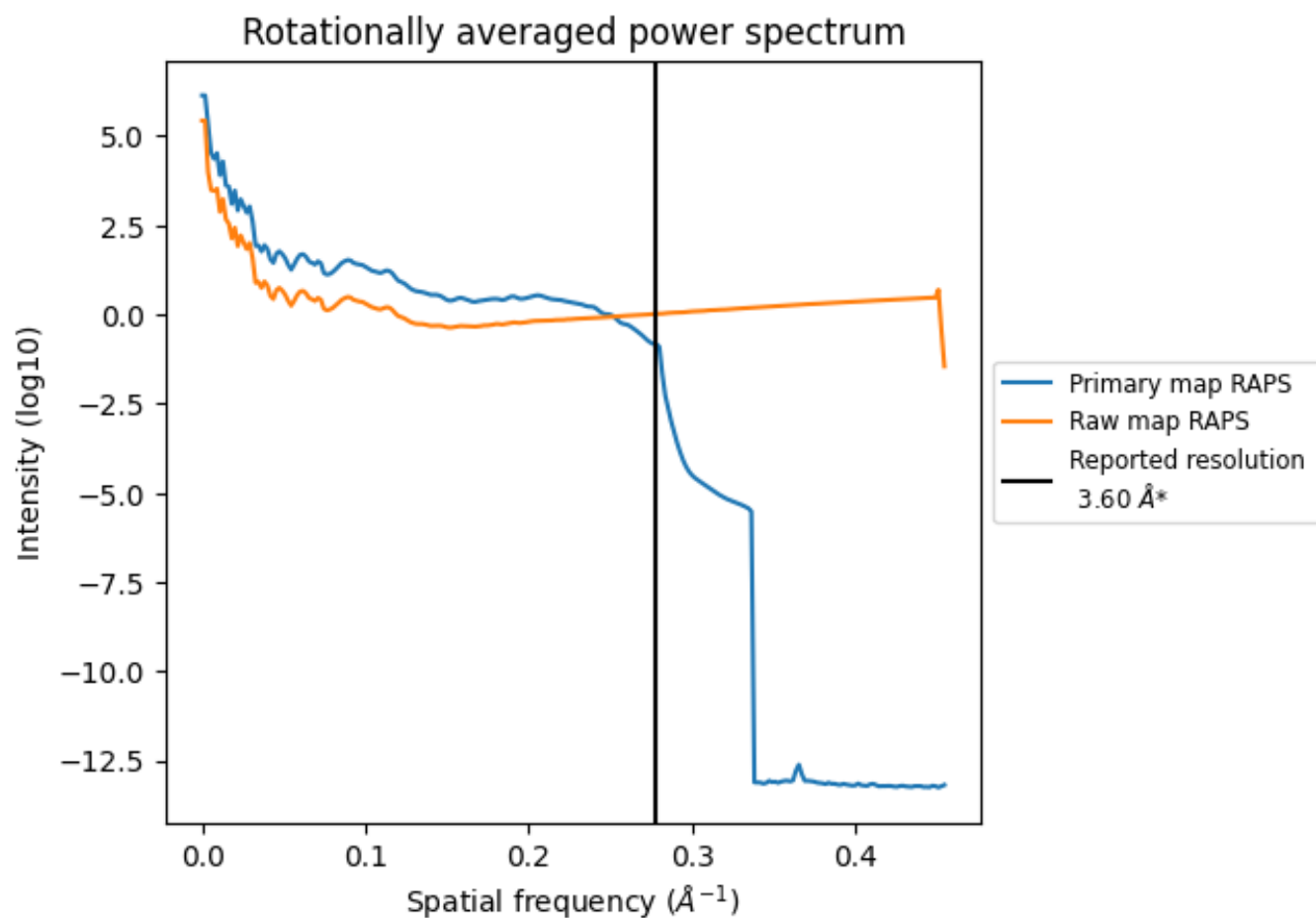
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8883 nm³; this corresponds to an approximate mass of 8024 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 ⓘ

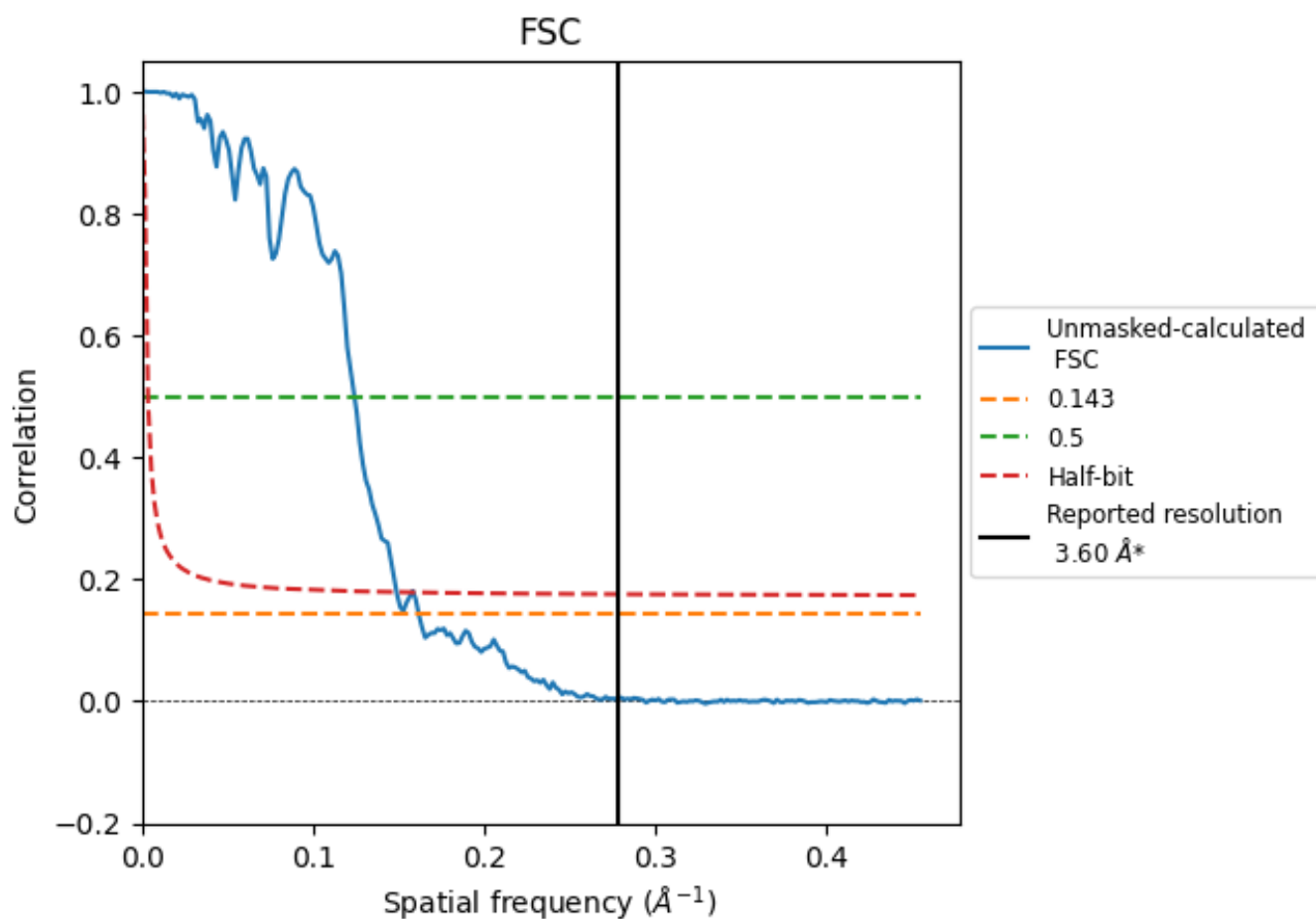


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

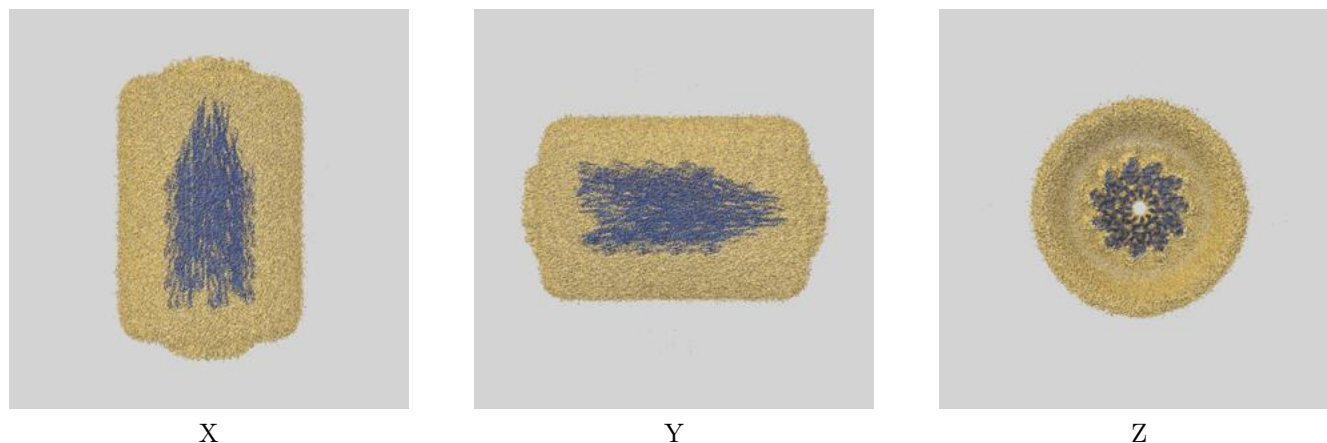
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.60 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 6.18 | 8.05 | 6.72 |

*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 6.18 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

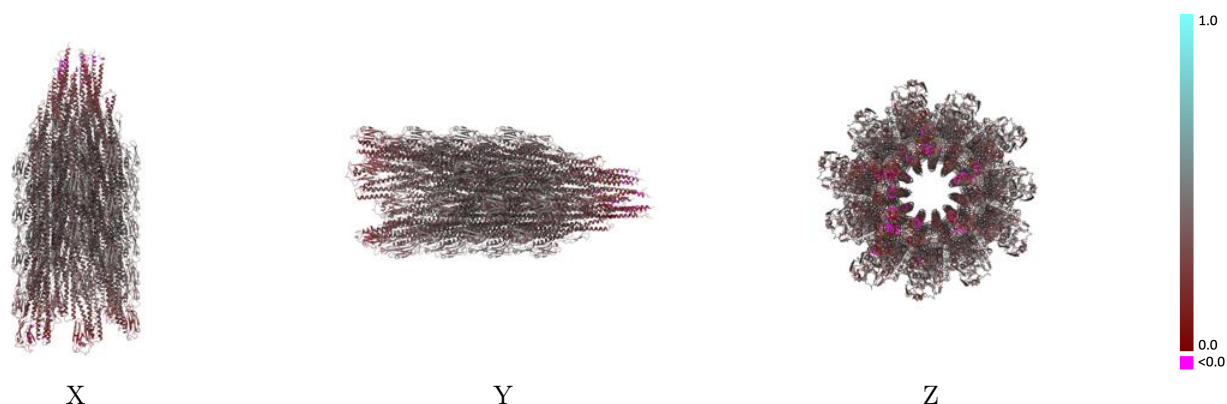
This section contains information regarding the fit between EMDB map EMD-53917 and PDB model 9RCD. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



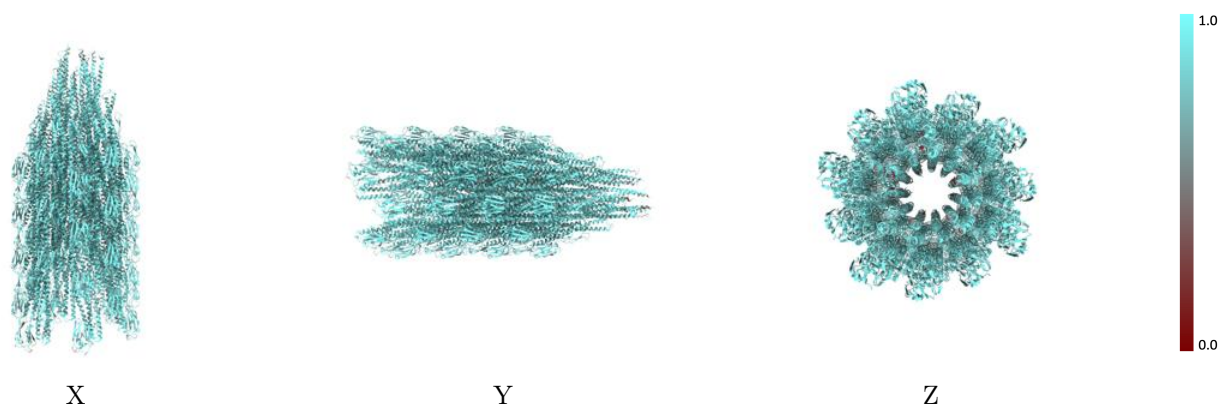
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



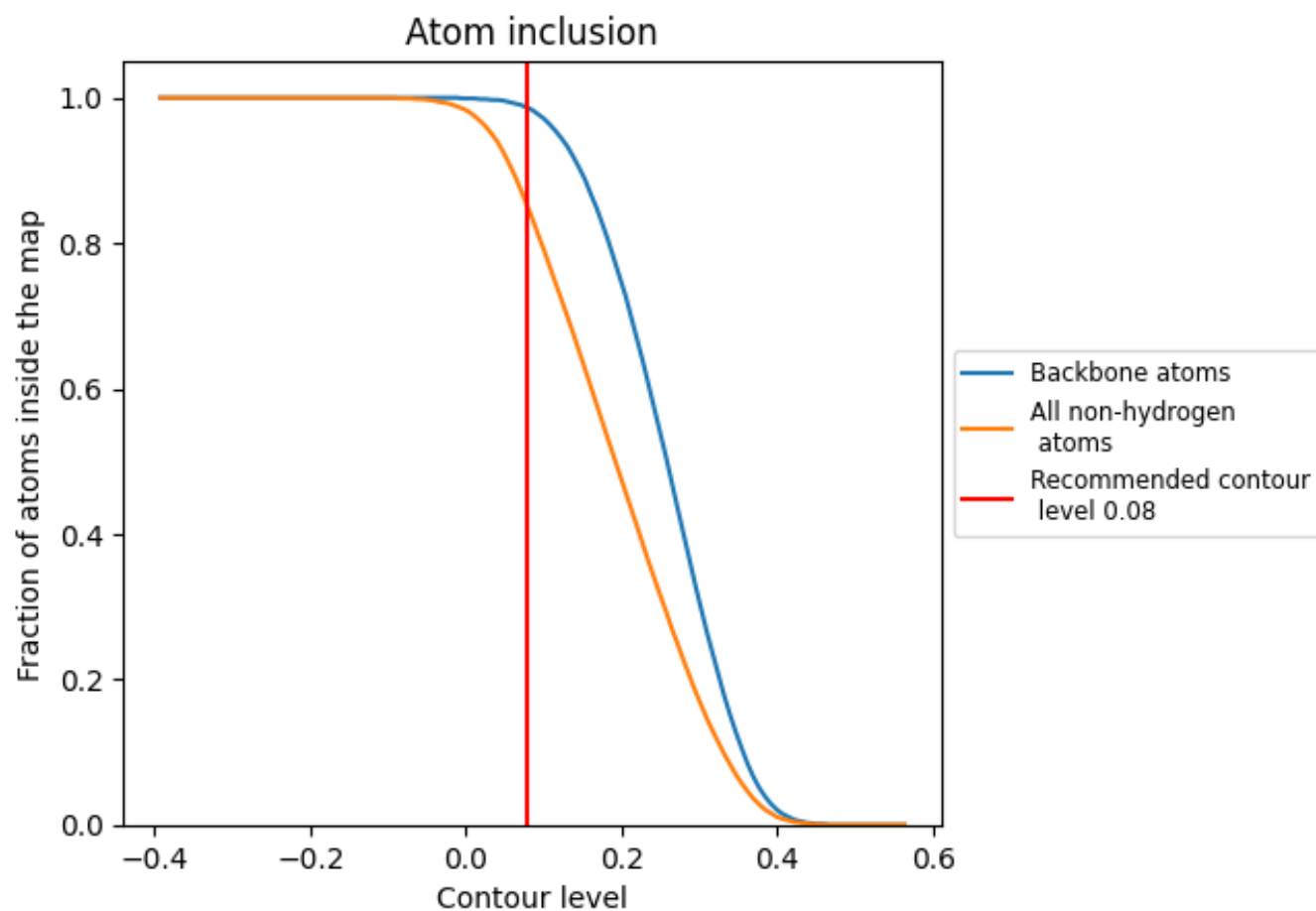
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.08).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 85% 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 (0.08) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.8490 |  0.3750 |
| 1 |  0.8170 |  0.3040 |
| 2 |  0.8330 |  0.3500 |
| 3 |  0.8230 |  0.3230 |
| A |  0.8650 |  0.3960 |
| B |  0.8650 |  0.4080 |
| C |  0.8600 |  0.4020 |
| D |  0.8620 |  0.4140 |
| E |  0.8550 |  0.3980 |
| F |  0.8600 |  0.4030 |
| G |  0.8540 |  0.4090 |
| H |  0.8670 |  0.4000 |
| I |  0.8630 |  0.4030 |
| J |  0.8590 |  0.3940 |
| K |  0.8620 |  0.4000 |
| L |  0.8320 |  0.3310 |
| M |  0.8660 |  0.3840 |
| N |  0.8330 |  0.3220 |
| O |  0.8490 |  0.3700 |
| P |  0.8210 |  0.3130 |
| Q |  0.8460 |  0.3580 |
| R |  0.8600 |  0.3900 |
| S |  0.8410 |  0.3500 |
| T |  0.8600 |  0.3810 |
| U |  0.8370 |  0.3380 |
| V |  0.8510 |  0.3750 |
| c |  0.8070 |  0.2900 |
| h |  0.8570 |  0.4020 |
| i |  0.8670 |  0.4000 |
| j |  0.8620 |  0.4150 |
| k |  0.8590 |  0.4020 |
| l |  0.8530 |  0.4080 |
| m |  0.8630 |  0.4040 |
| n |  0.8490 |  0.3810 |
| o |  0.8530 |  0.3990 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| p |  0.8540 |  0.3830 |
| q |  0.8550 |  0.3930 |
| r |  0.8550 |  0.3800 |
| s |  0.8470 |  0.3650 |
| t |  0.8420 |  0.3350 |
| u |  0.8460 |  0.3800 |
| v |  0.8350 |  0.3480 |
| w |  0.8450 |  0.3810 |
| x |  0.8400 |  0.3540 |
| z |  0.8320 |  0.3490 |