



# Full wwPDB X-ray Structure Validation Report i

Aug 16, 2023 – 10:37 AM EDT

PDB ID : 2A0F  
Title : Structure of D236A mutant E. coli Aspartate Transcarbamoylase in presence of Phosphonoacetamide at 2.90 Å resolution  
Authors : Stieglitz, K.A.; Dusinberre, K.J.; Cardia, J.P.; Tsuruta, H.; Kantrowitz, E.R.  
Deposited on : 2005-06-16  
Resolution : 2.90 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>  
with specific help available everywhere you see the i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

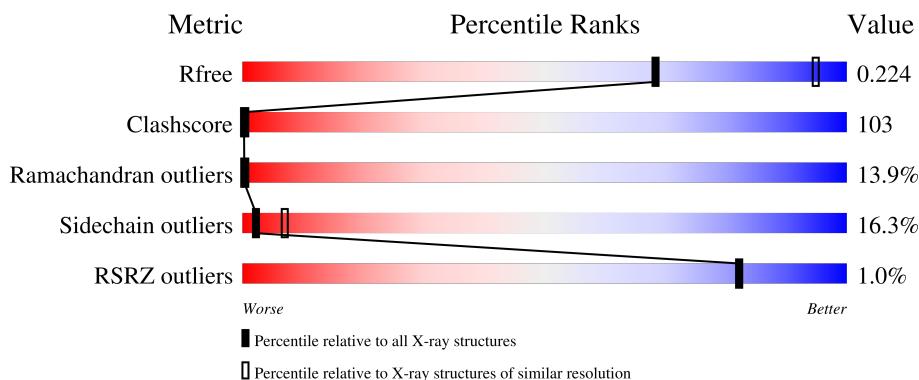
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

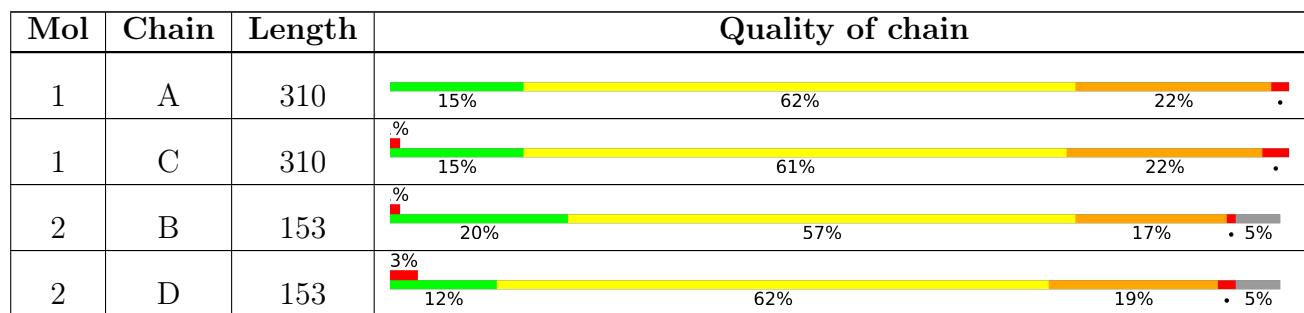
The reported resolution of this entry is 2.90 Å.

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) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|--------------------------|--|
| $R_{free}$            | 130704                   | 1957 (2.90-2.90)                                   |
| Clashscore            | 141614                   | 2172 (2.90-2.90)                                   |
| Ramachandran outliers | 138981                   | 2115 (2.90-2.90)                                   |
| Sidechain outliers    | 138945                   | 2117 (2.90-2.90)                                   |
| RSRZ outliers         | 127900                   | 1906 (2.90-2.90)                                   |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 electron density. The numeric value is given above the bar.



## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7489 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Aspartate carbamoyltransferase catalytic chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 310      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2412  | 1526 | 423 | 454 | 9 |         |         |       |

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | C     | 310      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2412  | 1526 | 423 | 454 | 9 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 236     | ALA      | ASP    | engineered mutation | UNP P0A786 |
| C     | 236     | ALA      | ASP    | engineered mutation | UNP P0A786 |

- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1138  | 714 | 201 | 218 | 5 |         |         |       |

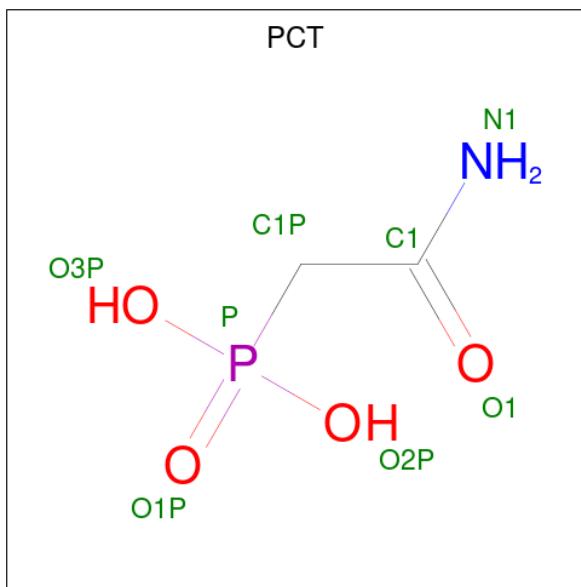
  

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | D     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1138  | 714 | 201 | 218 | 5 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | 1       | MET      | -      | initiating methionine | UNP P0A7F3 |
| D     | 1       | MET      | -      | initiating methionine | UNP P0A7F3 |

- Molecule 3 is PHOSPHONOACETAMIDE (three-letter code: PCT) (formula: C<sub>2</sub>H<sub>6</sub>NO<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
|     |       |          | Total | C | N | O | P |         |         |
| 3   | A     | 1        | 8     | 2 | 1 | 4 | 1 | 0       | 0       |

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms    |  | ZeroOcc | AltConf |
|-----|-------|----------|----------|--|---------|---------|
| 4   | B     | 1        | Total Zn |  | 0       | 0       |
| 4   | D     | 1        | Total Zn |  | 0       | 0       |

- Molecule 5 is water.

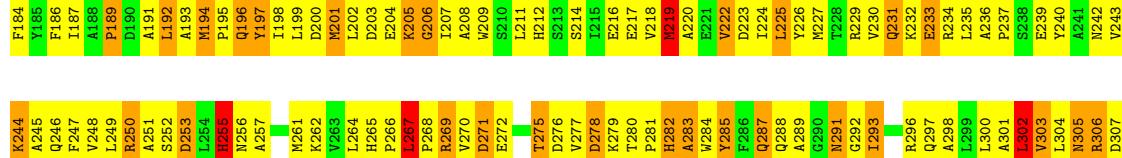
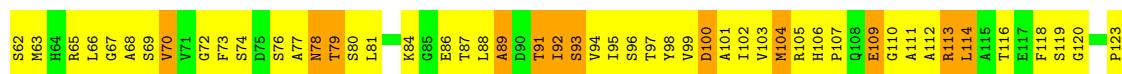
| Mol | Chain | Residues | Atoms              |  | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|--|---------|---------|
| 5   | A     | 130      | Total O<br>130 130 |  | 0       | 0       |
| 5   | B     | 82       | Total O<br>82 82   |  | 0       | 0       |
| 5   | C     | 110      | Total O<br>110 110 |  | 0       | 0       |
| 5   | D     | 57       | Total O<br>57 57   |  | 0       | 0       |

### 3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Aspartate carbamoyltransferase catalytic chain

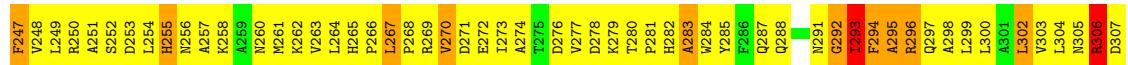
Chain A:  15% 62% 22% •



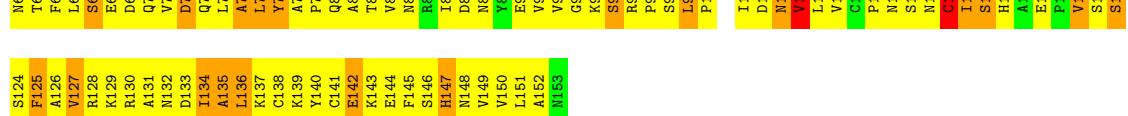
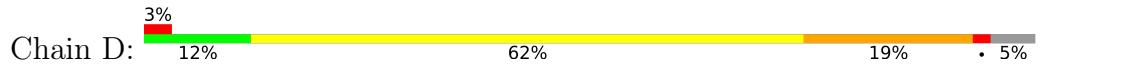
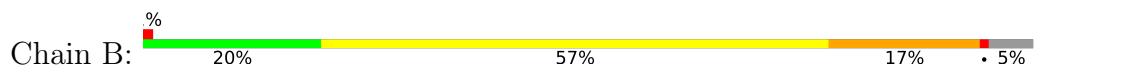
- Molecule 1: Aspartate carbamoyltransferase catalytic chain

Chain C:  15% 61% 22% •





- Molecule 2: Aspartate carbamoyltransferase regulatory chain



## 4 Data and refinement statistics (i)

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 3 2 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 120.45 Å    120.45 Å    155.24 Å<br>90.00°        90.00°        120.00° | Depositor        |
| Resolution (Å)  | 30.00 – 2.90<br>36.73 – 2.79  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (30.00-2.90)<br>80.8 (36.73-2.79)                       | Depositor<br>EDS |
| $R_{merge}$   | 0.09  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $< I/\sigma(I) >$ <sup>1</sup>  | 1.71 (at 2.81 Å)  | Xtriage          |
| Refinement program  | CNS   | Depositor        |
| $R$ , $R_{free}$  | 0.217 , 0.279<br>0.209 , 0.224  | Depositor<br>DCC |
| $R_{free}$ test set   | 2697 reflections (10.14%)   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 70.3  | Xtriage          |
| Anisotropy  | 0.131   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.22 , 122.3  | EDS              |
| L-test for twinning <sup>2</sup>  | $<  L  > = 0.37$ , $< L^2 > = 0.19$                                     | Xtriage          |
| Estimated twinning fraction   | 0.427 for -h,-k,l   | Xtriage          |
| $F_o, F_c$ correlation  | 0.94  | EDS              |
| Total number of atoms   | 7489  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 76.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [\(i\)](#)

### 5.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PCT

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   | A     | 0.62         | 1/2458 (0.0%) | 0.83        | 1/3335 (0.0%) |
| 1   | C     | 0.53         | 3/2458 (0.1%) | 0.71        | 0/3335        |
| 2   | B     | 0.52         | 0/1155        | 0.75        | 1/1561 (0.1%) |
| 2   | D     | 0.44         | 0/1155        | 0.68        | 0/1561        |
| All | All   | 0.55         | 4/7226 (0.1%) | 0.75        | 2/9792 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | C     | 60  | GLU  | CD-OE2 | 7.41 | 1.33        | 1.25     |
| 1   | A     | 60  | GLU  | CD-OE2 | 6.51 | 1.32        | 1.25     |
| 1   | C     | 147 | GLU  | CG-CD  | 5.70 | 1.60        | 1.51     |
| 1   | C     | 147 | GLU  | CD-OE1 | 5.10 | 1.31        | 1.25     |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 140 | LEU  | CA-CB-CG | 6.34  | 129.88      | 115.30   |
| 2   | B     | 74  | LEU  | CA-CB-CG | -5.01 | 103.78      | 115.30   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 98  | TYR  | Sidechain |

## 5.2 Too-close contacts [\(i\)](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2412  | 0        | 2423     | 452     | 0            |
| 1   | C     | 2412  | 0        | 2423     | 578     | 0            |
| 2   | B     | 1138  | 0        | 1152     | 209     | 0            |
| 2   | D     | 1138  | 0        | 1154     | 295     | 0            |
| 3   | A     | 8     | 0        | 4        | 3       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 130   | 0        | 0        | 22      | 0            |
| 5   | B     | 82    | 0        | 0        | 18      | 0            |
| 5   | C     | 110   | 0        | 0        | 32      | 0            |
| 5   | D     | 57    | 0        | 0        | 3       | 0            |
| All | All   | 7489  | 0        | 7156     | 1476    | 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 103.

All (1476) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:111:ASN:HD22 | 2:D:114:CYS:HB2  | 1.07                     | 1.16              |
| 1:A:158:ALA:HB2  | 1:A:222:VAL:HG11 | 1.26                     | 1.11              |
| 2:D:82:THR:HA    | 2:D:96:ARG:HH12  | 1.11                     | 1.08              |
| 2:B:44:ILE:HG23  | 2:D:44:ILE:HB    | 1.37                     | 1.06              |
| 2:D:20:HIS:HB3   | 2:D:80:GLN:HG2   | 1.37                     | 1.05              |
| 1:C:270:VAL:HG13 | 1:C:271:ASP:H    | 1.20                     | 1.04              |
| 2:B:75:ALA:HB1   | 2:B:99:LEU:HD12  | 1.36                     | 1.03              |
| 1:C:249:LEU:HG   | 1:C:254:LEU:HD11 | 1.40                     | 1.02              |
| 1:C:26:THR:O     | 1:C:30:LEU:HG    | 1.58                     | 1.02              |
| 1:A:229:ARG:HH21 | 1:A:270:VAL:HG21 | 1.22                     | 1.02              |
| 1:C:20:LEU:H     | 1:C:20:LEU:HD12  | 1.23                     | 1.02              |
| 1:A:164:LYS:HA   | 1:A:195:PRO:HD3  | 1.42                     | 1.01              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:76:LEU:H     | 2:B:76:LEU:HD23  | 1.23                     | 1.01              |
| 2:D:74:LEU:HG    | 2:D:97:PRO:HB3   | 1.40                     | 1.00              |
| 1:C:12:ILE:HD11  | 1:C:135:PRO:HA   | 1.43                     | 1.00              |
| 1:A:189:PRO:HG2  | 1:A:192:LEU:HD12 | 1.42                     | 0.99              |
| 1:C:219:MET:HB3  | 1:C:256:ASN:HD21 | 1.26                     | 0.99              |
| 2:D:103:ILE:HB   | 2:D:125:PHE:H    | 1.26                     | 0.99              |
| 2:D:146:SER:HB2  | 2:D:148:ASN:HD22 | 1.28                     | 0.98              |
| 1:A:216:GLU:O    | 1:A:219:MET:HB2  | 1.61                     | 0.98              |
| 1:C:9:ILE:HB     | 1:C:125:LEU:HA   | 1.43                     | 0.97              |
| 1:C:139:LEU:HA   | 1:C:142:LEU:HD12 | 1.42                     | 0.97              |
| 1:C:60:GLU:HA    | 1:C:63:MET:SD    | 2.05                     | 0.97              |
| 1:C:264:LEU:HD12 | 1:C:288:GLN:HB2  | 1.46                     | 0.97              |
| 2:D:111:ASN:ND2  | 2:D:114:CYS:HB2  | 1.79                     | 0.97              |
| 2:B:43:THR:HA    | 2:D:45:GLY:HA2   | 1.44                     | 0.97              |
| 1:A:145:ILE:HG23 | 1:A:224:ILE:HD12 | 1.44                     | 0.97              |
| 1:A:3:PRO:HD2    | 1:A:22:LEU:HD21  | 1.44                     | 0.96              |
| 2:D:46:LEU:HD23  | 2:D:46:LEU:H     | 1.29                     | 0.96              |
| 1:A:8:HIS:CD2    | 1:A:123:PRO:HA   | 2.01                     | 0.96              |
| 1:A:219:MET:HB3  | 1:A:256:ASN:HD21 | 1.30                     | 0.96              |
| 1:C:199:LEU:HA   | 1:C:202:LEU:HD21 | 1.48                     | 0.95              |
| 1:C:121:ASN:H    | 1:C:121:ASN:HD22 | 1.15                     | 0.94              |
| 1:A:267:LEU:HD23 | 1:A:268:PRO:HA   | 1.47                     | 0.93              |
| 1:C:237:PRO:HA   | 1:C:240:TYR:CE2  | 2.03                     | 0.93              |
| 1:A:52:SER:OG    | 1:A:55:THR:HG22  | 1.69                     | 0.92              |
| 2:D:137:LYS:HA   | 2:D:144:GLU:HA   | 1.50                     | 0.92              |
| 1:C:55:THR:O     | 1:C:59:PHE:HB2   | 1.70                     | 0.91              |
| 2:D:82:THR:HA    | 2:D:96:ARG:NH1   | 1.85                     | 0.91              |
| 1:A:109:GLU:HB3  | 2:B:141:CYS:HB3  | 1.52                     | 0.91              |
| 1:C:219:MET:HB3  | 1:C:256:ASN:ND2  | 1.84                     | 0.91              |
| 1:C:92:ILE:HG21  | 1:C:115:ALA:O    | 1.71                     | 0.91              |
| 1:C:92:ILE:HG13  | 1:C:115:ALA:HA   | 1.51                     | 0.90              |
| 1:C:237:PRO:HA   | 1:C:240:TYR:CZ   | 2.07                     | 0.90              |
| 1:C:169:VAL:HA   | 1:C:172:LEU:HD13 | 1.53                     | 0.90              |
| 2:B:102:ARG:HB3  | 2:B:126:ALA:HA   | 1.53                     | 0.90              |
| 1:C:19:ASP:O     | 1:C:22:LEU:HB3   | 1.72                     | 0.90              |
| 2:D:76:LEU:HB3   | 2:D:134:ILE:HG21 | 1.51                     | 0.90              |
| 1:A:91:THR:O     | 1:A:95:ILE:HG12  | 1.70                     | 0.89              |
| 1:A:125:LEU:HD12 | 1:A:125:LEU:N    | 1.87                     | 0.89              |
| 1:C:169:VAL:HB   | 1:C:172:LEU:HD22 | 1.53                     | 0.88              |
| 1:A:160:VAL:HG12 | 1:A:187:ILE:HB   | 1.52                     | 0.88              |
| 1:C:118:PHE:HB2  | 5:C:329:HOH:O    | 1.73                     | 0.88              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:59:PHE:O     | 1:C:63:MET:HG3   | 1.74                     | 0.88              |
| 1:C:152:LEU:H    | 1:C:152:LEU:HD12 | 1.37                     | 0.88              |
| 2:B:41:ARG:HG3   | 2:D:48:LEU:HD22  | 1.56                     | 0.87              |
| 1:C:109:GLU:HB2  | 2:D:141:CYS:SG   | 2.13                     | 0.87              |
| 2:D:111:ASN:ND2  | 2:D:114:CYS:H    | 1.72                     | 0.87              |
| 1:C:151:ARG:HH11 | 1:C:155:LEU:HD11 | 1.39                     | 0.87              |
| 1:A:219:MET:HB3  | 1:A:256:ASN:ND2  | 1.89                     | 0.87              |
| 2:B:27:PHE:N     | 2:B:46:LEU:HD21  | 1.90                     | 0.87              |
| 1:A:48:PHE:HE2   | 1:A:55:THR:HG23  | 1.38                     | 0.86              |
| 1:C:228:THR:HA   | 1:C:266:PRO:HG2  | 1.57                     | 0.86              |
| 2:D:78:ALA:HB3   | 2:D:81:ALA:HB2   | 1.58                     | 0.86              |
| 1:C:285:TYR:HA   | 1:C:288:GLN:OE1  | 1.76                     | 0.86              |
| 1:C:121:ASN:HD22 | 1:C:121:ASN:N    | 1.69                     | 0.86              |
| 1:A:94:VAL:HG23  | 1:A:95:ILE:HD13  | 1.57                     | 0.85              |
| 1:C:157:VAL:HG12 | 1:C:158:ALA:H    | 1.41                     | 0.85              |
| 1:A:200:ASP:O    | 1:A:203:ASP:HB2  | 1.75                     | 0.85              |
| 2:B:21:ILE:HB    | 2:B:57:ASP:HB2   | 1.58                     | 0.85              |
| 2:B:41:ARG:HA    | 2:D:47:ASN:HB2   | 1.57                     | 0.85              |
| 2:D:56:LYS:HD2   | 2:D:57:ASP:N     | 1.92                     | 0.84              |
| 2:D:42:ILE:HA    | 2:D:60:LYS:O     | 1.76                     | 0.84              |
| 1:C:207:ILE:HG13 | 1:C:208:ALA:H    | 1.38                     | 0.84              |
| 1:C:248:VAL:HG12 | 1:C:249:LEU:H    | 1.43                     | 0.84              |
| 1:C:109:GLU:HB3  | 5:C:419:HOH:O    | 1.77                     | 0.84              |
| 1:A:183:ARG:HH21 | 1:A:183:ARG:HG3  | 1.43                     | 0.83              |
| 1:C:104:MET:SD   | 1:C:112:ALA:HA   | 2.17                     | 0.83              |
| 1:A:51:ALA:O     | 1:A:52:SER:HB2   | 1.76                     | 0.83              |
| 1:A:54:ARG:HB2   | 3:A:1311:PCT:O3P | 1.79                     | 0.83              |
| 1:C:13:ASN:N     | 1:C:174:GLN:HE22 | 1.75                     | 0.83              |
| 2:D:82:THR:CA    | 2:D:96:ARG:HH12  | 1.92                     | 0.83              |
| 1:A:92:ILE:HG22  | 1:A:93:SER:N     | 1.94                     | 0.83              |
| 1:C:264:LEU:HB3  | 1:C:288:GLN:CD   | 1.99                     | 0.82              |
| 2:D:29:LEU:C     | 2:D:30:LEU:HD13  | 2.00                     | 0.82              |
| 2:D:138:CYS:SG   | 2:D:141:CYS:HB2  | 2.19                     | 0.82              |
| 2:B:70:GLN:H     | 2:B:70:GLN:NE2   | 1.77                     | 0.82              |
| 1:C:183:ARG:HE   | 1:C:208:ALA:HB1  | 1.44                     | 0.82              |
| 1:A:8:HIS:ND1    | 1:A:116:THR:HG22 | 1.95                     | 0.81              |
| 1:C:64:HIS:CD2   | 1:C:70:VAL:HG23  | 2.14                     | 0.81              |
| 1:C:109:GLU:OE1  | 1:C:132:ASN:HB2  | 1.81                     | 0.81              |
| 1:A:10:ILE:HG13  | 1:A:11:SER:N     | 1.95                     | 0.81              |
| 1:A:138:THR:HG23 | 1:A:172:LEU:HA   | 1.63                     | 0.81              |
| 2:B:137:LYS:HA   | 2:B:144:GLU:HA   | 1.63                     | 0.81              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:164:LYS:HB2  | 1:C:192:LEU:HA   | 1.62                     | 0.81              |
| 1:C:264:LEU:HD11 | 1:C:284:TRP:HB3  | 1.63                     | 0.81              |
| 2:D:104:ASP:O    | 2:D:106:VAL:HG23 | 1.82                     | 0.80              |
| 1:A:116:THR:HA   | 1:A:119:SER:OG   | 1.82                     | 0.80              |
| 2:B:70:GLN:H     | 2:B:70:GLN:HE21  | 1.29                     | 0.80              |
| 1:A:243:VAL:HG13 | 1:A:244:LYS:H    | 1.47                     | 0.80              |
| 1:C:91:THR:O     | 1:C:95:ILE:HG13  | 1.82                     | 0.79              |
| 2:D:20:HIS:HB3   | 2:D:80:GLN:CG    | 2.12                     | 0.79              |
| 1:C:142:LEU:HD23 | 1:C:145:ILE:CD1  | 2.12                     | 0.79              |
| 2:B:141:CYS:O    | 2:B:143:LYS:HG2  | 1.82                     | 0.79              |
| 1:C:96:SER:O     | 1:C:122:VAL:HG11 | 1.83                     | 0.79              |
| 2:D:146:SER:HB2  | 2:D:148:ASN:ND2  | 1.97                     | 0.79              |
| 1:C:218:VAL:O    | 1:C:222:VAL:HG13 | 1.82                     | 0.79              |
| 1:C:48:PHE:HZ    | 1:C:52:SER:H     | 1.30                     | 0.79              |
| 1:A:3:PRO:CD     | 1:A:22:LEU:HD21  | 2.13                     | 0.79              |
| 2:B:39:ASP:HA    | 2:D:55:ARG:HH22  | 1.47                     | 0.79              |
| 1:C:124:VAL:HG12 | 1:C:125:LEU:N    | 1.97                     | 0.78              |
| 1:C:225:LEU:HB2  | 1:C:261:MET:SD   | 2.24                     | 0.78              |
| 1:A:229:ARG:NH2  | 1:A:270:VAL:HG21 | 1.98                     | 0.78              |
| 2:D:126:ALA:O    | 2:D:127:VAL:HG13 | 1.83                     | 0.78              |
| 1:A:80:SER:O     | 1:A:84:LYS:HB2   | 1.82                     | 0.78              |
| 1:A:109:GLU:OE1  | 2:B:113:ASN:ND2  | 2.17                     | 0.78              |
| 1:C:108:GLN:NE2  | 2:D:115:ILE:HD12 | 1.99                     | 0.78              |
| 1:A:20:LEU:HD12  | 1:A:179:PHE:HZ   | 1.46                     | 0.78              |
| 1:C:132:ASN:OD1  | 2:D:143:LYS:NZ   | 2.16                     | 0.78              |
| 2:B:141:CYS:O    | 2:B:143:LYS:N    | 2.17                     | 0.77              |
| 1:C:105:ARG:HH11 | 1:C:167:ARG:HH12 | 1.29                     | 0.77              |
| 2:D:15:GLY:HA2   | 2:D:64:THR:O     | 1.85                     | 0.77              |
| 2:B:69:ASP:O     | 2:B:73:GLN:HG3   | 1.83                     | 0.77              |
| 1:C:183:ARG:HA   | 1:C:208:ALA:HB3  | 1.66                     | 0.77              |
| 2:B:30:LEU:HG    | 2:D:27:PHE:CZ    | 2.19                     | 0.77              |
| 2:D:96:ARG:HG3   | 2:D:97:PRO:HD2   | 1.65                     | 0.77              |
| 1:A:105:ARG:HB2  | 1:A:127:ALA:HB3  | 1.64                     | 0.77              |
| 1:A:287:GLN:HE21 | 1:A:287:GLN:N    | 1.82                     | 0.77              |
| 1:A:302:LEU:HD23 | 1:A:302:LEU:H    | 1.50                     | 0.77              |
| 1:A:81:LEU:HG    | 1:A:86:GLU:O     | 1.85                     | 0.77              |
| 1:C:171:SER:O    | 1:C:174:GLN:HG3  | 1.85                     | 0.77              |
| 2:B:44:ILE:HD11  | 2:B:46:LEU:HD23  | 1.65                     | 0.77              |
| 1:C:264:LEU:CD1  | 1:C:284:TRP:HB3  | 2.14                     | 0.77              |
| 1:C:160:VAL:HG12 | 1:C:161:GLY:H    | 1.50                     | 0.77              |
| 2:D:41:ARG:HB3   | 2:D:62:GLU:HB2   | 1.67                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:36:THR:HB    | 2:D:27:PHE:CD2   | 2.20                     | 0.77              |
| 1:C:264:LEU:HD12 | 1:C:288:GLN:CB   | 2.15                     | 0.77              |
| 1:A:38:LEU:HD23  | 1:A:38:LEU:O     | 1.84                     | 0.76              |
| 1:C:43:VAL:HG12  | 1:C:99:VAL:HG12  | 1.67                     | 0.76              |
| 1:A:61:THR:HG22  | 1:A:65:ARG:HD2   | 1.67                     | 0.76              |
| 2:B:30:LEU:HG    | 2:D:27:PHE:HZ    | 1.47                     | 0.76              |
| 1:C:56:ARG:HG2   | 1:C:56:ARG:NH2   | 1.99                     | 0.76              |
| 1:C:44:ILE:HG13  | 1:C:101:ALA:HB3  | 1.68                     | 0.76              |
| 1:C:56:ARG:HG2   | 1:C:56:ARG:HH21  | 1.50                     | 0.76              |
| 1:C:146:GLN:HA   | 1:C:150:GLY:HA2  | 1.68                     | 0.76              |
| 1:C:45:ALA:HB2   | 1:C:99:VAL:HG11  | 1.66                     | 0.76              |
| 1:A:156:HIS:ND1  | 1:A:156:HIS:N    | 2.31                     | 0.75              |
| 1:A:26:THR:HA    | 1:A:29:LYS:HE3   | 1.68                     | 0.75              |
| 1:A:109:GLU:HG3  | 1:A:132:ASN:HB2  | 1.67                     | 0.75              |
| 1:C:142:LEU:HD23 | 1:C:145:ILE:HD11 | 1.68                     | 0.75              |
| 2:D:24:GLN:NE2   | 2:D:47:ASN:HD21  | 1.85                     | 0.75              |
| 1:C:159:MET:CE   | 1:C:172:LEU:HD23 | 2.16                     | 0.75              |
| 1:A:43:VAL:HA    | 1:A:69:SER:O     | 1.85                     | 0.75              |
| 2:B:34:LYS:HB3   | 2:B:37:GLU:HB2   | 1.69                     | 0.75              |
| 5:B:204:HOH:O    | 2:D:39:ASP:HA    | 1.85                     | 0.75              |
| 2:D:62:GLU:HG2   | 2:D:63:ASN:ND2   | 2.02                     | 0.75              |
| 2:D:119:GLU:O    | 2:D:121:VAL:HG13 | 1.86                     | 0.75              |
| 1:A:166:GLY:HA2  | 1:A:231:GLN:NE2  | 2.01                     | 0.75              |
| 2:B:76:LEU:H     | 2:B:76:LEU:CD2   | 2.00                     | 0.75              |
| 1:A:2:ASN:CG     | 1:A:5:TYR:HB2    | 2.08                     | 0.74              |
| 1:A:81:LEU:O     | 1:A:81:LEU:HD23  | 1.86                     | 0.74              |
| 1:C:20:LEU:C     | 1:C:24:LEU:HG    | 2.07                     | 0.74              |
| 1:C:132:ASN:HA   | 1:C:170:HIS:ND1  | 2.01                     | 0.74              |
| 1:C:214:SER:HB2  | 1:C:216:GLU:HG3  | 1.69                     | 0.74              |
| 1:A:267:LEU:CD2  | 1:A:268:PRO:HA   | 2.16                     | 0.74              |
| 2:B:45:GLY:HA3   | 2:B:48:LEU:HD11  | 1.68                     | 0.74              |
| 2:B:75:ALA:CB    | 2:B:99:LEU:HD12  | 2.16                     | 0.74              |
| 1:C:149:GLN:HB2  | 5:C:326:HOH:O    | 1.87                     | 0.74              |
| 1:C:270:VAL:HG13 | 1:C:271:ASP:N    | 2.01                     | 0.74              |
| 1:A:48:PHE:CE2   | 1:A:55:THR:HG23  | 2.22                     | 0.74              |
| 1:C:245:ALA:HB2  | 1:C:272:GLU:OE1  | 1.87                     | 0.74              |
| 2:D:41:ARG:HB3   | 2:D:62:GLU:CB    | 2.17                     | 0.74              |
| 1:C:152:LEU:HD12 | 1:C:152:LEU:N    | 2.03                     | 0.74              |
| 2:B:42:ILE:HB    | 2:D:46:LEU:HD21  | 1.70                     | 0.74              |
| 1:C:228:THR:HA   | 1:C:266:PRO:CG   | 2.18                     | 0.74              |
| 1:A:231:GLN:HB3  | 1:A:234:ARG:HB2  | 1.69                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:174:GLN:O    | 1:C:178:LYS:HE2  | 1.87                     | 0.73              |
| 1:A:2:ASN:ND2    | 1:A:5:TYR:HB2    | 2.03                     | 0.73              |
| 1:A:59:PHE:HE2   | 1:A:300:LEU:HD21 | 1.54                     | 0.73              |
| 1:A:269:ARG:HH12 | 1:A:275:THR:HA   | 1.53                     | 0.73              |
| 1:C:146:GLN:HA   | 1:C:150:GLY:CA   | 2.18                     | 0.73              |
| 1:C:187:ILE:HD13 | 1:C:215:ILE:CD1  | 2.19                     | 0.73              |
| 1:C:296:ARG:C    | 1:C:300:LEU:HG   | 2.09                     | 0.73              |
| 2:D:148:ASN:O    | 2:D:152:ALA:HB2  | 1.87                     | 0.73              |
| 2:B:30:LEU:HD22  | 2:B:44:ILE:CD1   | 2.18                     | 0.73              |
| 2:D:138:CYS:HB3  | 2:D:143:LYS:H    | 1.53                     | 0.73              |
| 1:C:249:LEU:HG   | 1:C:254:LEU:CD1  | 2.17                     | 0.73              |
| 1:A:4:LEU:HD12   | 1:A:302:LEU:HD12 | 1.70                     | 0.72              |
| 1:A:141:ASP:O    | 1:A:145:ILE:HG12 | 1.88                     | 0.72              |
| 1:A:155:LEU:HD22 | 1:A:223:ASP:CG   | 2.10                     | 0.72              |
| 2:B:44:ILE:HG23  | 2:D:44:ILE:CB    | 2.16                     | 0.72              |
| 1:C:308:LEU:HD13 | 1:C:308:LEU:O    | 1.89                     | 0.72              |
| 1:A:237:PRO:HA   | 1:A:240:TYR:CD1  | 2.24                     | 0.72              |
| 1:C:287:GLN:H    | 1:C:287:GLN:NE2  | 1.86                     | 0.72              |
| 1:A:8:HIS:NE2    | 1:A:123:PRO:HA   | 2.03                     | 0.72              |
| 1:C:44:ILE:CG1   | 1:C:101:ALA:HB3  | 2.20                     | 0.72              |
| 1:C:151:ARG:HH11 | 1:C:155:LEU:CD1  | 2.03                     | 0.72              |
| 1:C:158:ALA:HA   | 1:C:185:TYR:O    | 1.89                     | 0.72              |
| 1:C:227:MET:O    | 1:C:266:PRO:HD3  | 1.89                     | 0.72              |
| 1:C:245:ALA:HB1  | 5:C:338:HOH:O    | 1.90                     | 0.72              |
| 1:C:310:LEU:N    | 1:C:310:LEU:HD12 | 2.05                     | 0.72              |
| 1:C:169:VAL:CA   | 1:C:172:LEU:HD13 | 2.20                     | 0.71              |
| 1:C:296:ARG:O    | 1:C:300:LEU:HG   | 1.90                     | 0.71              |
| 2:D:135:ALA:HB1  | 2:D:145:PHE:O    | 1.89                     | 0.71              |
| 1:C:226:TYR:CZ   | 1:C:266:PRO:HG3  | 2.24                     | 0.71              |
| 1:C:66:LEU:HD11  | 1:C:297:GLN:HA   | 1.73                     | 0.71              |
| 2:D:74:LEU:CG    | 2:D:97:PRO:HB3   | 2.18                     | 0.71              |
| 1:A:26:THR:HA    | 1:A:29:LYS:CE    | 2.21                     | 0.71              |
| 1:C:163:LEU:HG   | 1:C:188:ALA:HB2  | 1.71                     | 0.71              |
| 2:B:85:ARG:NH2   | 2:B:85:ARG:HB2   | 2.05                     | 0.71              |
| 2:D:29:LEU:O     | 2:D:30:LEU:HD13  | 1.90                     | 0.71              |
| 1:A:165:TYR:HE2  | 1:A:235:LEU:HD23 | 1.55                     | 0.71              |
| 1:C:285:TYR:HA   | 1:C:288:GLN:HB3  | 1.69                     | 0.71              |
| 1:C:105:ARG:NH1  | 1:C:167:ARG:HH12 | 1.89                     | 0.71              |
| 1:A:216:GLU:OE2  | 1:A:253:ASP:HA   | 1.89                     | 0.71              |
| 1:A:280:THR:HB   | 1:A:281:PRO:CD   | 2.21                     | 0.71              |
| 1:A:288:GLN:O    | 1:A:288:GLN:HG2  | 1.91                     | 0.71              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:99:LEU:CD1   | 2:D:129:LYS:HE3  | 2.21                     | 0.71              |
| 1:C:218:VAL:O    | 1:C:218:VAL:HG12 | 1.91                     | 0.70              |
| 1:C:164:LYS:HD3  | 1:C:191:ALA:O    | 1.91                     | 0.70              |
| 1:C:20:LEU:O     | 1:C:24:LEU:HG    | 1.91                     | 0.70              |
| 1:C:134:HIS:CE1  | 1:C:137:GLN:HB2  | 2.27                     | 0.70              |
| 1:C:139:LEU:CA   | 1:C:142:LEU:HD12 | 2.21                     | 0.70              |
| 1:C:160:VAL:HG12 | 1:C:161:GLY:N    | 2.05                     | 0.70              |
| 2:D:128:ARG:O    | 2:D:130:ARG:HG3  | 1.91                     | 0.70              |
| 1:A:229:ARG:HH21 | 1:A:270:VAL:CG2  | 2.01                     | 0.70              |
| 1:A:128:GLY:HA2  | 1:A:133:GLN:O    | 1.91                     | 0.70              |
| 1:A:164:LYS:HA   | 1:A:195:PRO:CD   | 2.20                     | 0.70              |
| 1:A:187:ILE:N    | 1:A:187:ILE:HD12 | 2.07                     | 0.70              |
| 1:A:230:VAL:O    | 1:A:232:LYS:N    | 2.24                     | 0.70              |
| 1:C:142:LEU:HA   | 1:C:145:ILE:CD1  | 2.22                     | 0.70              |
| 1:A:267:LEU:HD23 | 1:A:269:ARG:H    | 1.55                     | 0.69              |
| 1:A:287:GLN:NE2  | 1:A:287:GLN:H    | 1.90                     | 0.69              |
| 1:C:111:ALA:O    | 1:C:114:LEU:HB3  | 1.91                     | 0.69              |
| 1:C:195:PRO:O    | 1:C:199:LEU:HG   | 1.91                     | 0.69              |
| 1:C:30:LEU:HD12  | 1:C:298:ALA:HA   | 1.74                     | 0.69              |
| 1:C:222:VAL:HG21 | 1:C:225:LEU:HD13 | 1.75                     | 0.69              |
| 2:D:138:CYS:O    | 2:D:142:GLU:HA   | 1.93                     | 0.69              |
| 1:A:160:VAL:HG23 | 1:A:227:MET:SD   | 2.32                     | 0.69              |
| 2:B:46:LEU:O     | 2:D:42:ILE:HG13  | 1.93                     | 0.69              |
| 2:B:70:GLN:HA    | 2:B:73:GLN:OE1   | 1.93                     | 0.69              |
| 2:B:75:ALA:HB2   | 2:B:97:PRO:O     | 1.92                     | 0.69              |
| 1:C:133:GLN:O    | 1:C:167:ARG:HB2  | 1.92                     | 0.69              |
| 1:C:124:VAL:CG1  | 1:C:125:LEU:N    | 2.55                     | 0.69              |
| 1:A:2:ASN:HD22   | 1:A:306:ARG:CA   | 2.06                     | 0.69              |
| 1:C:50:GLU:OE2   | 1:C:107:PRO:HA   | 1.93                     | 0.69              |
| 1:A:9:ILE:HD13   | 1:A:125:LEU:HG   | 1.74                     | 0.69              |
| 1:C:11:SER:HA    | 1:C:133:GLN:OE1  | 1.92                     | 0.69              |
| 1:A:184:PHE:O    | 1:A:209:TRP:HA   | 1.93                     | 0.69              |
| 2:B:70:GLN:HE21  | 2:B:70:GLN:N     | 1.90                     | 0.69              |
| 2:D:12:ILE:HD13  | 2:D:12:ILE:H     | 1.58                     | 0.69              |
| 2:D:105:ASN:HA   | 2:D:123:SER:O    | 1.92                     | 0.69              |
| 1:C:169:VAL:HA   | 1:C:172:LEU:CD1  | 2.23                     | 0.68              |
| 1:C:228:THR:HA   | 1:C:266:PRO:CD   | 2.23                     | 0.68              |
| 1:C:248:VAL:HG12 | 1:C:249:LEU:N    | 2.07                     | 0.68              |
| 1:A:153:ASP:OD1  | 1:A:179:PHE:HB3  | 1.92                     | 0.68              |
| 1:C:112:ALA:C    | 1:C:114:LEU:H    | 1.97                     | 0.68              |
| 1:C:132:ASN:N    | 5:C:419:HOH:O    | 2.27                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:49:PHE:HB2   | 1:A:107:PRO:HD2  | 1.76                     | 0.68              |
| 1:C:124:VAL:CG1  | 1:C:125:LEU:H    | 2.06                     | 0.68              |
| 1:A:2:ASN:ND2    | 1:A:306:ARG:HA   | 2.09                     | 0.68              |
| 1:A:8:HIS:CE1    | 1:A:116:THR:HG22 | 2.29                     | 0.68              |
| 1:A:160:VAL:HG12 | 1:A:187:ILE:HD13 | 1.76                     | 0.68              |
| 1:A:202:LEU:HB3  | 1:A:207:ILE:HB   | 1.75                     | 0.68              |
| 1:A:255:HIS:CD2  | 1:A:255:HIS:H    | 2.11                     | 0.68              |
| 1:A:287:GLN:HE21 | 1:A:287:GLN:H    | 1.42                     | 0.68              |
| 1:C:9:ILE:HG21   | 1:C:125:LEU:HG   | 1.76                     | 0.68              |
| 1:A:47:CYS:HB3   | 1:A:73:PHE:CZ    | 2.29                     | 0.67              |
| 2:B:36:THR:HB    | 2:D:27:PHE:CE2   | 2.28                     | 0.67              |
| 2:B:41:ARG:HD3   | 2:D:48:LEU:HD13  | 1.76                     | 0.67              |
| 1:C:43:VAL:C     | 1:C:44:ILE:HD12  | 2.15                     | 0.67              |
| 1:C:159:MET:O    | 1:C:163:LEU:HD11 | 1.93                     | 0.67              |
| 1:C:295:ALA:O    | 1:C:297:GLN:N    | 2.27                     | 0.67              |
| 1:A:92:ILE:CG2   | 1:A:93:SER:N     | 2.58                     | 0.67              |
| 1:C:250:ARG:HB2  | 1:C:252:SER:OG   | 1.94                     | 0.67              |
| 1:A:45:ALA:HB1   | 1:A:47:CYS:SG    | 2.35                     | 0.67              |
| 1:C:42:LYS:HA    | 1:C:100:ASP:OD1  | 1.94                     | 0.67              |
| 1:C:262:LYS:HG3  | 1:C:282:HIS:HA   | 1.77                     | 0.67              |
| 1:C:269:ARG:HD3  | 1:C:273:ILE:H    | 1.57                     | 0.67              |
| 2:B:129:LYS:C    | 2:B:129:LYS:HE3  | 2.15                     | 0.67              |
| 2:D:66:LEU:HD22  | 2:D:83:VAL:HG21  | 1.77                     | 0.67              |
| 1:C:17:ARG:HG3   | 1:C:18:ASP:H     | 1.58                     | 0.67              |
| 1:C:266:PRO:O    | 1:C:267:LEU:HB2  | 1.94                     | 0.67              |
| 2:B:84:ASN:O     | 2:B:86:ILE:HG13  | 1.94                     | 0.67              |
| 1:C:102:ILE:HD13 | 1:C:102:ILE:N    | 2.09                     | 0.67              |
| 1:A:201:MET:HG2  | 1:A:205:LYS:HD2  | 1.77                     | 0.67              |
| 2:B:50:SER:HA    | 2:B:56:LYS:HE2   | 1.75                     | 0.67              |
| 1:C:160:VAL:HG12 | 5:C:338:HOH:O    | 1.95                     | 0.67              |
| 1:C:202:LEU:HA   | 1:C:205:LYS:NZ   | 2.10                     | 0.67              |
| 1:C:223:ASP:C    | 1:C:261:MET:HG2  | 2.16                     | 0.67              |
| 1:A:29:LYS:HB2   | 1:A:29:LYS:HZ2   | 1.60                     | 0.67              |
| 2:B:138:CYS:SG   | 5:B:221:HOH:O    | 2.53                     | 0.67              |
| 1:A:110:GLY:HA2  | 1:A:129:ASP:OD1  | 1.96                     | 0.66              |
| 2:B:69:ASP:HB3   | 2:B:70:GLN:HE21  | 1.59                     | 0.66              |
| 1:C:20:LEU:H     | 1:C:20:LEU:CD1   | 2.02                     | 0.66              |
| 1:C:29:LYS:HD3   | 1:C:310:LEU:HB2  | 1.77                     | 0.66              |
| 1:C:114:LEU:HD13 | 1:C:114:LEU:C    | 2.15                     | 0.66              |
| 2:B:62:GLU:C     | 2:B:64:THR:H     | 1.98                     | 0.66              |
| 1:C:112:ALA:O    | 1:C:114:LEU:N    | 2.28                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:30:LEU:HD22  | 2:B:44:ILE:HD13  | 1.78                     | 0.66              |
| 1:C:162:ASP:HB3  | 1:C:230:VAL:HA   | 1.76                     | 0.66              |
| 1:C:231:GLN:H    | 1:C:231:GLN:NE2  | 1.93                     | 0.66              |
| 2:D:34:LYS:HB3   | 2:D:37:GLU:OE1   | 1.95                     | 0.66              |
| 1:C:222:VAL:HG23 | 1:C:261:MET:HG3  | 1.77                     | 0.66              |
| 2:D:107:LEU:HD21 | 2:D:136:LEU:HD22 | 1.77                     | 0.66              |
| 1:A:2:ASN:N      | 1:A:306:ARG:O    | 2.26                     | 0.66              |
| 1:C:89:ALA:HB1   | 1:C:118:PHE:CG   | 2.30                     | 0.66              |
| 1:A:229:ARG:HH22 | 1:A:232:LYS:HE3  | 1.59                     | 0.66              |
| 2:D:132:ASN:ND2  | 2:D:133:ASP:H    | 1.93                     | 0.66              |
| 1:A:5:TYR:C      | 1:A:7:LYS:H      | 1.98                     | 0.66              |
| 1:A:138:THR:O    | 1:A:142:LEU:HG   | 1.96                     | 0.66              |
| 1:C:151:ARG:NH1  | 1:C:155:LEU:HD21 | 2.11                     | 0.66              |
| 1:A:99:VAL:HG23  | 1:A:101:ALA:H    | 1.61                     | 0.66              |
| 1:A:158:ALA:HB2  | 1:A:222:VAL:CG1  | 2.17                     | 0.66              |
| 2:B:17:VAL:HG13  | 2:B:59:ILE:O     | 1.95                     | 0.66              |
| 1:C:59:PHE:CD1   | 1:C:296:ARG:HD3  | 2.30                     | 0.65              |
| 1:C:88:LEU:O     | 1:C:92:ILE:HG12  | 1.95                     | 0.65              |
| 1:C:132:ASN:HA   | 1:C:170:HIS:CE1  | 2.30                     | 0.65              |
| 2:D:107:LEU:HD11 | 2:D:151:LEU:HD21 | 1.78                     | 0.65              |
| 1:C:38:LEU:HD12  | 1:C:39:LEU:CD1   | 2.26                     | 0.65              |
| 1:A:111:ALA:O    | 1:A:114:LEU:HB2  | 1.97                     | 0.65              |
| 1:A:308:LEU:HD23 | 1:A:309:VAL:O    | 1.96                     | 0.65              |
| 1:A:138:THR:OG1  | 1:A:171:SER:HB3  | 1.96                     | 0.65              |
| 1:A:284:TRP:CD1  | 1:A:287:GLN:HB2  | 2.31                     | 0.65              |
| 1:C:237:PRO:HG3  | 1:C:240:TYR:OH   | 1.96                     | 0.65              |
| 2:D:127:VAL:HG21 | 2:D:129:LYS:HZ2  | 1.61                     | 0.65              |
| 1:A:183:ARG:NH2  | 1:A:208:ALA:O    | 2.29                     | 0.65              |
| 1:A:293:ILE:O    | 1:A:297:GLN:HB2  | 1.97                     | 0.65              |
| 2:B:30:LEU:HD12  | 2:B:35:LEU:HB2   | 1.78                     | 0.65              |
| 1:C:100:ASP:O    | 1:C:122:VAL:HG13 | 1.96                     | 0.65              |
| 2:D:103:ILE:HB   | 2:D:125:PHE:N    | 2.07                     | 0.65              |
| 2:D:125:PHE:CE2  | 2:D:138:CYS:HA   | 2.32                     | 0.65              |
| 2:B:13:LYS:HG3   | 2:B:89:TYR:CE1   | 2.32                     | 0.64              |
| 1:A:26:THR:HA    | 1:A:29:LYS:NZ    | 2.12                     | 0.64              |
| 1:A:129:ASP:O    | 1:A:132:ASN:HB3  | 1.98                     | 0.64              |
| 2:B:41:ARG:HA    | 2:D:47:ASN:CB    | 2.27                     | 0.64              |
| 1:C:179:PHE:HD1  | 1:C:180:ASP:N    | 1.95                     | 0.64              |
| 1:C:205:LYS:H    | 1:C:205:LYS:HD2  | 1.62                     | 0.64              |
| 1:C:230:VAL:O    | 1:C:232:LYS:N    | 2.30                     | 0.64              |
| 1:C:263:VAL:HB   | 1:C:283:ALA:HA   | 1.79                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:59:PHE:CE1   | 1:C:296:ARG:NH2  | 2.65                     | 0.64              |
| 2:D:76:LEU:HB3   | 2:D:134:ILE:CG2  | 2.25                     | 0.64              |
| 2:D:13:LYS:HA    | 2:D:88:ASN:HA    | 1.78                     | 0.64              |
| 1:A:169:VAL:O    | 1:A:170:HIS:C    | 2.36                     | 0.64              |
| 1:C:162:ASP:OD2  | 1:C:165:TYR:HB2  | 1.98                     | 0.64              |
| 1:A:25:ALA:O     | 1:A:29:LYS:HG3   | 1.97                     | 0.64              |
| 1:A:269:ARG:NH1  | 1:A:275:THR:HA   | 2.12                     | 0.64              |
| 1:C:227:MET:SD   | 1:C:272:GLU:HB3  | 2.36                     | 0.64              |
| 2:D:114:CYS:O    | 2:D:116:SER:N    | 2.30                     | 0.64              |
| 2:D:86:ILE:HG23  | 2:D:90:GLU:C     | 2.17                     | 0.64              |
| 2:D:103:ILE:CB   | 2:D:125:PHE:H    | 2.04                     | 0.64              |
| 1:A:229:ARG:HH12 | 1:A:232:LYS:HG2  | 1.63                     | 0.64              |
| 1:A:40:LYS:O     | 1:A:42:LYS:N     | 2.31                     | 0.64              |
| 1:A:292:GLY:O    | 1:A:293:ILE:C    | 2.35                     | 0.64              |
| 1:C:48:PHE:HZ    | 1:C:52:SER:N     | 1.96                     | 0.64              |
| 1:C:144:THR:HA   | 1:C:147:GLU:HB2  | 1.80                     | 0.63              |
| 1:C:157:VAL:O    | 1:C:185:TYR:HB2  | 1.98                     | 0.63              |
| 1:A:134:HIS:HB2  | 1:A:167:ARG:HB2  | 1.80                     | 0.63              |
| 2:B:53:MET:SD    | 2:B:54:GLY:N     | 2.71                     | 0.63              |
| 1:C:11:SER:CB    | 1:C:133:GLN:HG3  | 2.27                     | 0.63              |
| 1:C:274:ALA:O    | 1:C:277:VAL:HG23 | 1.98                     | 0.63              |
| 2:D:135:ALA:HA   | 2:D:147:HIS:H    | 1.63                     | 0.63              |
| 2:B:68:GLU:HA    | 2:B:71:VAL:CG2   | 2.27                     | 0.63              |
| 1:C:171:SER:HA   | 1:C:174:GLN:HG2  | 1.80                     | 0.63              |
| 2:D:48:LEU:HB2   | 2:D:56:LYS:HZ2   | 1.61                     | 0.63              |
| 1:C:183:ARG:NE   | 1:C:208:ALA:HB1  | 2.13                     | 0.63              |
| 1:A:23:VAL:HA    | 1:A:302:LEU:HD11 | 1.81                     | 0.63              |
| 1:A:113:ARG:HH22 | 2:B:139:LYS:HB2  | 1.62                     | 0.63              |
| 1:A:125:LEU:N    | 1:A:125:LEU:CD1  | 2.60                     | 0.63              |
| 2:B:38:THR:HG23  | 2:B:42:ILE:HD11  | 1.81                     | 0.63              |
| 2:B:39:ASP:O     | 2:D:47:ASN:HB3   | 1.98                     | 0.63              |
| 2:B:86:ILE:HG12  | 2:B:91:VAL:HA    | 1.80                     | 0.63              |
| 1:C:5:TYR:HA     | 1:C:303:VAL:HA   | 1.81                     | 0.63              |
| 1:A:223:ASP:O    | 1:A:261:MET:HA   | 1.99                     | 0.62              |
| 2:D:46:LEU:H     | 2:D:46:LEU:CD2   | 2.09                     | 0.62              |
| 1:A:134:HIS:CE1  | 1:A:136:THR:OG1  | 2.52                     | 0.62              |
| 1:A:176:LEU:HD12 | 1:A:184:PHE:CZ   | 2.34                     | 0.62              |
| 2:B:34:LYS:C     | 2:B:36:THR:H     | 2.01                     | 0.62              |
| 2:B:39:ASP:CA    | 2:D:55:ARG:HH22  | 2.12                     | 0.62              |
| 2:D:56:LYS:HE2   | 2:D:58:LEU:HB3   | 1.81                     | 0.62              |
| 2:B:71:VAL:HG23  | 5:B:190:HOH:O    | 2.00                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:48:LEU:HB2   | 2:D:56:LYS:NZ    | 2.14                     | 0.62              |
| 2:D:72:ASP:HA    | 2:D:98:SER:O     | 2.00                     | 0.62              |
| 1:A:59:PHE:CE1   | 1:A:296:ARG:HG2  | 2.34                     | 0.62              |
| 1:A:235:LEU:HB3  | 1:A:240:TYR:CE2  | 2.35                     | 0.62              |
| 1:C:187:ILE:HD13 | 1:C:215:ILE:HD13 | 1.79                     | 0.62              |
| 2:D:44:ILE:HG22  | 2:D:45:GLY:H     | 1.63                     | 0.62              |
| 2:D:110:PRO:HD3  | 2:D:150:VAL:HG13 | 1.81                     | 0.62              |
| 2:D:128:ARG:NH1  | 2:D:130:ARG:HD2  | 2.15                     | 0.62              |
| 1:A:111:ALA:HA   | 2:B:115:ILE:HG21 | 1.81                     | 0.62              |
| 1:A:201:MET:CG   | 1:A:205:LYS:HD2  | 2.30                     | 0.62              |
| 1:A:205:LYS:C    | 1:A:207:ILE:H    | 2.03                     | 0.62              |
| 1:A:306:ARG:HG3  | 1:A:307:ASP:N    | 2.14                     | 0.62              |
| 2:B:104:ASP:O    | 2:B:106:VAL:HG22 | 1.98                     | 0.62              |
| 2:B:129:LYS:HZ1  | 2:B:131:ALA:N    | 1.98                     | 0.62              |
| 1:C:103:VAL:HA   | 1:C:125:LEU:O    | 1.99                     | 0.62              |
| 1:C:306:ARG:HG3  | 1:C:307:ASP:H    | 1.65                     | 0.62              |
| 1:C:306:ARG:NH2  | 1:C:306:ARG:HB3  | 2.14                     | 0.62              |
| 1:A:5:TYR:O      | 1:A:7:LYS:N      | 2.32                     | 0.62              |
| 1:A:40:LYS:HA    | 1:A:67:GLY:O     | 2.00                     | 0.62              |
| 1:A:161:GLY:O    | 1:A:163:LEU:HG   | 2.00                     | 0.62              |
| 1:C:105:ARG:NH1  | 1:C:167:ARG:NH1  | 2.48                     | 0.62              |
| 1:C:265:HIS:ND1  | 1:C:266:PRO:HD2  | 2.15                     | 0.62              |
| 1:C:23:VAL:HG11  | 1:C:299:LEU:HD12 | 1.81                     | 0.61              |
| 1:C:264:LEU:N    | 1:C:264:LEU:HD22 | 2.14                     | 0.61              |
| 1:A:186:PHE:O    | 1:A:211:LEU:HD23 | 1.99                     | 0.61              |
| 2:B:40:GLN:HB3   | 2:B:63:ASN:HD22  | 1.65                     | 0.61              |
| 1:A:77:ALA:O     | 1:A:79:THR:N     | 2.28                     | 0.61              |
| 2:B:20:HIS:NE2   | 2:B:52:GLU:CD    | 2.54                     | 0.61              |
| 1:C:65:ARG:NE    | 5:C:351:HOH:O    | 2.33                     | 0.61              |
| 2:D:137:LYS:HE3  | 2:D:142:GLU:OE2  | 1.99                     | 0.61              |
| 1:C:144:THR:HG21 | 1:C:288:GLN:HA   | 1.83                     | 0.61              |
| 1:C:306:ARG:CB   | 1:C:306:ARG:HH21 | 2.14                     | 0.61              |
| 2:D:73:GLN:O     | 2:D:77:TYR:HB2   | 2.00                     | 0.61              |
| 1:A:145:ILE:HG23 | 1:A:224:ILE:CD1  | 2.26                     | 0.61              |
| 1:C:149:GLN:CB   | 1:C:151:ARG:HH12 | 2.13                     | 0.61              |
| 1:C:284:TRP:HD1  | 1:C:288:GLN:HB2  | 1.64                     | 0.61              |
| 1:C:303:VAL:HG12 | 1:C:303:VAL:O    | 2.01                     | 0.61              |
| 2:D:81:ALA:O     | 2:D:97:PRO:HD3   | 2.01                     | 0.61              |
| 1:A:53:THR:O     | 1:A:57:LEU:HD12  | 1.99                     | 0.61              |
| 2:B:50:SER:OG    | 2:B:53:MET:HB3   | 2.00                     | 0.61              |
| 1:C:104:MET:HG3  | 1:C:126:ASN:HB2  | 1.81                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:99:LEU:HD22  | 2:D:99:LEU:O     | 2.01                     | 0.61              |
| 2:B:44:ILE:O     | 2:D:44:ILE:HG12  | 2.01                     | 0.61              |
| 1:C:9:ILE:HB     | 1:C:125:LEU:CA   | 2.27                     | 0.61              |
| 2:D:138:CYS:HB3  | 2:D:143:LYS:N    | 2.15                     | 0.61              |
| 1:A:138:THR:CG2  | 1:A:172:LEU:HA   | 2.31                     | 0.60              |
| 1:A:183:ARG:HG3  | 1:A:183:ARG:NH2  | 2.10                     | 0.60              |
| 1:A:284:TRP:HA   | 1:A:287:GLN:NE2  | 2.16                     | 0.60              |
| 1:C:176:LEU:C    | 1:C:178:LYS:H    | 2.05                     | 0.60              |
| 2:D:103:ILE:HD11 | 2:D:127:VAL:HG22 | 1.81                     | 0.60              |
| 1:A:267:LEU:HD21 | 1:A:269:ARG:HG2  | 1.82                     | 0.60              |
| 1:C:36:PRO:O     | 1:C:38:LEU:N     | 2.35                     | 0.60              |
| 1:C:56:ARG:HH21  | 1:C:56:ARG:C     | 2.04                     | 0.60              |
| 1:C:269:ARG:NE   | 1:C:273:ILE:HB   | 2.15                     | 0.60              |
| 1:A:245:ALA:HB2  | 1:A:271:ASP:OD2  | 2.00                     | 0.60              |
| 1:C:125:LEU:O    | 1:C:125:LEU:HD23 | 2.01                     | 0.60              |
| 1:A:138:THR:HG23 | 1:A:172:LEU:CD1  | 2.31                     | 0.60              |
| 1:A:291:ASN:HB2  | 5:A:1344:HOH:O   | 2.00                     | 0.60              |
| 2:B:105:ASN:C    | 2:B:106:VAL:HG22 | 2.20                     | 0.60              |
| 1:C:54:ARG:NH2   | 1:C:267:LEU:HD12 | 2.17                     | 0.60              |
| 1:C:162:ASP:OD1  | 1:C:192:LEU:HD22 | 2.01                     | 0.60              |
| 1:C:215:ILE:CG2  | 1:C:219:MET:HE2  | 2.31                     | 0.60              |
| 1:A:39:LEU:HD13  | 1:A:304:LEU:HD12 | 1.83                     | 0.60              |
| 1:A:49:PHE:CB    | 1:A:107:PRO:HD2  | 2.31                     | 0.60              |
| 2:B:27:PHE:HB2   | 2:D:36:THR:HG21  | 1.82                     | 0.60              |
| 1:C:219:MET:HB3  | 1:C:256:ASN:CG   | 2.20                     | 0.60              |
| 1:C:17:ARG:HG3   | 1:C:18:ASP:N     | 2.16                     | 0.60              |
| 1:C:140:LEU:HD12 | 1:C:140:LEU:C    | 2.21                     | 0.60              |
| 2:D:28:LYS:HE2   | 2:D:32:LEU:HB2   | 1.82                     | 0.60              |
| 1:A:4:LEU:O      | 1:A:7:LYS:HB2    | 2.00                     | 0.60              |
| 1:A:160:VAL:HG12 | 1:A:187:ILE:CB   | 2.31                     | 0.60              |
| 1:C:38:LEU:HD12  | 1:C:39:LEU:HG    | 1.83                     | 0.60              |
| 1:C:162:ASP:CB   | 1:C:230:VAL:HA   | 2.31                     | 0.60              |
| 2:D:149:VAL:HA   | 2:D:152:ALA:HB3  | 1.83                     | 0.60              |
| 1:C:189:PRO:HG3  | 1:C:246:GLN:OE1  | 2.02                     | 0.60              |
| 1:C:199:LEU:O    | 1:C:202:LEU:HG   | 2.01                     | 0.60              |
| 2:D:83:VAL:O     | 2:D:94:LYS:HA    | 2.01                     | 0.60              |
| 1:A:267:LEU:HD23 | 1:A:269:ARG:N    | 2.16                     | 0.60              |
| 2:B:22:PRO:O     | 2:B:25:ILE:HB    | 2.02                     | 0.60              |
| 2:B:42:ILE:HB    | 2:D:46:LEU:CD2   | 2.31                     | 0.60              |
| 2:B:105:ASN:OD1  | 2:B:105:ASN:O    | 2.18                     | 0.60              |
| 2:B:105:ASN:O    | 2:B:106:VAL:HG13 | 2.01                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:183:ARG:NH2  | 1:C:184:PHE:O    | 2.34                     | 0.60              |
| 1:C:214:SER:HB2  | 1:C:216:GLU:OE2  | 2.02                     | 0.60              |
| 1:C:270:VAL:CG1  | 1:C:271:ASP:H    | 2.04                     | 0.60              |
| 2:D:30:LEU:N     | 2:D:30:LEU:HD22  | 2.16                     | 0.60              |
| 1:A:119:SER:OG   | 1:A:120:GLY:N    | 2.35                     | 0.59              |
| 2:B:21:ILE:CD1   | 2:B:59:ILE:HG12  | 2.32                     | 0.59              |
| 1:C:13:ASN:N     | 1:C:174:GLN:NE2  | 2.48                     | 0.59              |
| 1:A:176:LEU:HD12 | 1:A:184:PHE:HZ   | 1.68                     | 0.59              |
| 1:C:195:PRO:HG2  | 1:C:198:ILE:HG12 | 1.82                     | 0.59              |
| 2:D:138:CYS:SG   | 2:D:141:CYS:N    | 2.75                     | 0.59              |
| 1:A:166:GLY:HA2  | 1:A:231:GLN:HE22 | 1.66                     | 0.59              |
| 1:C:30:LEU:CD1   | 1:C:298:ALA:HA   | 2.33                     | 0.59              |
| 1:C:228:THR:CA   | 1:C:266:PRO:HG2  | 2.30                     | 0.59              |
| 1:A:172:LEU:O    | 1:A:176:LEU:HG   | 2.02                     | 0.59              |
| 1:A:172:LEU:O    | 1:A:175:ALA:HB3  | 2.03                     | 0.59              |
| 2:B:21:ILE:HB    | 2:B:57:ASP:CB    | 2.30                     | 0.59              |
| 1:C:214:SER:HB2  | 1:C:216:GLU:CG   | 2.31                     | 0.59              |
| 1:A:48:PHE:CE2   | 1:A:56:ARG:HB2   | 2.36                     | 0.59              |
| 1:A:306:ARG:HG3  | 1:A:307:ASP:H    | 1.66                     | 0.59              |
| 1:C:45:ALA:HB1   | 1:C:72:GLY:H     | 1.68                     | 0.59              |
| 2:D:125:PHE:CD2  | 2:D:138:CYS:HA   | 2.38                     | 0.59              |
| 1:A:55:THR:HG21  | 1:A:105:ARG:HH11 | 1.68                     | 0.59              |
| 1:C:56:ARG:HH21  | 1:C:56:ARG:CG    | 2.16                     | 0.59              |
| 1:A:44:ILE:CG2   | 1:A:103:VAL:HG23 | 2.33                     | 0.59              |
| 1:A:229:ARG:HG3  | 1:A:270:VAL:HG23 | 1.85                     | 0.59              |
| 2:B:16:THR:HG22  | 2:B:17:VAL:N     | 2.18                     | 0.59              |
| 1:C:89:ALA:HA    | 5:C:329:HOH:O    | 2.02                     | 0.59              |
| 1:C:92:ILE:HA    | 1:C:95:ILE:HB    | 1.85                     | 0.59              |
| 1:C:220:ALA:N    | 1:C:256:ASN:ND2  | 2.50                     | 0.59              |
| 2:D:99:LEU:HD13  | 2:D:129:LYS:HE3  | 1.85                     | 0.59              |
| 1:A:23:VAL:HG22  | 1:A:302:LEU:CD1  | 2.33                     | 0.59              |
| 1:C:141:ASP:O    | 1:C:144:THR:N    | 2.36                     | 0.59              |
| 1:C:142:LEU:HA   | 1:C:145:ILE:HG13 | 1.85                     | 0.59              |
| 1:C:269:ARG:HD2  | 1:C:270:VAL:N    | 2.18                     | 0.59              |
| 1:A:140:LEU:HD13 | 1:A:288:GLN:O    | 2.03                     | 0.59              |
| 1:A:235:LEU:CB   | 1:A:240:TYR:HE2  | 2.16                     | 0.58              |
| 2:D:75:ALA:HA    | 2:D:97:PRO:HB2   | 1.85                     | 0.58              |
| 1:A:29:LYS:HB2   | 1:A:29:LYS:NZ    | 2.18                     | 0.58              |
| 1:A:49:PHE:HB2   | 1:A:106:HIS:HA   | 1.84                     | 0.58              |
| 2:B:30:LEU:HD22  | 2:B:44:ILE:HD12  | 1.84                     | 0.58              |
| 1:C:131:SER:N    | 5:C:419:HOH:O    | 2.36                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:136:THR:HB   | 1:C:296:ARG:NH2  | 2.18                     | 0.58              |
| 1:A:30:LEU:C     | 1:A:32:ALA:N     | 2.56                     | 0.58              |
| 1:A:264:LEU:HD22 | 1:A:288:GLN:HG3  | 1.86                     | 0.58              |
| 1:A:284:TRP:O    | 1:A:288:GLN:N    | 2.33                     | 0.58              |
| 1:C:215:ILE:HG22 | 1:C:219:MET:HE2  | 1.84                     | 0.58              |
| 2:D:84:ASN:ND2   | 2:D:91:VAL:HG11  | 2.17                     | 0.58              |
| 1:A:146:GLN:HE21 | 1:A:152:LEU:CB   | 2.16                     | 0.58              |
| 2:B:44:ILE:O     | 2:D:44:ILE:N     | 2.36                     | 0.58              |
| 2:B:62:GLU:HG2   | 2:B:63:ASN:N     | 2.18                     | 0.58              |
| 1:A:164:LYS:CA   | 1:A:195:PRO:HD3  | 2.26                     | 0.58              |
| 2:D:115:ILE:C    | 2:D:117:HIS:H    | 2.07                     | 0.58              |
| 1:C:144:THR:CG2  | 1:C:288:GLN:HA   | 2.34                     | 0.58              |
| 1:C:282:HIS:O    | 1:C:284:TRP:N    | 2.37                     | 0.58              |
| 2:B:102:ARG:HA   | 2:B:127:VAL:HG23 | 1.85                     | 0.58              |
| 1:C:113:ARG:HA   | 1:C:116:THR:OG1  | 2.04                     | 0.58              |
| 2:D:66:LEU:HD13  | 2:D:83:VAL:HG21  | 1.84                     | 0.58              |
| 2:D:111:ASN:ND2  | 2:D:114:CYS:N    | 2.49                     | 0.58              |
| 2:B:69:ASP:HB3   | 2:B:70:GLN:NE2   | 2.19                     | 0.58              |
| 1:C:121:ASN:H    | 1:C:121:ASN:ND2  | 1.94                     | 0.58              |
| 1:C:179:PHE:CD1  | 1:C:180:ASP:N    | 2.72                     | 0.58              |
| 1:A:124:VAL:C    | 1:A:125:LEU:HD12 | 2.24                     | 0.58              |
| 2:D:12:ILE:HG23  | 2:D:41:ARG:NH2   | 2.19                     | 0.58              |
| 2:B:18:ILE:HB    | 2:B:21:ILE:HD11  | 1.85                     | 0.57              |
| 1:A:2:ASN:HD22   | 1:A:306:ARG:C    | 2.08                     | 0.57              |
| 1:C:134:HIS:HB2  | 1:C:167:ARG:O    | 2.04                     | 0.57              |
| 1:C:152:LEU:HB2  | 1:C:179:PHE:CZ   | 2.39                     | 0.57              |
| 2:D:126:ALA:HB3  | 2:D:137:LYS:O    | 2.04                     | 0.57              |
| 1:A:296:ARG:O    | 1:A:300:LEU:HG   | 2.03                     | 0.57              |
| 1:A:308:LEU:HD23 | 1:A:309:VAL:N    | 2.19                     | 0.57              |
| 1:C:184:PHE:HB2  | 1:C:209:TRP:HA   | 1.87                     | 0.57              |
| 2:B:50:SER:HB3   | 2:B:53:MET:C     | 2.25                     | 0.57              |
| 1:C:151:ARG:HH11 | 1:C:155:LEU:CG   | 2.16                     | 0.57              |
| 1:C:237:PRO:CA   | 1:C:240:TYR:CZ   | 2.85                     | 0.57              |
| 1:A:177:ALA:HB2  | 1:A:202:LEU:HD23 | 1.86                     | 0.57              |
| 1:C:4:LEU:HB3    | 1:C:22:LEU:CD2   | 2.35                     | 0.57              |
| 1:C:23:VAL:HG12  | 1:C:302:LEU:HD12 | 1.85                     | 0.57              |
| 1:C:112:ALA:C    | 1:C:114:LEU:N    | 2.57                     | 0.57              |
| 1:C:188:ALA:O    | 1:C:193:ALA:HB2  | 2.04                     | 0.57              |
| 2:B:62:GLU:HG2   | 2:B:63:ASN:H     | 1.69                     | 0.57              |
| 1:C:66:LEU:HD11  | 1:C:297:GLN:CA   | 2.34                     | 0.57              |
| 1:C:207:ILE:HG13 | 1:C:208:ALA:N    | 2.16                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:16:THR:HG22  | 2:D:65:PHE:HA    | 1.86                     | 0.57              |
| 2:D:143:LYS:HB2  | 2:D:145:PHE:CE1  | 2.39                     | 0.57              |
| 1:A:26:THR:HG21  | 1:A:302:LEU:HD21 | 1.85                     | 0.57              |
| 1:A:204:GLU:C    | 1:A:206:GLY:H    | 2.08                     | 0.57              |
| 1:A:288:GLN:C    | 5:A:1344:HOH:O   | 2.43                     | 0.57              |
| 1:C:89:ALA:HB1   | 1:C:118:PHE:CD2  | 2.40                     | 0.57              |
| 1:C:115:ALA:HA   | 5:C:329:HOH:O    | 2.05                     | 0.57              |
| 1:C:171:SER:HA   | 1:C:174:GLN:CG   | 2.35                     | 0.57              |
| 1:C:237:PRO:O    | 1:C:239:GLU:N    | 2.38                     | 0.57              |
| 2:D:103:ILE:HD11 | 2:D:127:VAL:HG13 | 1.85                     | 0.57              |
| 2:D:114:CYS:C    | 2:D:116:SER:H    | 2.08                     | 0.57              |
| 1:A:189:PRO:HB3  | 1:A:242:ASN:ND2  | 2.18                     | 0.57              |
| 1:C:44:ILE:CD1   | 1:C:101:ALA:HB3  | 2.34                     | 0.57              |
| 1:A:163:LEU:HD13 | 1:A:194:MET:HB2  | 1.87                     | 0.56              |
| 1:A:183:ARG:NE   | 1:A:208:ALA:HB3  | 2.20                     | 0.56              |
| 1:C:114:LEU:HD13 | 5:C:329:HOH:O    | 2.05                     | 0.56              |
| 1:C:254:LEU:O    | 1:C:256:ASN:N    | 2.35                     | 0.56              |
| 2:D:128:ARG:HH12 | 2:D:130:ARG:CZ   | 2.19                     | 0.56              |
| 1:C:149:GLN:HB3  | 1:C:151:ARG:HH12 | 1.69                     | 0.56              |
| 1:A:3:PRO:CG     | 1:A:22:LEU:HD21  | 2.35                     | 0.56              |
| 1:A:55:THR:HG21  | 1:A:105:ARG:HE   | 1.70                     | 0.56              |
| 1:A:138:THR:HG23 | 1:A:172:LEU:HD13 | 1.88                     | 0.56              |
| 1:A:160:VAL:CG1  | 1:A:187:ILE:HB   | 2.30                     | 0.56              |
| 2:B:52:GLU:CD    | 2:B:52:GLU:H     | 2.09                     | 0.56              |
| 2:B:128:ARG:O    | 2:B:134:ILE:HG22 | 2.04                     | 0.56              |
| 1:C:127:ALA:HA   | 1:C:135:PRO:HD2  | 1.86                     | 0.56              |
| 1:C:180:ASP:O    | 1:C:182:ASN:OD1  | 2.24                     | 0.56              |
| 1:A:285:TYR:HA   | 1:A:288:GLN:OE1  | 2.06                     | 0.56              |
| 1:C:3:PRO:O      | 1:C:7:LYS:HD3    | 2.05                     | 0.56              |
| 1:C:29:LYS:CD    | 1:C:310:LEU:HB2  | 2.36                     | 0.56              |
| 1:C:67:GLY:O     | 1:C:68:ALA:HB2   | 2.05                     | 0.56              |
| 1:C:237:PRO:C    | 1:C:239:GLU:H    | 2.09                     | 0.56              |
| 2:D:125:PHE:CD1  | 2:D:136:LEU:HD13 | 2.40                     | 0.56              |
| 1:A:248:VAL:HG13 | 1:A:271:ASP:O    | 2.05                     | 0.56              |
| 1:C:75:ASP:C     | 1:C:77:ALA:H     | 2.09                     | 0.56              |
| 1:C:103:VAL:HG13 | 1:C:125:LEU:CD2  | 2.35                     | 0.56              |
| 1:C:155:LEU:HD13 | 1:C:224:ILE:HD11 | 1.87                     | 0.56              |
| 1:A:165:TYR:HB3  | 1:A:231:GLN:HG2  | 1.86                     | 0.56              |
| 2:B:30:LEU:HD12  | 2:B:35:LEU:CB    | 2.35                     | 0.56              |
| 1:C:131:SER:O    | 1:C:170:HIS:CE1  | 2.58                     | 0.56              |
| 1:A:5:TYR:C      | 1:A:7:LYS:N      | 2.58                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:9:ILE:CG2    | 1:C:125:LEU:HG   | 2.35                     | 0.56              |
| 1:C:207:ILE:HG23 | 1:C:208:ALA:N    | 2.20                     | 0.56              |
| 2:B:12:ILE:HG12  | 2:B:13:LYS:N     | 2.20                     | 0.56              |
| 2:B:38:THR:CG2   | 2:B:42:ILE:HD11  | 2.34                     | 0.56              |
| 1:C:60:GLU:CA    | 1:C:63:MET:SD    | 2.90                     | 0.56              |
| 1:C:104:MET:HG3  | 1:C:126:ASN:CB   | 2.35                     | 0.56              |
| 1:C:171:SER:C    | 1:C:174:GLN:HG3  | 2.25                     | 0.56              |
| 2:D:96:ARG:NH2   | 2:D:97:PRO:HD2   | 2.21                     | 0.56              |
| 2:D:137:LYS:HD2  | 2:D:142:GLU:O    | 2.06                     | 0.56              |
| 1:A:94:VAL:HG23  | 1:A:95:ILE:N     | 2.19                     | 0.56              |
| 1:C:44:ILE:HD11  | 1:C:101:ALA:HB3  | 1.88                     | 0.56              |
| 1:C:104:MET:CE   | 1:C:112:ALA:HA   | 2.36                     | 0.56              |
| 1:C:113:ARG:O    | 1:C:117:GLU:HG3  | 2.06                     | 0.56              |
| 2:D:24:GLN:NE2   | 2:D:47:ASN:ND2   | 2.54                     | 0.56              |
| 1:A:2:ASN:HD22   | 1:A:306:ARG:HA   | 1.67                     | 0.56              |
| 1:A:78:ASN:HD22  | 1:A:78:ASN:N     | 2.04                     | 0.56              |
| 1:A:113:ARG:HG2  | 1:A:113:ARG:HH21 | 1.70                     | 0.56              |
| 1:A:287:GLN:N    | 1:A:287:GLN:NE2  | 2.50                     | 0.55              |
| 1:C:135:PRO:HG2  | 1:C:136:THR:H    | 1.70                     | 0.55              |
| 1:C:273:ILE:HG21 | 1:C:285:TYR:OH   | 2.06                     | 0.55              |
| 2:D:138:CYS:HB3  | 2:D:142:GLU:N    | 2.21                     | 0.55              |
| 1:A:5:TYR:CE1    | 1:A:306:ARG:HB3  | 2.41                     | 0.55              |
| 1:A:54:ARG:HH12  | 1:A:268:PRO:HB3  | 1.71                     | 0.55              |
| 1:A:146:GLN:HE21 | 1:A:152:LEU:HG   | 1.70                     | 0.55              |
| 1:A:196:GLN:C    | 1:A:198:ILE:H    | 2.09                     | 0.55              |
| 1:C:253:ASP:OD1  | 1:C:254:LEU:HD12 | 2.05                     | 0.55              |
| 1:A:20:LEU:HD12  | 1:A:179:PHE:CZ   | 2.36                     | 0.55              |
| 2:B:50:SER:HB3   | 2:B:53:MET:O     | 2.06                     | 0.55              |
| 1:C:228:THR:HA   | 1:C:266:PRO:HD2  | 1.88                     | 0.55              |
| 2:D:126:ALA:HB3  | 2:D:137:LYS:HB3  | 1.88                     | 0.55              |
| 1:C:104:MET:CG   | 1:C:126:ASN:HB2  | 2.35                     | 0.55              |
| 1:C:178:LYS:HZ3  | 1:C:201:MET:CE   | 2.20                     | 0.55              |
| 2:D:15:GLY:HA3   | 2:D:61:ILE:O     | 2.05                     | 0.55              |
| 2:D:137:LYS:HD2  | 2:D:142:GLU:HG3  | 1.87                     | 0.55              |
| 2:D:84:ASN:O     | 2:D:86:ILE:HD12  | 2.06                     | 0.55              |
| 1:A:166:GLY:O    | 1:A:167:ARG:C    | 2.45                     | 0.55              |
| 1:C:46:SER:O     | 1:C:72:GLY:HA3   | 2.07                     | 0.55              |
| 1:C:219:MET:CB   | 1:C:256:ASN:HD21 | 2.09                     | 0.55              |
| 1:C:30:LEU:HD12  | 1:C:298:ALA:CA   | 2.36                     | 0.55              |
| 1:C:192:LEU:C    | 1:C:194:MET:H    | 2.11                     | 0.55              |
| 1:C:226:TYR:OH   | 1:C:266:PRO:HG3  | 2.06                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:67:SER:O     | 2:D:71:VAL:HG23  | 2.07                     | 0.55              |
| 1:A:59:PHE:O     | 1:A:63:MET:HE2   | 2.06                     | 0.55              |
| 2:B:41:ARG:HB2   | 2:D:47:ASN:O     | 2.07                     | 0.55              |
| 2:B:137:LYS:HA   | 2:B:143:LYS:O    | 2.07                     | 0.55              |
| 1:C:9:ILE:HG22   | 1:C:135:PRO:HG3  | 1.89                     | 0.55              |
| 1:C:11:SER:HB2   | 1:C:133:GLN:HG3  | 1.88                     | 0.55              |
| 1:C:129:ASP:O    | 5:C:419:HOH:O    | 2.18                     | 0.55              |
| 1:C:141:ASP:C    | 1:C:143:PHE:N    | 2.59                     | 0.55              |
| 1:C:306:ARG:CG   | 1:C:307:ASP:H    | 2.19                     | 0.55              |
| 2:D:59:ILE:N     | 2:D:59:ILE:HD12  | 2.22                     | 0.55              |
| 2:D:103:ILE:HD11 | 2:D:127:VAL:CG2  | 2.37                     | 0.55              |
| 2:D:105:ASN:O    | 2:D:106:VAL:HG22 | 2.07                     | 0.55              |
| 2:B:31:SER:HA    | 2:D:27:PHE:HE1   | 1.72                     | 0.55              |
| 1:C:280:THR:C    | 1:C:282:HIS:H    | 2.11                     | 0.55              |
| 2:D:124:SER:HB2  | 2:D:139:LYS:HD3  | 1.89                     | 0.55              |
| 2:D:127:VAL:CG2  | 2:D:129:LYS:HZ2  | 2.19                     | 0.55              |
| 1:A:146:GLN:NE2  | 1:A:152:LEU:HG   | 2.22                     | 0.54              |
| 1:A:208:ALA:HA   | 5:A:1437:HOH:O   | 2.06                     | 0.54              |
| 2:B:9:VAL:HG13   | 2:B:43:THR:HG21  | 1.88                     | 0.54              |
| 1:A:235:LEU:HB3  | 1:A:240:TYR:HE2  | 1.72                     | 0.54              |
| 1:C:142:LEU:HD23 | 1:C:145:ILE:HD12 | 1.88                     | 0.54              |
| 1:C:148:THR:HB   | 5:C:331:HOH:O    | 2.08                     | 0.54              |
| 1:C:151:ARG:HB3  | 1:C:151:ARG:NH2  | 2.22                     | 0.54              |
| 1:C:152:LEU:H    | 1:C:152:LEU:CD1  | 2.14                     | 0.54              |
| 1:C:237:PRO:HA   | 1:C:240:TYR:CD2  | 2.41                     | 0.54              |
| 2:D:108:VAL:HG23 | 2:D:150:VAL:O    | 2.07                     | 0.54              |
| 1:A:10:ILE:HG13  | 1:A:11:SER:H     | 1.72                     | 0.54              |
| 1:A:92:ILE:HG22  | 1:A:93:SER:H     | 1.67                     | 0.54              |
| 1:A:155:LEU:HD22 | 1:A:223:ASP:OD2  | 2.06                     | 0.54              |
| 1:A:168:THR:OG1  | 1:A:169:VAL:N    | 2.40                     | 0.54              |
| 2:B:85:ARG:HB2   | 2:B:85:ARG:HH21  | 1.71                     | 0.54              |
| 1:C:26:THR:HA    | 1:C:29:LYS:HG2   | 1.88                     | 0.54              |
| 1:C:131:SER:HA   | 1:C:167:ARG:HB3  | 1.88                     | 0.54              |
| 1:C:160:VAL:CG1  | 1:C:161:GLY:H    | 2.20                     | 0.54              |
| 1:C:269:ARG:CD   | 1:C:273:ILE:HB   | 2.37                     | 0.54              |
| 2:D:30:LEU:O     | 2:D:34:LYS:HA    | 2.07                     | 0.54              |
| 2:D:122:SER:HB3  | 5:D:170:HOH:O    | 2.07                     | 0.54              |
| 1:A:8:HIS:ND1    | 1:A:116:THR:CG2  | 2.67                     | 0.54              |
| 1:C:103:VAL:HG13 | 1:C:125:LEU:O    | 2.05                     | 0.54              |
| 1:C:20:LEU:HD12  | 1:C:20:LEU:N     | 2.08                     | 0.54              |
| 1:C:167:ARG:NH1  | 1:C:234:ARG:HH12 | 2.06                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:13:LYS:CA    | 2:D:88:ASN:HA    | 2.37                     | 0.54              |
| 2:D:74:LEU:HD11  | 2:D:81:ALA:HB1   | 1.90                     | 0.54              |
| 1:A:59:PHE:HD2   | 1:A:63:MET:HE2   | 1.71                     | 0.54              |
| 2:D:46:LEU:HD23  | 2:D:46:LEU:N     | 2.11                     | 0.54              |
| 2:D:127:VAL:HG12 | 2:D:136:LEU:HB3  | 1.88                     | 0.54              |
| 1:A:47:CYS:HB3   | 1:A:73:PHE:CE2   | 2.42                     | 0.54              |
| 2:B:62:GLU:O     | 2:B:64:THR:N     | 2.40                     | 0.54              |
| 1:A:177:ALA:HB2  | 1:A:202:LEU:CD2  | 2.38                     | 0.54              |
| 2:B:13:LYS:O     | 2:B:88:ASN:N     | 2.41                     | 0.54              |
| 1:C:103:VAL:HG13 | 1:C:125:LEU:HD23 | 1.89                     | 0.54              |
| 1:C:153:ASP:CG   | 1:C:179:PHE:HE1  | 2.11                     | 0.54              |
| 2:D:44:ILE:N     | 2:D:44:ILE:HD13  | 2.23                     | 0.54              |
| 2:D:99:LEU:HD11  | 2:D:129:LYS:HE3  | 1.89                     | 0.54              |
| 2:D:125:PHE:CE1  | 2:D:136:LEU:HD13 | 2.43                     | 0.54              |
| 1:A:129:ASP:CG   | 1:A:132:ASN:HD22 | 2.11                     | 0.54              |
| 1:A:139:LEU:O    | 1:A:142:LEU:HB2  | 2.07                     | 0.54              |
| 1:A:174:GLN:HG2  | 1:A:198:ILE:HG23 | 1.90                     | 0.54              |
| 1:A:177:ALA:CB   | 1:A:202:LEU:HD23 | 2.37                     | 0.54              |
| 2:B:9:VAL:HG13   | 2:B:43:THR:CG2   | 2.38                     | 0.54              |
| 2:B:27:PHE:HE1   | 2:D:34:LYS:HZ2   | 1.55                     | 0.54              |
| 1:C:81:LEU:HA    | 1:C:86:GLU:HB2   | 1.90                     | 0.54              |
| 1:C:105:ARG:NH1  | 1:C:167:ARG:HH22 | 2.06                     | 0.54              |
| 2:D:103:ILE:HG21 | 2:D:125:PHE:HB2  | 1.89                     | 0.54              |
| 2:B:47:ASN:HB2   | 2:D:42:ILE:HD11  | 1.88                     | 0.54              |
| 1:C:82:GLY:O     | 1:C:83:LYS:C     | 2.47                     | 0.54              |
| 1:C:153:ASP:HA   | 1:C:179:PHE:CE1  | 2.43                     | 0.54              |
| 2:D:87:ASP:O     | 2:D:88:ASN:HB3   | 2.07                     | 0.54              |
| 2:D:111:ASN:ND2  | 2:D:114:CYS:CB   | 2.63                     | 0.54              |
| 1:A:109:GLU:O    | 2:B:115:ILE:HG22 | 2.08                     | 0.53              |
| 1:A:280:THR:HB   | 1:A:281:PRO:HD2  | 1.89                     | 0.53              |
| 1:C:96:SER:HB2   | 1:C:122:VAL:HB   | 1.90                     | 0.53              |
| 2:D:99:LEU:HD22  | 2:D:129:LYS:NZ   | 2.22                     | 0.53              |
| 2:B:129:LYS:NZ   | 2:B:130:ARG:N    | 2.57                     | 0.53              |
| 1:C:265:HIS:N    | 1:C:288:GLN:OE1  | 2.39                     | 0.53              |
| 1:A:10:ILE:CG1   | 1:A:11:SER:N     | 2.68                     | 0.53              |
| 1:A:165:TYR:C    | 1:A:231:GLN:HE21 | 2.11                     | 0.53              |
| 1:A:225:LEU:HD12 | 1:A:226:TYR:N    | 2.23                     | 0.53              |
| 2:B:38:THR:HG21  | 2:B:61:ILE:HD11  | 1.91                     | 0.53              |
| 1:C:306:ARG:HG3  | 1:C:307:ASP:N    | 2.24                     | 0.53              |
| 2:D:90:GLU:OE1   | 2:D:92:VAL:HG22  | 2.08                     | 0.53              |
| 1:A:2:ASN:ND2    | 1:A:305:ASN:O    | 2.41                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:54:ARG:NH1   | 1:A:268:PRO:HB3  | 2.24                     | 0.53              |
| 1:C:44:ILE:O     | 1:C:70:VAL:HA    | 2.08                     | 0.53              |
| 1:C:49:PHE:HB2   | 1:C:105:ARG:O    | 2.09                     | 0.53              |
| 1:A:20:LEU:O     | 1:A:22:LEU:N     | 2.41                     | 0.53              |
| 1:A:251:ALA:O    | 1:A:253:ASP:N    | 2.42                     | 0.53              |
| 2:B:111:ASN:OD1  | 2:B:114:CYS:N    | 2.41                     | 0.53              |
| 1:C:45:ALA:CB    | 1:C:99:VAL:HG11  | 2.38                     | 0.53              |
| 1:C:92:ILE:HG22  | 1:C:118:PHE:O    | 2.09                     | 0.53              |
| 1:A:95:ILE:HD13  | 1:A:95:ILE:N     | 2.23                     | 0.53              |
| 1:A:284:TRP:HA   | 1:A:287:GLN:CD   | 2.28                     | 0.53              |
| 1:C:162:ASP:OD2  | 1:C:231:GLN:HB2  | 2.09                     | 0.53              |
| 1:A:113:ARG:HB3  | 2:B:140:TYR:HD1  | 1.74                     | 0.53              |
| 1:C:4:LEU:HD21   | 1:C:299:LEU:CD1  | 2.39                     | 0.53              |
| 1:C:64:HIS:NE2   | 1:C:70:VAL:HG23  | 2.24                     | 0.53              |
| 1:C:145:ILE:HA   | 5:C:320:HOH:O    | 2.09                     | 0.53              |
| 2:D:83:VAL:O     | 2:D:83:VAL:HG13  | 2.09                     | 0.53              |
| 1:C:262:LYS:O    | 1:C:264:LEU:HD22 | 2.09                     | 0.53              |
| 2:D:9:VAL:C      | 2:D:11:ALA:H     | 2.12                     | 0.53              |
| 2:D:28:LYS:O     | 2:D:30:LEU:N     | 2.42                     | 0.53              |
| 2:D:41:ARG:HB3   | 2:D:62:GLU:HB3   | 1.90                     | 0.53              |
| 2:D:130:ARG:C    | 2:D:132:ASN:H    | 2.12                     | 0.53              |
| 1:A:169:VAL:HG23 | 1:A:170:HIS:HD2  | 1.74                     | 0.53              |
| 1:A:287:GLN:O    | 5:A:1344:HOH:O   | 2.19                     | 0.53              |
| 1:C:106:HIS:ND1  | 1:C:108:GLN:OE1  | 2.37                     | 0.53              |
| 2:B:129:LYS:HZ1  | 2:B:130:ARG:C    | 2.12                     | 0.53              |
| 2:B:141:CYS:N    | 5:B:221:HOH:O    | 2.15                     | 0.53              |
| 1:C:250:ARG:O    | 1:C:251:ALA:C    | 2.47                     | 0.53              |
| 2:D:41:ARG:H     | 2:D:62:GLU:HB3   | 1.74                     | 0.53              |
| 2:D:132:ASN:ND2  | 2:D:133:ASP:OD1  | 2.42                     | 0.53              |
| 1:A:49:PHE:HA    | 1:A:76:SER:HB2   | 1.90                     | 0.52              |
| 1:A:309:VAL:HG22 | 5:A:1403:HOH:O   | 2.08                     | 0.52              |
| 1:C:178:LYS:NZ   | 1:C:201:MET:CE   | 2.73                     | 0.52              |
| 2:D:137:LYS:CE   | 2:D:142:GLU:HG3  | 2.39                     | 0.52              |
| 1:C:184:PHE:HB3  | 1:C:186:PHE:CE1  | 2.44                     | 0.52              |
| 1:A:2:ASN:ND2    | 1:A:5:TYR:CG     | 2.77                     | 0.52              |
| 1:A:146:GLN:HG2  | 1:A:152:LEU:HB3  | 1.90                     | 0.52              |
| 1:A:229:ARG:CG   | 1:A:270:VAL:HG23 | 2.39                     | 0.52              |
| 1:A:278:ASP:HA   | 1:A:285:TYR:OH   | 2.09                     | 0.52              |
| 2:B:17:VAL:HG13  | 2:B:60:LYS:HG2   | 1.91                     | 0.52              |
| 1:C:136:THR:CB   | 1:C:296:ARG:NH2  | 2.72                     | 0.52              |
| 1:C:231:GLN:H    | 1:C:231:GLN:HE21 | 1.57                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:287:GLN:HG2  | 5:A:1326:HOH:O   | 2.09                     | 0.52              |
| 2:B:128:ARG:HD3  | 5:B:201:HOH:O    | 2.09                     | 0.52              |
| 1:C:219:MET:HB3  | 1:C:256:ASN:OD1  | 2.08                     | 0.52              |
| 2:D:24:GLN:HE21  | 2:D:47:ASN:HD21  | 1.58                     | 0.52              |
| 2:D:107:LEU:HD21 | 2:D:136:LEU:CD2  | 2.39                     | 0.52              |
| 2:D:124:SER:O    | 2:D:139:LYS:HB3  | 2.09                     | 0.52              |
| 1:A:76:SER:HA    | 5:A:1399:HOH:O   | 2.09                     | 0.52              |
| 1:A:126:ASN:ND2  | 1:A:128:GLY:H    | 2.07                     | 0.52              |
| 1:C:155:LEU:HD13 | 1:C:224:ILE:CD1  | 2.40                     | 0.52              |
| 1:C:201:MET:HA   | 5:C:337:HOH:O    | 2.09                     | 0.52              |
| 1:A:201:MET:O    | 1:A:202:LEU:C    | 2.48                     | 0.52              |
| 1:A:205:LYS:O    | 1:A:207:ILE:N    | 2.43                     | 0.52              |
| 1:A:269:ARG:HH22 | 1:A:278:ASP:CG   | 2.11                     | 0.52              |
| 1:C:54:ARG:NE    | 1:C:267:LEU:HB3  | 2.25                     | 0.52              |
| 1:C:66:LEU:HG    | 1:C:297:GLN:HG2  | 1.92                     | 0.52              |
| 1:C:193:ALA:HB1  | 1:C:211:LEU:HD22 | 1.92                     | 0.52              |
| 1:A:2:ASN:ND2    | 1:A:5:TYR:CB     | 2.72                     | 0.52              |
| 1:A:169:VAL:HG23 | 1:A:170:HIS:N    | 2.25                     | 0.52              |
| 1:C:38:LEU:HD12  | 1:C:39:LEU:CG    | 2.39                     | 0.52              |
| 1:C:45:ALA:HB1   | 1:C:72:GLY:N     | 2.25                     | 0.52              |
| 2:D:33:PHE:HB3   | 2:D:35:LEU:HG    | 1.92                     | 0.52              |
| 1:A:30:LEU:C     | 1:A:32:ALA:H     | 2.13                     | 0.52              |
| 1:A:128:GLY:HA3  | 1:A:167:ARG:CZ   | 2.40                     | 0.52              |
| 1:C:92:ILE:O     | 1:C:93:SER:C     | 2.47                     | 0.52              |
| 1:C:157:VAL:HG12 | 1:C:158:ALA:N    | 2.17                     | 0.52              |
| 1:A:265:HIS:O    | 1:A:288:GLN:OE1  | 2.27                     | 0.52              |
| 2:B:41:ARG:CD    | 2:D:48:LEU:HD13  | 2.40                     | 0.52              |
| 1:C:192:LEU:O    | 1:C:194:MET:N    | 2.36                     | 0.52              |
| 1:C:202:LEU:HA   | 1:C:205:LYS:HZ2  | 1.74                     | 0.52              |
| 1:A:157:VAL:HA   | 1:A:224:ILE:O    | 2.10                     | 0.52              |
| 2:B:18:ILE:HD12  | 2:B:18:ILE:N     | 2.24                     | 0.52              |
| 1:C:26:THR:HA    | 1:C:29:LYS:CG    | 2.40                     | 0.52              |
| 2:D:86:ILE:HD12  | 2:D:86:ILE:H     | 1.75                     | 0.52              |
| 2:D:108:VAL:HG23 | 2:D:108:VAL:O    | 2.10                     | 0.52              |
| 1:A:187:ILE:HG23 | 1:A:212:HIS:O    | 2.10                     | 0.51              |
| 1:C:48:PHE:CZ    | 1:C:52:SER:N     | 2.70                     | 0.51              |
| 1:C:155:LEU:HA   | 5:C:363:HOH:O    | 2.10                     | 0.51              |
| 1:C:273:ILE:HG21 | 1:C:285:TYR:CZ   | 2.45                     | 0.51              |
| 2:D:24:GLN:HE21  | 2:D:47:ASN:ND2   | 2.08                     | 0.51              |
| 1:A:16:SER:O     | 1:A:178:LYS:HD3  | 2.11                     | 0.51              |
| 1:A:26:THR:HG21  | 1:A:302:LEU:CD2  | 2.39                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:103:ILE:O    | 2:B:103:ILE:HG13 | 2.10                     | 0.51              |
| 1:C:164:LYS:CB   | 1:C:192:LEU:HA   | 2.38                     | 0.51              |
| 1:A:50:GLU:HG2   | 1:A:105:ARG:HD3  | 1.92                     | 0.51              |
| 1:C:141:ASP:C    | 1:C:143:PHE:H    | 2.13                     | 0.51              |
| 1:C:142:LEU:HA   | 1:C:145:ILE:CG1  | 2.40                     | 0.51              |
| 1:C:155:LEU:HD22 | 1:C:224:ILE:CD1  | 2.40                     | 0.51              |
| 1:C:274:ALA:HB3  | 1:C:277:VAL:HG23 | 1.92                     | 0.51              |
| 2:D:135:ALA:CB   | 2:D:146:SER:HA   | 2.40                     | 0.51              |
| 1:A:23:VAL:O     | 1:A:26:THR:HB    | 2.10                     | 0.51              |
| 2:B:109:CYS:SG   | 2:B:110:PRO:HD2  | 2.50                     | 0.51              |
| 1:C:136:THR:OG1  | 1:C:296:ARG:NH2  | 2.43                     | 0.51              |
| 1:A:26:THR:OG1   | 1:A:302:LEU:HD21 | 2.10                     | 0.51              |
| 1:A:177:ALA:O    | 1:A:207:ILE:HD11 | 2.11                     | 0.51              |
| 2:B:20:HIS:HA    | 2:B:56:LYS:HD2   | 1.91                     | 0.51              |
| 1:C:13:ASN:OD1   | 1:C:178:LYS:CE   | 2.59                     | 0.51              |
| 2:D:28:LYS:C     | 2:D:30:LEU:H     | 2.13                     | 0.51              |
| 2:D:103:ILE:HD11 | 2:D:127:VAL:CG1  | 2.40                     | 0.51              |
| 2:B:21:ILE:O     | 2:B:57:ASP:HB2   | 2.11                     | 0.51              |
| 1:C:2:ASN:HB2    | 1:C:3:PRO:HD2    | 1.93                     | 0.51              |
| 1:C:124:VAL:HG12 | 1:C:125:LEU:H    | 1.64                     | 0.51              |
| 1:C:178:LYS:HZ3  | 1:C:201:MET:HE1  | 1.75                     | 0.51              |
| 1:C:188:ALA:HB3  | 1:C:193:ALA:HA   | 1.92                     | 0.51              |
| 2:B:28:LYS:C     | 2:B:30:LEU:H     | 2.12                     | 0.51              |
| 1:A:279:LYS:HB2  | 5:A:1418:HOH:O   | 2.11                     | 0.51              |
| 2:B:27:PHE:H     | 2:B:46:LEU:HD21  | 1.74                     | 0.51              |
| 2:B:84:ASN:O     | 2:B:86:ILE:N     | 2.44                     | 0.51              |
| 2:B:114:CYS:O    | 2:B:117:HIS:HE1  | 1.93                     | 0.51              |
| 1:C:4:LEU:HD23   | 1:C:303:VAL:HG22 | 1.93                     | 0.51              |
| 1:C:159:MET:HE3  | 1:C:172:LEU:HD23 | 1.91                     | 0.51              |
| 1:C:261:MET:C    | 1:C:262:LYS:HD2  | 2.31                     | 0.51              |
| 2:D:16:THR:CG2   | 2:D:65:PHE:HA    | 2.41                     | 0.51              |
| 2:D:34:LYS:O     | 2:D:37:GLU:OE1   | 2.29                     | 0.51              |
| 1:A:155:LEU:O    | 1:A:182:ASN:HA   | 2.10                     | 0.51              |
| 1:A:191:ALA:C    | 1:A:193:ALA:H    | 2.14                     | 0.51              |
| 1:C:291:ASN:O    | 1:C:292:GLY:C    | 2.49                     | 0.51              |
| 2:D:45:GLY:O     | 2:D:48:LEU:HD23  | 2.10                     | 0.51              |
| 2:D:133:ASP:HB2  | 2:D:147:HIS:HE1  | 1.74                     | 0.51              |
| 1:A:131:SER:HB2  | 1:A:165:TYR:HA   | 1.93                     | 0.51              |
| 2:B:36:THR:O     | 2:D:24:GLN:NE2   | 2.43                     | 0.51              |
| 1:C:46:SER:N     | 1:C:72:GLY:HA3   | 2.26                     | 0.51              |
| 1:C:136:THR:CB   | 1:C:296:ARG:HH22 | 2.23                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:129:ASP:OD2  | 1:A:132:ASN:HB3  | 2.10                     | 0.50              |
| 1:C:186:PHE:C    | 1:C:187:ILE:HG13 | 2.31                     | 0.50              |
| 1:C:31:LYS:HZ3   | 1:C:143:PHE:HE2  | 1.53                     | 0.50              |
| 1:C:80:SER:HA    | 1:C:84:LYS:HB2   | 1.93                     | 0.50              |
| 1:A:225:LEU:HD12 | 1:A:225:LEU:C    | 2.32                     | 0.50              |
| 1:A:16:SER:HA    | 5:A:1389:HOH:O   | 2.11                     | 0.50              |
| 1:A:174:GLN:CG   | 1:A:198:ILE:HG23 | 2.41                     | 0.50              |
| 2:B:42:ILE:O     | 2:D:46:LEU:N     | 2.45                     | 0.50              |
| 1:C:129:ASP:O    | 1:C:130:GLY:C    | 2.49                     | 0.50              |
| 1:C:220:ALA:HB2  | 1:C:256:ASN:HD22 | 1.77                     | 0.50              |
| 1:A:157:VAL:HG12 | 1:A:224:ILE:HB   | 1.92                     | 0.50              |
| 1:A:191:ALA:O    | 1:A:193:ALA:N    | 2.42                     | 0.50              |
| 2:B:58:LEU:HD22  | 2:B:60:LYS:HG3   | 1.92                     | 0.50              |
| 1:C:189:PRO:O    | 1:C:192:LEU:N    | 2.45                     | 0.50              |
| 1:C:190:ASP:OD1  | 1:C:191:ALA:N    | 2.36                     | 0.50              |
| 2:D:125:PHE:O    | 2:D:139:LYS:HB2  | 2.11                     | 0.50              |
| 1:C:2:ASN:OD1    | 1:C:5:TYR:HB2    | 2.10                     | 0.50              |
| 1:C:81:LEU:C     | 1:C:81:LEU:HD23  | 2.32                     | 0.50              |
| 1:C:155:LEU:HD23 | 1:C:223:ASP:CG   | 2.32                     | 0.50              |
| 1:C:224:ILE:N    | 1:C:261:MET:HG2  | 2.26                     | 0.50              |
| 2:D:137:LYS:CD   | 2:D:142:GLU:HG3  | 2.42                     | 0.50              |
| 2:D:149:VAL:HA   | 2:D:152:ALA:CB   | 2.42                     | 0.50              |
| 1:A:16:SER:OG    | 1:A:19:ASP:HB2   | 2.11                     | 0.50              |
| 1:A:160:VAL:CG1  | 1:A:187:ILE:HD13 | 2.42                     | 0.50              |
| 1:A:189:PRO:HD2  | 1:A:192:LEU:HB2  | 1.92                     | 0.50              |
| 2:B:9:VAL:O      | 2:B:10:GLU:HB2   | 2.11                     | 0.50              |
| 2:B:96:ARG:HD2   | 2:B:97:PRO:HD2   | 1.93                     | 0.50              |
| 1:C:263:VAL:HG23 | 1:C:282:HIS:HB3  | 1.94                     | 0.50              |
| 2:B:83:VAL:HG11  | 2:B:85:ARG:NH1   | 2.26                     | 0.50              |
| 2:B:36:THR:HG23  | 2:B:37:GLU:H     | 1.77                     | 0.49              |
| 1:C:26:THR:HA    | 1:C:29:LYS:CD    | 2.42                     | 0.49              |
| 1:C:26:THR:CA    | 1:C:29:LYS:HG2   | 2.42                     | 0.49              |
| 1:C:43:VAL:O     | 1:C:44:ILE:HD12  | 2.12                     | 0.49              |
| 1:C:237:PRO:HA   | 1:C:240:TYR:CE1  | 2.47                     | 0.49              |
| 1:C:248:VAL:CG1  | 1:C:249:LEU:H    | 2.19                     | 0.49              |
| 1:C:295:ALA:O    | 1:C:296:ARG:C    | 2.49                     | 0.49              |
| 1:A:128:GLY:HA3  | 1:A:167:ARG:NH2  | 2.27                     | 0.49              |
| 2:B:55:ARG:O     | 2:B:56:LYS:HB3   | 2.13                     | 0.49              |
| 2:B:61:ILE:HG23  | 2:B:61:ILE:O     | 2.11                     | 0.49              |
| 1:C:21:ASN:HA    | 1:C:24:LEU:HD12  | 1.94                     | 0.49              |
| 1:C:26:THR:OG1   | 1:C:302:LEU:HD11 | 2.12                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:46:SER:O     | 1:C:73:PHE:N     | 2.45                     | 0.49              |
| 1:A:2:ASN:ND2    | 1:A:306:ARG:CA   | 2.70                     | 0.49              |
| 1:A:48:PHE:CD2   | 1:A:105:ARG:HD2  | 2.47                     | 0.49              |
| 1:A:109:GLU:OE2  | 1:A:132:ASN:HB2  | 2.12                     | 0.49              |
| 1:A:134:HIS:ND1  | 1:A:136:THR:OG1  | 2.42                     | 0.49              |
| 1:A:267:LEU:CD2  | 1:A:269:ARG:HG2  | 2.41                     | 0.49              |
| 1:C:5:TYR:O      | 1:C:6:GLN:HB2    | 2.12                     | 0.49              |
| 1:C:38:LEU:HB3   | 1:C:39:LEU:HD12  | 1.94                     | 0.49              |
| 1:C:140:LEU:O    | 1:C:291:ASN:OD1  | 2.29                     | 0.49              |
| 1:C:183:ARG:HA   | 1:C:208:ALA:CB   | 2.40                     | 0.49              |
| 1:A:160:VAL:HA   | 1:A:187:ILE:O    | 2.12                     | 0.49              |
| 1:A:243:VAL:O    | 1:A:244:LYS:O    | 2.29                     | 0.49              |
| 1:C:159:MET:HE2  | 1:C:172:LEU:HD23 | 1.91                     | 0.49              |
| 2:D:16:THR:HG21  | 2:D:66:LEU:HD12  | 1.94                     | 0.49              |
| 1:A:39:LEU:HD21  | 1:A:301:ALA:HA   | 1.94                     | 0.49              |
| 1:C:61:THR:CG2   | 5:C:351:HOH:O    | 2.60                     | 0.49              |
| 1:C:234:ARG:C    | 1:C:235:LEU:HD23 | 2.33                     | 0.49              |
| 2:D:25:ILE:HG23  | 5:D:191:HOH:O    | 2.12                     | 0.49              |
| 1:A:78:ASN:HD22  | 1:A:78:ASN:H     | 1.61                     | 0.49              |
| 1:A:105:ARG:HG2  | 5:A:1388:HOH:O   | 2.13                     | 0.49              |
| 1:C:260:ASN:O    | 1:C:262:LYS:HD2  | 2.12                     | 0.49              |
| 1:A:137:GLN:NE2  | 1:A:266:PRO:HB3  | 2.28                     | 0.49              |
| 1:A:183:ARG:NH2  | 1:A:183:ARG:CG   | 2.74                     | 0.49              |
| 2:B:12:ILE:HG12  | 2:B:13:LYS:H     | 1.78                     | 0.49              |
| 2:B:42:ILE:O     | 2:D:45:GLY:HA2   | 2.12                     | 0.49              |
| 1:A:202:LEU:HA   | 1:A:207:ILE:HB   | 1.94                     | 0.49              |
| 1:A:302:LEU:HD23 | 1:A:302:LEU:N    | 2.21                     | 0.49              |
| 2:B:70:GLN:HB3   | 5:B:164:HOH:O    | 2.13                     | 0.49              |
| 1:C:60:GLU:O     | 1:C:63:MET:HB2   | 2.13                     | 0.49              |
| 1:C:109:GLU:CB   | 5:C:419:HOH:O    | 2.49                     | 0.49              |
| 1:C:110:GLY:HA2  | 2:D:140:TYR:O    | 2.12                     | 0.49              |
| 1:C:128:GLY:HA2  | 1:C:133:GLN:O    | 2.13                     | 0.49              |
| 1:C:249:LEU:HD11 | 1:C:254:LEU:HD21 | 1.94                     | 0.49              |
| 1:A:34:PRO:O     | 1:A:35:GLN:HG3   | 2.13                     | 0.49              |
| 1:A:160:VAL:CG2  | 1:A:227:MET:SD   | 3.00                     | 0.49              |
| 1:A:255:HIS:CD2  | 1:A:255:HIS:N    | 2.75                     | 0.49              |
| 1:A:267:LEU:HD23 | 1:A:268:PRO:CA   | 2.33                     | 0.49              |
| 1:C:5:TYR:CE2    | 1:C:305:ASN:N    | 2.81                     | 0.49              |
| 1:C:134:HIS:CE1  | 1:C:137:GLN:CB   | 2.95                     | 0.49              |
| 1:C:155:LEU:HD22 | 1:C:224:ILE:HD11 | 1.94                     | 0.49              |
| 1:C:292:GLY:HA2  | 1:C:296:ARG:HG3  | 1.94                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:33:PHE:O     | 2:D:34:LYS:C     | 2.51                     | 0.49              |
| 1:A:92:ILE:HG21  | 1:A:118:PHE:HB2  | 1.94                     | 0.49              |
| 1:C:229:ARG:O    | 1:C:231:GLN:NE2  | 2.46                     | 0.49              |
| 1:A:134:HIS:CE1  | 1:A:136:THR:HG1  | 2.31                     | 0.48              |
| 1:A:202:LEU:CB   | 1:A:207:ILE:HB   | 2.41                     | 0.48              |
| 1:C:13:ASN:HB2   | 1:C:174:GLN:NE2  | 2.27                     | 0.48              |
| 1:C:160:VAL:CG1  | 1:C:161:GLY:N    | 2.75                     | 0.48              |
| 1:C:276:ASP:HA   | 1:C:279:LYS:NZ   | 2.27                     | 0.48              |
| 1:A:9:ILE:HD12   | 1:A:9:ILE:N      | 2.28                     | 0.48              |
| 1:C:37:GLU:HA    | 1:C:40:LYS:HE3   | 1.93                     | 0.48              |
| 1:C:141:ASP:OD1  | 1:C:288:GLN:HG2  | 2.13                     | 0.48              |
| 1:C:167:ARG:HG3  | 1:C:167:ARG:HH21 | 1.78                     | 0.48              |
| 1:A:160:VAL:HG12 | 1:A:187:ILE:CD1  | 2.43                     | 0.48              |
| 1:A:289:ALA:N    | 5:A:1344:HOH:O   | 2.46                     | 0.48              |
| 2:B:86:ILE:HA    | 2:B:91:VAL:HA    | 1.95                     | 0.48              |
| 1:C:9:ILE:CB     | 1:C:125:LEU:HG   | 2.43                     | 0.48              |
| 1:C:4:LEU:HD13   | 1:C:23:VAL:HG13  | 1.96                     | 0.48              |
| 1:C:107:PRO:HB2  | 5:C:316:HOH:O    | 2.13                     | 0.48              |
| 1:C:142:LEU:HA   | 1:C:145:ILE:HD12 | 1.94                     | 0.48              |
| 1:C:219:MET:HE1  | 1:C:254:LEU:HG   | 1.95                     | 0.48              |
| 1:C:228:THR:HG23 | 1:C:266:PRO:HG2  | 1.96                     | 0.48              |
| 1:C:260:ASN:O    | 1:C:262:LYS:CD   | 2.61                     | 0.48              |
| 1:A:48:PHE:CZ    | 1:A:56:ARG:HA    | 2.49                     | 0.48              |
| 1:A:55:THR:HB    | 3:A:1311:PCT:C1  | 2.43                     | 0.48              |
| 1:A:162:ASP:OD1  | 1:A:192:LEU:HD22 | 2.13                     | 0.48              |
| 1:A:164:LYS:HD3  | 5:A:1376:HOH:O   | 2.12                     | 0.48              |
| 1:C:146:GLN:N    | 1:C:146:GLN:OE1  | 2.47                     | 0.48              |
| 1:A:13:ASN:OD1   | 1:A:174:GLN:CD   | 2.51                     | 0.48              |
| 1:A:146:GLN:HE21 | 1:A:152:LEU:CG   | 2.26                     | 0.48              |
| 2:B:50:SER:OG    | 2:B:56:LYS:HD3   | 2.13                     | 0.48              |
| 1:C:49:PHE:CD1   | 1:C:49:PHE:N     | 2.82                     | 0.48              |
| 1:C:105:ARG:NH1  | 1:C:167:ARG:NH2  | 2.60                     | 0.48              |
| 1:C:137:GLN:HG3  | 1:C:137:GLN:O    | 2.14                     | 0.48              |
| 1:A:167:ARG:HD2  | 5:A:1319:HOH:O   | 2.13                     | 0.48              |
| 1:C:65:ARG:C     | 1:C:67:GLY:H     | 2.16                     | 0.48              |
| 1:C:231:GLN:NE2  | 1:C:231:GLN:N    | 2.60                     | 0.48              |
| 1:C:310:LEU:N    | 1:C:310:LEU:CD1  | 2.74                     | 0.48              |
| 2:D:147:HIS:HB2  | 2:D:151:LEU:CD1  | 2.44                     | 0.48              |
| 1:A:87:THR:O     | 1:A:91:THR:OG1   | 2.31                     | 0.48              |
| 2:B:74:LEU:HB2   | 2:B:97:PRO:HB3   | 1.96                     | 0.48              |
| 2:B:75:ALA:CB    | 2:B:97:PRO:O     | 2.60                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:92:ILE:HG13  | 1:C:115:ALA:CA   | 2.32                     | 0.48              |
| 1:C:125:LEU:HD23 | 1:C:125:LEU:C    | 2.33                     | 0.48              |
| 1:C:151:ARG:NH1  | 1:C:155:LEU:HD11 | 2.19                     | 0.48              |
| 1:C:306:ARG:NH2  | 1:C:306:ARG:CB   | 2.73                     | 0.48              |
| 1:C:163:LEU:CG   | 1:C:188:ALA:HB2  | 2.41                     | 0.48              |
| 1:C:202:LEU:HA   | 1:C:205:LYS:HZ3  | 1.77                     | 0.48              |
| 1:C:245:ALA:O    | 1:C:247:PHE:N    | 2.46                     | 0.48              |
| 1:A:106:HIS:HB3  | 1:A:111:ALA:HB3  | 1.95                     | 0.48              |
| 2:B:30:LEU:O     | 2:B:33:PHE:O     | 2.31                     | 0.48              |
| 2:B:47:ASN:O     | 2:B:48:LEU:HD23  | 2.14                     | 0.48              |
| 1:C:219:MET:O    | 1:C:257:ALA:HA   | 2.14                     | 0.48              |
| 2:D:72:ASP:OD2   | 2:D:72:ASP:N     | 2.46                     | 0.48              |
| 1:A:57:LEU:O     | 1:A:60:GLU:N     | 2.47                     | 0.47              |
| 1:A:165:TYR:CE2  | 1:A:235:LEU:HD23 | 2.43                     | 0.47              |
| 1:C:228:THR:CB   | 1:C:266:PRO:HG2  | 2.43                     | 0.47              |
| 2:D:28:LYS:HE2   | 2:D:32:LEU:HD22  | 1.96                     | 0.47              |
| 2:D:62:GLU:O     | 2:D:63:ASN:HB2   | 2.13                     | 0.47              |
| 2:D:86:ILE:HD12  | 2:D:86:ILE:N     | 2.29                     | 0.47              |
| 1:A:44:ILE:HG21  | 1:A:103:VAL:CG2  | 2.44                     | 0.47              |
| 1:A:237:PRO:HD3  | 5:A:1392:HOH:O   | 2.14                     | 0.47              |
| 1:C:5:TYR:HE2    | 1:C:305:ASN:N    | 2.12                     | 0.47              |
| 1:C:26:THR:HG23  | 1:C:310:LEU:HD22 | 1.95                     | 0.47              |
| 1:C:54:ARG:HH11  | 1:C:268:PRO:HD3  | 1.78                     | 0.47              |
| 1:C:287:GLN:N    | 1:C:287:GLN:CD   | 2.67                     | 0.47              |
| 2:D:28:LYS:HB3   | 2:D:32:LEU:HB3   | 1.97                     | 0.47              |
| 2:D:137:LYS:HB2  | 2:D:144:GLU:CG   | 2.44                     | 0.47              |
| 1:A:50:GLU:HB3   | 1:A:107:PRO:HD3  | 1.96                     | 0.47              |
| 1:A:109:GLU:HB3  | 2:B:141:CYS:CB   | 2.34                     | 0.47              |
| 1:A:197:TYR:CZ   | 1:A:198:ILE:HD11 | 2.50                     | 0.47              |
| 2:B:129:LYS:HE3  | 2:B:129:LYS:O    | 2.14                     | 0.47              |
| 1:C:146:GLN:HA   | 1:C:150:GLY:N    | 2.30                     | 0.47              |
| 2:D:23:ALA:HB2   | 2:D:55:ARG:HG3   | 1.95                     | 0.47              |
| 2:D:56:LYS:HD2   | 2:D:57:ASP:CA    | 2.44                     | 0.47              |
| 2:D:96:ARG:CZ    | 2:D:96:ARG:HA    | 2.44                     | 0.47              |
| 1:A:160:VAL:HG22 | 1:A:225:LEU:HD11 | 1.95                     | 0.47              |
| 1:A:170:HIS:H    | 1:A:170:HIS:CD2  | 2.30                     | 0.47              |
| 1:C:100:ASP:O    | 1:C:122:VAL:CG1  | 2.62                     | 0.47              |
| 1:C:291:ASN:O    | 1:C:293:ILE:N    | 2.47                     | 0.47              |
| 2:D:149:VAL:O    | 2:D:150:VAL:C    | 2.53                     | 0.47              |
| 1:A:41:HIS:O     | 1:A:42:LYS:C     | 2.53                     | 0.47              |
| 1:A:48:PHE:HE2   | 1:A:55:THR:CG2   | 2.19                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:233:GLU:H    | 1:A:233:GLU:CD   | 2.17                     | 0.47              |
| 1:C:80:SER:OG    | 1:C:84:LYS:HD2   | 2.14                     | 0.47              |
| 1:C:208:ALA:O    | 1:C:209:TRP:HB3  | 2.14                     | 0.47              |
| 1:C:253:ASP:OD1  | 1:C:254:LEU:CD1  | 2.63                     | 0.47              |
| 1:C:287:GLN:NE2  | 1:C:287:GLN:N    | 2.60                     | 0.47              |
| 2:D:115:ILE:HG12 | 2:D:115:ILE:O    | 2.15                     | 0.47              |
| 1:A:3:PRO:C      | 1:A:5:TYR:H      | 2.16                     | 0.47              |
| 1:A:119:SER:HG   | 1:A:120:GLY:H    | 1.60                     | 0.47              |
| 2:B:21:ILE:HD13  | 2:B:59:ILE:HG12  | 1.96                     | 0.47              |
| 2:B:42:ILE:O     | 2:D:46:LEU:HD23  | 2.15                     | 0.47              |
| 2:B:77:TYR:O     | 2:B:79:PRO:HD3   | 2.14                     | 0.47              |
| 2:B:84:ASN:HB3   | 2:B:91:VAL:HG13  | 1.96                     | 0.47              |
| 2:B:141:CYS:C    | 2:B:143:LYS:H    | 2.18                     | 0.47              |
| 1:C:89:ALA:HB1   | 1:C:118:PHE:CD1  | 2.49                     | 0.47              |
| 1:C:108:GLN:HE22 | 2:D:115:ILE:HD12 | 1.74                     | 0.47              |
| 1:C:126:ASN:ND2  | 1:C:128:GLY:H    | 2.12                     | 0.47              |
| 1:C:204:GLU:OE2  | 1:C:204:GLU:N    | 2.48                     | 0.47              |
| 1:C:237:PRO:C    | 1:C:239:GLU:N    | 2.68                     | 0.47              |
| 1:C:249:LEU:O    | 1:C:249:LEU:HD23 | 2.15                     | 0.47              |
| 1:C:303:VAL:O    | 1:C:304:LEU:HD23 | 2.15                     | 0.47              |
| 2:D:104:ASP:O    | 2:D:106:VAL:N    | 2.48                     | 0.47              |
| 2:D:146:SER:CB   | 2:D:148:ASN:HD22 | 2.13                     | 0.47              |
| 1:A:93:SER:O     | 1:A:96:SER:OG    | 2.33                     | 0.47              |
| 2:B:18:ILE:HD13  | 2:B:59:ILE:HB    | 1.97                     | 0.47              |
| 2:B:86:ILE:HG12  | 2:B:91:VAL:HG22  | 1.95                     | 0.47              |
| 1:C:43:VAL:O     | 1:C:99:VAL:HA    | 2.15                     | 0.47              |
| 1:C:148:THR:HB   | 1:C:149:GLN:OE1  | 2.15                     | 0.47              |
| 1:A:4:LEU:O      | 1:A:303:VAL:HG13 | 2.15                     | 0.47              |
| 1:A:9:ILE:HB     | 1:A:125:LEU:HA   | 1.96                     | 0.47              |
| 2:B:108:VAL:HA   | 5:B:178:HOH:O    | 2.15                     | 0.47              |
| 1:C:66:LEU:CD1   | 1:C:300:LEU:HB2  | 2.45                     | 0.47              |
| 2:D:12:ILE:HD13  | 2:D:12:ILE:N     | 2.29                     | 0.47              |
| 1:A:8:HIS:CD2    | 1:A:124:VAL:H    | 2.33                     | 0.47              |
| 1:C:253:ASP:CG   | 1:C:254:LEU:HD12 | 2.34                     | 0.47              |
| 2:D:114:CYS:C    | 2:D:116:SER:N    | 2.69                     | 0.47              |
| 1:A:284:TRP:CG   | 1:A:287:GLN:HB2  | 2.50                     | 0.46              |
| 2:B:62:GLU:C     | 2:B:64:THR:N     | 2.67                     | 0.46              |
| 2:B:86:ILE:HG12  | 2:B:91:VAL:CA    | 2.42                     | 0.46              |
| 2:B:137:LYS:HB2  | 2:B:144:GLU:OE2  | 2.15                     | 0.46              |
| 2:B:137:LYS:HB2  | 2:B:144:GLU:CD   | 2.36                     | 0.46              |
| 1:C:23:VAL:HG12  | 1:C:302:LEU:CD1  | 2.45                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:44:ILE:HG13  | 1:C:101:ALA:O    | 2.16                     | 0.46              |
| 1:C:88:LEU:HD13  | 1:C:106:HIS:NE2  | 2.30                     | 0.46              |
| 1:C:196:GLN:O    | 1:C:196:GLN:OE1  | 2.33                     | 0.46              |
| 1:C:264:LEU:HB3  | 1:C:288:GLN:OE1  | 2.15                     | 0.46              |
| 2:D:16:THR:HG23  | 2:D:61:ILE:HD12  | 1.97                     | 0.46              |
| 2:D:74:LEU:O     | 2:D:75:ALA:O     | 2.33                     | 0.46              |
| 1:A:264:LEU:HD22 | 1:A:288:GLN:CG   | 2.45                     | 0.46              |
| 2:B:21:ILE:O     | 2:B:57:ASP:N     | 2.49                     | 0.46              |
| 2:B:39:ASP:CG    | 2:D:55:ARG:HH12  | 2.18                     | 0.46              |
| 2:B:55:ARG:NH1   | 5:B:204:HOH:O    | 2.47                     | 0.46              |
| 2:D:113:ASN:O    | 2:D:115:ILE:N    | 2.48                     | 0.46              |
| 1:A:23:VAL:HG22  | 1:A:302:LEU:HD12 | 1.98                     | 0.46              |
| 1:A:176:LEU:HB2  | 1:A:184:PHE:HZ   | 1.79                     | 0.46              |
| 1:C:26:THR:C     | 1:C:29:LYS:HG2   | 2.36                     | 0.46              |
| 1:C:105:ARG:HH11 | 1:C:167:ARG:NH1  | 2.05                     | 0.46              |
| 1:A:169:VAL:O    | 1:A:173:THR:N    | 2.42                     | 0.46              |
| 1:C:10:ILE:O     | 1:C:135:PRO:HD3  | 2.15                     | 0.46              |
| 1:C:38:LEU:HD12  | 1:C:39:LEU:HD12  | 1.95                     | 0.46              |
| 1:C:105:ARG:NH2  | 1:C:134:HIS:NE2  | 2.63                     | 0.46              |
| 1:C:145:ILE:HB   | 1:C:146:GLN:OE1  | 2.15                     | 0.46              |
| 2:D:81:ALA:O     | 2:D:96:ARG:NH2   | 2.48                     | 0.46              |
| 2:D:135:ALA:HB1  | 2:D:146:SER:HA   | 1.98                     | 0.46              |
| 1:A:38:LEU:HD23  | 1:A:38:LEU:C     | 2.36                     | 0.46              |
| 1:A:131:SER:HB2  | 1:A:165:TYR:CA   | 2.46                     | 0.46              |
| 1:A:222:VAL:HG23 | 1:A:222:VAL:O    | 2.15                     | 0.46              |
| 2:B:59:ILE:HG22  | 2:B:60:LYS:N     | 2.30                     | 0.46              |
| 2:B:113:ASN:O    | 2:B:114:CYS:C    | 2.53                     | 0.46              |
| 1:C:59:PHE:CE1   | 1:C:296:ARG:HD3  | 2.50                     | 0.46              |
| 1:C:199:LEU:HD13 | 1:C:209:TRP:CE3  | 2.51                     | 0.46              |
| 1:C:220:ALA:HA   | 1:C:256:ASN:O    | 2.15                     | 0.46              |
| 1:A:243:VAL:HG22 | 1:A:244:LYS:N    | 2.29                     | 0.46              |
| 2:B:79:PRO:HG2   | 2:B:80:GLN:H     | 1.80                     | 0.46              |
| 2:D:127:VAL:CG1  | 2:D:136:LEU:HB3  | 2.46                     | 0.46              |
| 1:A:152:LEU:HD12 | 1:A:152:LEU:H    | 1.79                     | 0.46              |
| 2:B:31:SER:HA    | 2:D:27:PHE:CE1   | 2.51                     | 0.46              |
| 1:C:21:ASN:HA    | 1:C:24:LEU:HB2   | 1.97                     | 0.46              |
| 1:C:288:GLN:O    | 1:C:291:ASN:OD1  | 2.33                     | 0.46              |
| 2:D:99:LEU:HD22  | 2:D:99:LEU:C     | 2.36                     | 0.46              |
| 2:B:56:LYS:HE3   | 5:B:228:HOH:O    | 2.15                     | 0.46              |
| 1:C:139:LEU:HA   | 1:C:142:LEU:CD1  | 2.29                     | 0.46              |
| 1:A:154:ASN:N    | 1:A:181:GLY:O    | 2.49                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:176:LEU:HG   | 1:A:176:LEU:H    | 1.57                     | 0.46              |
| 1:A:202:LEU:CA   | 1:A:207:ILE:HB   | 2.45                     | 0.46              |
| 1:A:236:ALA:HA   | 5:A:1392:HOH:O   | 2.16                     | 0.46              |
| 1:A:246:GLN:HB3  | 1:A:247:PHE:CD1  | 2.50                     | 0.46              |
| 1:A:277:VAL:HA   | 1:A:280:THR:HG23 | 1.97                     | 0.46              |
| 2:B:117:HIS:O    | 2:B:119:GLU:N    | 2.49                     | 0.46              |
| 1:C:195:PRO:HB2  | 1:C:197:TYR:CD2  | 2.50                     | 0.46              |
| 2:D:66:LEU:CD2   | 2:D:83:VAL:HG21  | 2.44                     | 0.46              |
| 2:D:84:ASN:O     | 2:D:86:ILE:CD1   | 2.63                     | 0.46              |
| 1:A:3:PRO:CG     | 1:A:22:LEU:CD2   | 2.94                     | 0.46              |
| 1:A:92:ILE:O     | 1:A:94:VAL:N     | 2.49                     | 0.46              |
| 2:B:83:VAL:HG11  | 2:B:85:ARG:HH12  | 1.80                     | 0.46              |
| 1:C:121:ASN:N    | 1:C:121:ASN:ND2  | 2.43                     | 0.46              |
| 1:C:280:THR:CG2  | 1:C:281:PRO:HD2  | 2.46                     | 0.46              |
| 2:D:111:ASN:O    | 2:D:117:HIS:CE1  | 2.69                     | 0.46              |
| 1:A:12:ILE:HD13  | 5:A:1429:HOH:O   | 2.16                     | 0.45              |
| 1:A:44:ILE:HG21  | 1:A:103:VAL:HG23 | 1.97                     | 0.45              |
| 1:C:227:MET:HG3  | 1:C:265:HIS:ND1  | 2.30                     | 0.45              |
| 1:C:280:THR:C    | 1:C:282:HIS:N    | 2.70                     | 0.45              |
| 2:D:143:LYS:CB   | 2:D:145:PHE:CE1  | 2.99                     | 0.45              |
| 1:A:30:LEU:O     | 1:A:32:ALA:N     | 2.50                     | 0.45              |
| 1:A:92:ILE:CG2   | 1:A:118:PHE:HB2  | 2.46                     | 0.45              |
| 1:A:132:ASN:ND2  | 2:B:142:GLU:OE1  | 2.37                     | 0.45              |
| 1:A:249:LEU:HG   | 1:A:250:ARG:N    | 2.31                     | 0.45              |
| 1:C:92:ILE:O     | 1:C:95:ILE:N     | 2.48                     | 0.45              |
| 1:C:293:ILE:HB   | 1:C:294:PHE:H    | 1.62                     | 0.45              |
| 2:D:34:LYS:HD3   | 2:D:37:GLU:OE2   | 2.16                     | 0.45              |
| 2:D:110:PRO:HG3  | 2:D:150:VAL:HG22 | 1.97                     | 0.45              |
| 2:D:146:SER:O    | 2:D:148:ASN:N    | 2.49                     | 0.45              |
| 1:A:106:HIS:HA   | 5:A:1388:HOH:O   | 2.15                     | 0.45              |
| 1:A:278:ASP:OD2  | 1:A:278:ASP:N    | 2.49                     | 0.45              |
| 1:C:145:ILE:HG23 | 5:C:320:HOH:O    | 2.16                     | 0.45              |
| 1:C:151:ARG:CG   | 1:C:153:ASP:HB2  | 2.46                     | 0.45              |
| 2:D:16:THR:CG2   | 2:D:61:ILE:HD12  | 2.46                     | 0.45              |
| 2:D:72:ASP:HB3   | 2:D:100:PRO:HD2  | 1.97                     | 0.45              |
| 2:D:99:LEU:HD22  | 2:D:100:PRO:O    | 2.16                     | 0.45              |
| 1:A:283:ALA:O    | 1:A:287:GLN:OE1  | 2.34                     | 0.45              |
| 2:B:103:ILE:HG22 | 5:B:187:HOH:O    | 2.16                     | 0.45              |
| 1:C:205:LYS:HD2  | 1:C:205:LYS:N    | 2.28                     | 0.45              |
| 1:A:3:PRO:HB2    | 1:A:22:LEU:CD2   | 2.46                     | 0.45              |
| 1:A:86:GLU:OE1   | 1:A:91:THR:HG23  | 2.17                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:103:VAL:HG22 | 1:A:125:LEU:HD13 | 1.97                     | 0.45              |
| 2:B:44:ILE:HG13  | 5:B:188:HOH:O    | 2.15                     | 0.45              |
| 1:C:48:PHE:O     | 1:C:74:SER:O     | 2.34                     | 0.45              |
| 1:C:265:HIS:CE1  | 1:C:266:PRO:HD2  | 2.52                     | 0.45              |
| 2:D:149:VAL:O    | 2:D:152:ALA:N    | 2.50                     | 0.45              |
| 1:C:157:VAL:O    | 1:C:158:ALA:HB2  | 2.16                     | 0.45              |
| 1:C:163:LEU:HB2  | 1:C:192:LEU:O    | 2.17                     | 0.45              |
| 1:C:176:LEU:C    | 1:C:178:LYS:N    | 2.70                     | 0.45              |
| 2:D:13:LYS:C     | 2:D:88:ASN:HA    | 2.36                     | 0.45              |
| 2:D:64:THR:HG22  | 2:D:65:PHE:N     | 2.32                     | 0.45              |
| 2:D:76:LEU:HD12  | 2:D:77:TYR:N     | 2.32                     | 0.45              |
| 2:D:128:ARG:HG2  | 2:D:128:ARG:HH21 | 1.82                     | 0.45              |
| 1:A:2:ASN:OD1    | 1:A:5:TYR:HB2    | 2.15                     | 0.45              |
| 1:A:10:ILE:HD12  | 1:A:113:ARG:CD   | 2.47                     | 0.45              |
| 1:A:39:LEU:HD12  | 1:A:66:LEU:HD12  | 1.99                     | 0.45              |
| 1:A:81:LEU:HA    | 1:A:86:GLU:HB3   | 1.99                     | 0.45              |
| 1:A:189:PRO:HA   | 1:A:246:GLN:OE1  | 2.17                     | 0.45              |
| 1:C:59:PHE:CG    | 1:C:296:ARG:HD3  | 2.51                     | 0.45              |
| 1:C:154:ASN:O    | 1:C:155:LEU:HG   | 2.16                     | 0.45              |
| 2:D:126:ALA:N    | 2:D:137:LYS:O    | 2.50                     | 0.45              |
| 1:A:44:ILE:O     | 1:A:70:VAL:HG23  | 2.17                     | 0.45              |
| 1:A:49:PHE:CZ    | 1:A:73:PHE:HZ    | 2.35                     | 0.45              |
| 1:A:109:GLU:HB2  | 2:B:114:CYS:HA   | 1.98                     | 0.45              |
| 1:A:146:GLN:NE2  | 1:A:151:ARG:C    | 2.71                     | 0.45              |
| 1:A:227:MET:CE   | 1:A:272:GLU:HB2  | 2.47                     | 0.45              |
| 1:A:284:TRP:O    | 1:A:285:TYR:C    | 2.55                     | 0.45              |
| 1:C:249:LEU:HD23 | 1:C:249:LEU:C    | 2.38                     | 0.45              |
| 2:D:76:LEU:CB    | 2:D:134:ILE:HG21 | 2.37                     | 0.45              |
| 2:D:128:ARG:CZ   | 2:D:130:ARG:HD2  | 2.47                     | 0.45              |
| 2:D:141:CYS:O    | 2:D:143:LYS:N    | 2.49                     | 0.45              |
| 1:A:109:GLU:CG   | 1:A:132:ASN:HB2  | 2.41                     | 0.45              |
| 2:B:41:ARG:HG3   | 2:D:48:LEU:CD2   | 2.37                     | 0.45              |
| 2:B:61:ILE:HG23  | 2:B:64:THR:HB    | 1.99                     | 0.45              |
| 1:C:264:LEU:HD12 | 1:C:288:GLN:CG   | 2.47                     | 0.45              |
| 2:D:138:CYS:SG   | 2:D:141:CYS:CB   | 3.00                     | 0.45              |
| 1:C:132:ASN:CB   | 5:C:419:HOH:O    | 2.65                     | 0.44              |
| 1:C:262:LYS:O    | 1:C:264:LEU:CD2  | 2.65                     | 0.44              |
| 1:A:308:LEU:HD23 | 1:A:309:VAL:C    | 2.38                     | 0.44              |
| 2:B:114:CYS:O    | 2:B:117:HIS:CE1  | 2.70                     | 0.44              |
| 2:B:123:SER:O    | 2:B:124:SER:HB2  | 2.17                     | 0.44              |
| 1:C:31:LYS:HG3   | 5:C:391:HOH:O    | 2.16                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:151:ARG:CZ   | 1:C:151:ARG:O    | 2.65                     | 0.44              |
| 1:C:226:TYR:O    | 1:C:226:TYR:CD1  | 2.70                     | 0.44              |
| 1:C:263:VAL:O    | 1:C:264:LEU:HD13 | 2.17                     | 0.44              |
| 2:D:69:ASP:OD2   | 2:D:70:GLN:NE2   | 2.49                     | 0.44              |
| 2:D:125:PHE:HD1  | 2:D:136:LEU:HB2  | 1.82                     | 0.44              |
| 1:A:39:LEU:O     | 1:A:68:ALA:N     | 2.50                     | 0.44              |
| 1:A:237:PRO:HA   | 1:A:240:TYR:CE1  | 2.52                     | 0.44              |
| 2:B:12:ILE:CG1   | 2:B:13:LYS:N     | 2.80                     | 0.44              |
| 1:C:5:TYR:H      | 1:C:7:LYS:HG2    | 1.82                     | 0.44              |
| 1:C:61:THR:O     | 1:C:64:HIS:HB2   | 2.16                     | 0.44              |
| 2:D:9:VAL:HG13   | 2:D:9:VAL:O      | 2.18                     | 0.44              |
| 2:D:75:ALA:CA    | 2:D:97:PRO:HB2   | 2.47                     | 0.44              |
| 2:D:105:ASN:C    | 2:D:106:VAL:HG22 | 2.37                     | 0.44              |
| 1:A:59:PHE:CD2   | 1:A:63:MET:HE2   | 2.51                     | 0.44              |
| 1:A:166:GLY:O    | 1:A:168:THR:N    | 2.50                     | 0.44              |
| 1:A:169:VAL:HG23 | 1:A:170:HIS:H    | 1.82                     | 0.44              |
| 1:C:39:LEU:C     | 1:C:41:HIS:H     | 2.20                     | 0.44              |
| 1:C:80:SER:CA    | 1:C:84:LYS:HB2   | 2.47                     | 0.44              |
| 1:C:151:ARG:HB3  | 1:C:151:ARG:HH21 | 1.82                     | 0.44              |
| 2:D:58:LEU:C     | 2:D:59:ILE:HD12  | 2.37                     | 0.44              |
| 1:A:3:PRO:HG2    | 1:A:22:LEU:CD2   | 2.47                     | 0.44              |
| 1:A:113:ARG:HG2  | 1:A:113:ARG:NH2  | 2.31                     | 0.44              |
| 2:B:84:ASN:HB3   | 2:B:91:VAL:CG1   | 2.47                     | 0.44              |
| 1:C:152:LEU:HB2  | 1:C:179:PHE:CE2  | 2.53                     | 0.44              |
| 1:C:295:ALA:O    | 1:C:298:ALA:N    | 2.42                     | 0.44              |
| 2:D:24:GLN:NE2   | 2:D:47:ASN:OD1   | 2.50                     | 0.44              |
| 2:D:24:GLN:HE21  | 2:D:47:ASN:CG    | 2.21                     | 0.44              |
| 2:D:66:LEU:HD13  | 2:D:83:VAL:CG2   | 2.47                     | 0.44              |
| 2:D:66:LEU:HB3   | 2:D:67:SER:H     | 1.64                     | 0.44              |
| 2:D:72:ASP:HB3   | 2:D:100:PRO:CD   | 2.47                     | 0.44              |
| 2:D:133:ASP:OD2  | 2:D:148:ASN:ND2  | 2.50                     | 0.44              |
| 1:A:172:LEU:HG   | 1:A:176:LEU:HD11 | 1.99                     | 0.44              |
| 1:A:243:VAL:HG13 | 1:A:244:LYS:N    | 2.25                     | 0.44              |
| 1:C:234:ARG:HD3  | 5:C:406:HOH:O    | 2.18                     | 0.44              |
| 2:D:24:GLN:HG2   | 2:D:47:ASN:OD1   | 2.17                     | 0.44              |
| 1:A:88:LEU:N     | 2:B:119:GLU:OE1  | 2.49                     | 0.44              |
| 2:B:34:LYS:C     | 2:B:36:THR:N     | 2.68                     | 0.44              |
| 1:C:44:ILE:HG22  | 1:C:70:VAL:HG13  | 2.00                     | 0.44              |
| 1:C:131:SER:O    | 1:C:170:HIS:HE1  | 2.01                     | 0.44              |
| 1:C:159:MET:HG2  | 1:C:172:LEU:CD2  | 2.48                     | 0.44              |
| 2:D:41:ARG:CB    | 2:D:62:GLU:HB3   | 2.48                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:145:ILE:O    | 1:A:149:GLN:HB2  | 2.18                     | 0.44              |
| 2:B:140:TYR:HB2  | 5:B:221:HOH:O    | 2.17                     | 0.44              |
| 1:C:38:LEU:C     | 1:C:38:LEU:HD13  | 2.38                     | 0.44              |
| 1:A:129:ASP:O    | 1:A:129:ASP:OD2  | 2.35                     | 0.44              |
| 1:A:195:PRO:HB2  | 1:A:198:ILE:CD1  | 2.48                     | 0.44              |
| 2:B:16:THR:CG2   | 2:B:17:VAL:N     | 2.81                     | 0.44              |
| 2:B:43:THR:CG2   | 2:D:44:ILE:O     | 2.66                     | 0.44              |
| 2:B:50:SER:HA    | 2:B:56:LYS:CE    | 2.46                     | 0.44              |
| 1:C:161:GLY:HA2  | 5:C:338:HOH:O    | 2.18                     | 0.44              |
| 1:C:227:MET:HE1  | 1:C:273:ILE:HD13 | 2.00                     | 0.44              |
| 1:C:237:PRO:CA   | 1:C:240:TYR:CE2  | 2.90                     | 0.44              |
| 2:D:84:ASN:HD22  | 2:D:91:VAL:HG21  | 1.82                     | 0.44              |
| 1:A:13:ASN:OD1   | 1:A:174:GLN:OE1  | 2.36                     | 0.43              |
| 1:A:46:SER:H     | 1:A:72:GLY:HA3   | 1.83                     | 0.43              |
| 1:A:89:ALA:O     | 1:A:93:SER:N     | 2.45                     | 0.43              |
| 1:A:143:PHE:CD1  | 1:A:143:PHE:C    | 2.91                     | 0.43              |
| 1:A:198:ILE:HD12 | 1:A:198:ILE:N    | 2.33                     | 0.43              |
| 1:A:236:ALA:HB3  | 1:A:239:GLU:OE2  | 2.18                     | 0.43              |
| 2:B:17:VAL:CG1   | 2:B:58:LEU:HD21  | 2.48                     | 0.43              |
| 1:C:250:ARG:O    | 1:C:253:ASP:N    | 2.47                     | 0.43              |
| 1:C:274:ALA:H    | 1:C:277:VAL:HG21 | 1.83                     | 0.43              |
| 1:A:87:THR:HB    | 2:B:119:GLU:OE2  | 2.18                     | 0.43              |
| 1:A:94:VAL:CG2   | 1:A:95:ILE:N     | 2.82                     | 0.43              |
| 1:A:148:THR:OG1  | 1:A:149:GLN:HG2  | 2.17                     | 0.43              |
| 1:A:280:THR:HA   | 5:A:1411:HOH:O   | 2.18                     | 0.43              |
| 1:C:4:LEU:HD23   | 1:C:4:LEU:O      | 2.18                     | 0.43              |
| 1:C:227:MET:O    | 1:C:266:PRO:CD   | 2.62                     | 0.43              |
| 1:C:284:TRP:CD1  | 1:C:284:TRP:O    | 2.71                     | 0.43              |
| 2:D:124:SER:CB   | 2:D:139:LYS:HD3  | 2.48                     | 0.43              |
| 1:A:21:ASN:OD1   | 1:A:21:ASN:N     | 2.49                     | 0.43              |
| 1:A:173:THR:HG21 | 1:A:194:MET:CE   | 2.48                     | 0.43              |
| 2:B:39:ASP:CG    | 2:D:55:ARG:NH1   | 2.71                     | 0.43              |
| 2:B:100:PRO:O    | 2:B:127:VAL:HB   | 2.18                     | 0.43              |
| 1:C:150:GLY:O    | 1:C:151:ARG:C    | 2.57                     | 0.43              |
| 2:D:41:ARG:NH2   | 2:D:60:LYS:HD3   | 2.34                     | 0.43              |
| 1:A:17:ARG:HG2   | 1:A:179:PHE:CE1  | 2.53                     | 0.43              |
| 1:A:133:GLN:HG3  | 2:B:142:GLU:OE1  | 2.19                     | 0.43              |
| 1:C:46:SER:C     | 1:C:72:GLY:HA3   | 2.39                     | 0.43              |
| 1:C:112:ALA:O    | 1:C:116:THR:HG23 | 2.18                     | 0.43              |
| 1:A:220:ALA:HB2  | 1:A:256:ASN:HD22 | 1.83                     | 0.43              |
| 1:C:16:SER:O     | 1:C:19:ASP:OD2   | 2.37                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:97:THR:O     | 1:C:98:TYR:C     | 2.57                     | 0.43              |
| 1:A:81:LEU:HD12  | 1:A:88:LEU:HA    | 2.01                     | 0.43              |
| 1:A:102:ILE:O    | 1:A:124:VAL:HA   | 2.19                     | 0.43              |
| 1:A:181:GLY:O    | 1:A:182:ASN:CG   | 2.57                     | 0.43              |
| 2:B:19:ASP:HA    | 2:B:58:LEU:HG    | 2.00                     | 0.43              |
| 1:C:66:LEU:HD12  | 1:C:300:LEU:HB2  | 2.00                     | 0.43              |
| 1:C:66:LEU:HD21  | 1:C:297:GLN:HB3  | 1.99                     | 0.43              |
| 1:C:126:ASN:HD21 | 1:C:128:GLY:C    | 2.21                     | 0.43              |
| 1:C:157:VAL:HA   | 1:C:224:ILE:O    | 2.19                     | 0.43              |
| 1:C:218:VAL:O    | 1:C:218:VAL:CG1  | 2.62                     | 0.43              |
| 1:C:267:LEU:HD13 | 1:C:268:PRO:HA   | 2.01                     | 0.43              |
| 1:C:306:ARG:HH21 | 1:C:306:ARG:HB2  | 1.82                     | 0.43              |
| 1:A:284:TRP:CD1  | 1:A:284:TRP:O    | 2.71                     | 0.43              |
| 1:C:114:LEU:C    | 1:C:114:LEU:CD1  | 2.83                     | 0.43              |
| 1:C:151:ARG:HG2  | 1:C:153:ASP:H    | 1.84                     | 0.43              |
| 2:D:9:VAL:C      | 2:D:11:ALA:N     | 2.71                     | 0.43              |
| 1:A:110:GLY:C    | 1:A:112:ALA:N    | 2.70                     | 0.43              |
| 1:A:167:ARG:HG3  | 1:A:168:THR:H    | 1.82                     | 0.43              |
| 1:C:12:ILE:HG22  | 1:C:12:ILE:O     | 2.18                     | 0.43              |
| 1:C:59:PHE:HE1   | 1:C:296:ARG:NH2  | 2.16                     | 0.43              |
| 2:D:126:ALA:O    | 2:D:136:LEU:CB   | 2.66                     | 0.43              |
| 2:D:132:ASN:CG   | 2:D:133:ASP:H    | 2.21                     | 0.43              |
| 1:A:205:LYS:O    | 1:A:207:ILE:HG12 | 2.18                     | 0.43              |
| 1:C:45:ALA:CB    | 1:C:72:GLY:H     | 2.31                     | 0.43              |
| 1:C:137:GLN:HG3  | 5:C:325:HOH:O    | 2.18                     | 0.43              |
| 1:C:244:LYS:HE3  | 5:C:376:HOH:O    | 2.19                     | 0.43              |
| 2:D:105:ASN:C    | 2:D:106:VAL:CG2  | 2.87                     | 0.43              |
| 2:D:111:ASN:O    | 2:D:113:ASN:N    | 2.52                     | 0.43              |
| 1:A:2:ASN:OD1    | 1:A:5:TYR:N      | 2.52                     | 0.43              |
| 2:B:150:VAL:HG12 | 2:B:150:VAL:O    | 2.18                     | 0.43              |
| 1:C:169:VAL:C    | 1:C:172:LEU:HD13 | 2.39                     | 0.43              |
| 1:C:250:ARG:C    | 1:C:252:SER:N    | 2.71                     | 0.43              |
| 2:D:76:LEU:HA    | 2:D:134:ILE:HG13 | 2.01                     | 0.43              |
| 1:A:5:TYR:CG     | 1:A:306:ARG:HA   | 2.54                     | 0.42              |
| 1:A:183:ARG:CZ   | 1:A:208:ALA:HB3  | 2.49                     | 0.42              |
| 1:A:187:ILE:N    | 1:A:187:ILE:CD1  | 2.75                     | 0.42              |
| 1:A:309:VAL:HG23 | 1:A:310:LEU:N    | 2.34                     | 0.42              |
| 2:B:25:ILE:O     | 2:B:25:ILE:HG22  | 2.19                     | 0.42              |
| 2:B:107:LEU:HB2  | 2:B:125:PHE:CE1  | 2.54                     | 0.42              |
| 1:C:130:GLY:O    | 1:C:167:ARG:HD3  | 2.20                     | 0.42              |
| 1:C:235:LEU:HD23 | 1:C:235:LEU:N    | 2.33                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:9:VAL:O      | 2:D:11:ALA:N     | 2.52                     | 0.42              |
| 2:D:28:LYS:O     | 2:D:32:LEU:N     | 2.52                     | 0.42              |
| 2:D:56:LYS:CD    | 2:D:57:ASP:N     | 2.74                     | 0.42              |
| 1:A:26:THR:CG2   | 1:A:302:LEU:HD21 | 2.50                     | 0.42              |
| 1:A:119:SER:HG   | 1:A:120:GLY:N    | 2.17                     | 0.42              |
| 1:A:204:GLU:C    | 1:A:206:GLY:N    | 2.72                     | 0.42              |
| 1:A:205:LYS:C    | 1:A:207:ILE:N    | 2.70                     | 0.42              |
| 2:B:115:ILE:HA   | 5:B:173:HOH:O    | 2.19                     | 0.42              |
| 1:C:4:LEU:HB3    | 1:C:22:LEU:HD23  | 2.01                     | 0.42              |
| 1:C:252:SER:O    | 1:C:255:HIS:CE1  | 2.73                     | 0.42              |
| 1:C:261:MET:SD   | 1:C:262:LYS:N    | 2.92                     | 0.42              |
| 2:D:99:LEU:CD2   | 2:D:129:LYS:NZ   | 2.82                     | 0.42              |
| 1:A:73:PHE:CD2   | 1:A:79:THR:HG21  | 2.55                     | 0.42              |
| 1:A:261:MET:SD   | 1:A:262:LYS:N    | 2.92                     | 0.42              |
| 1:A:265:HIS:HA   | 1:A:266:PRO:HD2  | 1.75                     | 0.42              |
| 2:B:12:ILE:CG1   | 2:B:13:LYS:H     | 2.31                     | 0.42              |
| 2:B:24:GLN:NE2   | 2:D:38:THR:O     | 2.52                     | 0.42              |
| 2:D:103:ILE:HG13 | 2:D:126:ALA:N    | 2.34                     | 0.42              |
| 1:A:23:VAL:HG22  | 1:A:302:LEU:HD11 | 2.01                     | 0.42              |
| 1:A:92:ILE:O     | 1:A:93:SER:C     | 2.58                     | 0.42              |
| 1:A:104:MET:O    | 1:A:127:ALA:N    | 2.47                     | 0.42              |
| 1:A:149:GLN:O    | 1:A:150:GLY:C    | 2.58                     | 0.42              |
| 1:A:174:GLN:HA   | 1:A:201:MET:HE1  | 2.02                     | 0.42              |
| 1:C:139:LEU:O    | 1:C:142:LEU:N    | 2.52                     | 0.42              |
| 1:C:262:LYS:HB2  | 5:C:377:HOH:O    | 2.19                     | 0.42              |
| 1:C:263:VAL:O    | 1:C:284:TRP:N    | 2.42                     | 0.42              |
| 2:D:12:ILE:HG23  | 2:D:41:ARG:HH21  | 1.83                     | 0.42              |
| 2:D:26:GLY:O     | 2:D:30:LEU:CD2   | 2.68                     | 0.42              |
| 2:D:79:PRO:HG2   | 2:D:80:GLN:H     | 1.84                     | 0.42              |
| 2:D:137:LYS:HB2  | 2:D:144:GLU:CD   | 2.39                     | 0.42              |
| 1:A:22:LEU:HD12  | 5:A:1421:HOH:O   | 2.20                     | 0.42              |
| 1:A:187:ILE:HA   | 5:A:1327:HOH:O   | 2.19                     | 0.42              |
| 2:B:42:ILE:HG12  | 2:B:61:ILE:HG13  | 2.01                     | 0.42              |
| 1:C:45:ALA:HB3   | 1:C:102:ILE:HG22 | 2.00                     | 0.42              |
| 1:C:132:ASN:CA   | 1:C:170:HIS:ND1  | 2.76                     | 0.42              |
| 2:D:16:THR:CB    | 2:D:65:PHE:HA    | 2.50                     | 0.42              |
| 2:D:37:GLU:HB3   | 5:D:173:HOH:O    | 2.18                     | 0.42              |
| 1:A:109:GLU:CB   | 2:B:114:CYS:HA   | 2.49                     | 0.42              |
| 1:A:196:GLN:C    | 1:A:198:ILE:N    | 2.72                     | 0.42              |
| 1:A:255:HIS:HB3  | 5:A:1396:HOH:O   | 2.19                     | 0.42              |
| 2:B:28:LYS:C     | 2:B:30:LEU:N     | 2.72                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:76:LEU:HD23  | 2:B:76:LEU:N     | 2.09                     | 0.42              |
| 2:B:140:TYR:N    | 5:B:221:HOH:O    | 2.52                     | 0.42              |
| 1:C:104:MET:HG3  | 1:C:126:ASN:OD1  | 2.20                     | 0.42              |
| 1:C:167:ARG:HH11 | 1:C:234:ARG:HH22 | 1.68                     | 0.42              |
| 1:C:285:TYR:CA   | 1:C:288:GLN:OE1  | 2.60                     | 0.42              |
| 2:D:107:LEU:CD1  | 2:D:151:LEU:HD21 | 2.47                     | 0.42              |
| 1:A:131:SER:N    | 1:A:234:ARG:NE   | 2.67                     | 0.42              |
| 1:A:186:PHE:C    | 1:A:187:ILE:HD12 | 2.40                     | 0.42              |
| 2:B:75:ALA:HB2   | 2:B:98:SER:O     | 2.20                     | 0.42              |
| 2:D:126:ALA:O    | 2:D:127:VAL:CG1  | 2.62                     | 0.42              |
| 1:A:89:ALA:O     | 1:A:93:SER:OG    | 2.38                     | 0.42              |
| 1:A:217:GLU:C    | 1:A:219:MET:H    | 2.22                     | 0.42              |
| 1:A:264:LEU:CD2  | 1:A:288:GLN:HB2  | 2.50                     | 0.42              |
| 1:C:165:TYR:CE2  | 1:C:192:LEU:HD21 | 2.55                     | 0.42              |
| 2:D:96:ARG:NH2   | 2:D:97:PRO:CD    | 2.81                     | 0.42              |
| 1:A:55:THR:HG21  | 1:A:105:ARG:NH1  | 2.33                     | 0.42              |
| 2:B:39:ASP:CA    | 2:D:55:ARG:NH2   | 2.81                     | 0.42              |
| 2:B:129:LYS:C    | 2:B:129:LYS:CE   | 2.86                     | 0.42              |
| 1:C:45:ALA:N     | 1:C:99:VAL:HG11  | 2.35                     | 0.42              |
| 1:C:127:ALA:HB1  | 1:C:136:THR:HG1  | 1.85                     | 0.42              |
| 1:C:280:THR:O    | 1:C:282:HIS:N    | 2.53                     | 0.42              |
| 2:D:16:THR:HB    | 2:D:65:PHE:HA    | 2.02                     | 0.42              |
| 2:D:18:ILE:HG22  | 2:D:21:ILE:HD11  | 2.02                     | 0.42              |
| 1:A:55:THR:HB    | 3:A:1311:PCT:O1  | 2.19                     | 0.42              |
| 1:A:109:GLU:OE2  | 1:A:132:ASN:CB   | 2.68                     | 0.42              |
| 1:A:214:SER:HB3  | 1:A:217:GLU:HG3  | 2.02                     | 0.42              |
| 2:B:44:ILE:CG2   | 2:D:44:ILE:HB    | 2.27                     | 0.42              |
| 2:B:94:LYS:HD2   | 2:B:94:LYS:HA    | 1.81                     | 0.42              |
| 2:B:134:ILE:O    | 2:B:147:HIS:HB3  | 2.20                     | 0.42              |
| 2:B:136:LEU:O    | 2:B:145:PHE:N    | 2.53                     | 0.42              |
| 1:C:48:PHE:CE2   | 1:C:51:ALA:HA    | 2.55                     | 0.42              |
| 1:C:172:LEU:O    | 1:C:174:GLN:N    | 2.43                     | 0.42              |
| 1:A:280:THR:CB   | 1:A:281:PRO:CD   | 2.87                     | 0.41              |
| 1:C:13:ASN:HB2   | 1:C:174:GLN:CD   | 2.41                     | 0.41              |
| 1:C:59:PHE:O     | 1:C:60:GLU:C     | 2.58                     | 0.41              |
| 2:D:111:ASN:C    | 2:D:113:ASN:N    | 2.73                     | 0.41              |
| 1:A:10:ILE:CG1   | 1:A:11:SER:H     | 2.32                     | 0.41              |
| 1:A:136:THR:HB   | 1:A:296:ARG:HH11 | 1.84                     | 0.41              |
| 1:A:202:LEU:H    | 1:A:202:LEU:HG   | 1.54                     | 0.41              |
| 2:B:76:LEU:HG    | 2:B:77:TYR:CD2   | 2.55                     | 0.41              |
| 1:C:61:THR:HG21  | 5:C:351:HOH:O    | 2.17                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:178:LYS:HA   | 5:C:367:HOH:O    | 2.21                     | 0.41              |
| 1:C:223:ASP:C    | 1:C:224:ILE:HG13 | 2.41                     | 0.41              |
| 1:C:292:GLY:O    | 1:C:296:ARG:HB2  | 2.20                     | 0.41              |
| 1:A:277:VAL:O    | 1:A:283:ALA:HB2  | 2.19                     | 0.41              |
| 2:B:104:ASP:HB2  | 5:B:172:HOH:O    | 2.19                     | 0.41              |
| 1:C:26:THR:HG22  | 1:C:30:LEU:HG    | 2.01                     | 0.41              |
| 1:C:260:ASN:O    | 5:C:331:HOH:O    | 2.21                     | 0.41              |
| 2:D:28:LYS:C     | 2:D:30:LEU:N     | 2.73                     | 0.41              |
| 2:D:86:ILE:CG2   | 2:D:90:GLU:N     | 2.84                     | 0.41              |
| 2:D:143:LYS:HB3  | 2:D:145:PHE:CZ   | 2.55                     | 0.41              |
| 1:A:189:PRO:CG   | 1:A:192:LEU:HD12 | 2.30                     | 0.41              |
| 2:B:60:LYS:HG3   | 5:B:186:HOH:O    | 2.19                     | 0.41              |
| 1:C:6:GLN:H      | 1:C:303:VAL:HG13 | 1.86                     | 0.41              |
| 1:C:59:PHE:CE2   | 1:C:300:LEU:HD21 | 2.55                     | 0.41              |
| 2:D:56:LYS:HD2   | 2:D:57:ASP:H     | 1.77                     | 0.41              |
| 1:A:219:MET:HE2  | 1:A:257:ALA:HA   | 2.02                     | 0.41              |
| 1:A:229:ARG:HD2  | 1:A:270:VAL:HG23 | 2.02                     | 0.41              |
| 1:C:4:LEU:HA     | 1:C:7:LYS:HG3    | 2.01                     | 0.41              |
| 1:C:274:ALA:O    | 1:C:277:VAL:CG2  | 2.67                     | 0.41              |
| 2:D:134:ILE:H    | 2:D:147:HIS:CE1  | 2.39                     | 0.41              |
| 1:A:4:LEU:HD23   | 1:A:7:LYS:HD2    | 2.02                     | 0.41              |
| 1:A:26:THR:CB    | 1:A:302:LEU:HD21 | 2.50                     | 0.41              |
| 1:A:176:LEU:CD1  | 1:A:184:PHE:CZ   | 3.03                     | 0.41              |
| 1:A:197:TYR:CE1  | 1:A:198:ILE:HD11 | 2.56                     | 0.41              |
| 2:B:38:THR:HG23  | 2:B:38:THR:O     | 2.21                     | 0.41              |
| 1:C:60:GLU:O     | 1:C:70:VAL:HG21  | 2.20                     | 0.41              |
| 1:C:65:ARG:CZ    | 5:C:351:HOH:O    | 2.69                     | 0.41              |
| 1:C:183:ARG:HG2  | 1:C:208:ALA:CB   | 2.51                     | 0.41              |
| 1:C:187:ILE:HG21 | 1:C:215:ILE:HD11 | 2.02                     | 0.41              |
| 1:C:204:GLU:HG2  | 1:C:205:LYS:HZ2  | 1.85                     | 0.41              |
| 1:C:229:ARG:HH12 | 1:C:233:GLU:CG   | 2.34                     | 0.41              |
| 2:D:67:SER:O     | 2:D:71:VAL:CG2   | 2.68                     | 0.41              |
| 2:D:68:GLU:O     | 2:D:72:ASP:OD2   | 2.38                     | 0.41              |
| 2:D:93:GLY:C     | 2:D:95:SER:H     | 2.24                     | 0.41              |
| 2:D:99:LEU:CD2   | 2:D:129:LYS:HZ2  | 2.33                     | 0.41              |
| 2:D:125:PHE:HB3  | 2:D:126:ALA:H    | 1.55                     | 0.41              |
| 2:D:141:CYS:C    | 2:D:143:LYS:N    | 2.73                     | 0.41              |
| 1:A:114:LEU:CD2  | 2:B:115:ILE:HG23 | 2.50                     | 0.41              |
| 1:A:146:GLN:HE21 | 1:A:152:LEU:N    | 2.19                     | 0.41              |
| 1:A:196:GLN:HA   | 1:A:199:LEU:HB2  | 2.02                     | 0.41              |
| 1:C:12:ILE:C     | 1:C:174:GLN:HE22 | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:50:GLU:HB3   | 1:C:51:ALA:H     | 1.65                     | 0.41              |
| 1:C:88:LEU:HD22  | 1:C:106:HIS:NE2  | 2.36                     | 0.41              |
| 1:C:109:GLU:C    | 1:C:111:ALA:H    | 2.24                     | 0.41              |
| 1:C:186:PHE:HE1  | 1:C:209:TRP:HB2  | 1.86                     | 0.41              |
| 1:A:41:HIS:O     | 1:A:42:LYS:O     | 2.39                     | 0.41              |
| 2:B:30:LEU:HA    | 2:B:35:LEU:HD12  | 2.01                     | 0.41              |
| 2:B:58:LEU:HD23  | 2:B:59:ILE:O     | 2.21                     | 0.41              |
| 1:C:110:GLY:N    | 1:C:129:ASP:OD1  | 2.49                     | 0.41              |
| 1:C:157:VAL:CG1  | 1:C:158:ALA:H    | 2.12                     | 0.41              |
| 2:D:30:LEU:HB3   | 2:D:36:THR:OG1   | 2.21                     | 0.41              |
| 1:A:10:ILE:HD12  | 1:A:113:ARG:HD2  | 2.02                     | 0.41              |
| 1:A:56:ARG:HG2   | 1:A:60:GLU:OE2   | 2.21                     | 0.41              |
| 1:A:110:GLY:C    | 1:A:112:ALA:H    | 2.24                     | 0.41              |
| 1:A:126:ASN:HD22 | 1:A:135:PRO:HD2  | 1.86                     | 0.41              |
| 1:C:26:THR:HA    | 1:C:29:LYS:HD2   | 2.02                     | 0.41              |
| 1:C:44:ILE:HG13  | 1:C:101:ALA:CB   | 2.42                     | 0.41              |
| 1:C:54:ARG:NH1   | 1:C:268:PRO:HD3  | 2.35                     | 0.41              |
| 1:C:92:ILE:HD13  | 1:C:95:ILE:HD12  | 2.02                     | 0.41              |
| 1:C:116:THR:HG22 | 1:C:124:VAL:HG11 | 2.03                     | 0.41              |
| 1:C:126:ASN:ND2  | 1:C:126:ASN:C    | 2.74                     | 0.41              |
| 1:C:163:LEU:CD1  | 1:C:188:ALA:HB2  | 2.51                     | 0.41              |
| 1:C:186:PHE:O    | 1:C:187:ILE:HG13 | 2.21                     | 0.41              |
| 2:D:111:ASN:C    | 2:D:113:ASN:H    | 2.23                     | 0.41              |
| 2:B:23:ALA:C     | 2:B:25:ILE:H     | 2.23                     | 0.41              |
| 1:C:214:SER:HB2  | 1:C:216:GLU:CD   | 2.40                     | 0.41              |
| 2:D:41:ARG:CB    | 2:D:62:GLU:CB    | 2.93                     | 0.41              |
| 2:D:105:ASN:HA   | 2:D:123:SER:C    | 2.42                     | 0.41              |
| 1:A:100:ASP:HB2  | 5:A:1410:HOH:O   | 2.21                     | 0.40              |
| 1:A:146:GLN:NE2  | 1:A:152:LEU:N    | 2.68                     | 0.40              |
| 1:A:176:LEU:HB2  | 1:A:184:PHE:CZ   | 2.55                     | 0.40              |
| 1:A:195:PRO:O    | 1:A:198:ILE:HD13 | 2.22                     | 0.40              |
| 1:A:266:PRO:O    | 1:A:267:LEU:O    | 2.38                     | 0.40              |
| 2:B:34:LYS:HD3   | 2:B:37:GLU:OE2   | 2.21                     | 0.40              |
| 2:B:138:CYS:CB   | 5:B:221:HOH:O    | 2.69                     | 0.40              |
| 1:C:9:ILE:HB     | 1:C:125:LEU:HG   | 2.02                     | 0.40              |
| 1:C:12:ILE:CD1   | 1:C:135:PRO:HA   | 2.32                     | 0.40              |
| 1:C:48:PHE:HB3   | 1:C:74:SER:O     | 2.20                     | 0.40              |
| 1:C:92:ILE:CD1   | 1:C:115:ALA:HB1  | 2.52                     | 0.40              |
| 1:C:261:MET:O    | 1:C:282:HIS:ND1  | 2.54                     | 0.40              |
| 2:D:22:PRO:HB2   | 2:D:25:ILE:HG13  | 2.03                     | 0.40              |
| 2:D:75:ALA:N     | 2:D:97:PRO:HB2   | 2.36                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:141:CYS:C    | 2:D:143:LYS:H    | 2.25                     | 0.40              |
| 1:A:55:THR:HG21  | 1:A:105:ARG:NE   | 2.35                     | 0.40              |
| 1:A:250:ARG:NH2  | 1:A:276:ASP:OD2  | 2.54                     | 0.40              |
| 1:A:262:LYS:HG2  | 1:A:282:HIS:HA   | 2.03                     | 0.40              |
| 1:A:298:ALA:O    | 1:A:302:LEU:CD2  | 2.69                     | 0.40              |
| 5:B:165:HOH:O    | 2:D:49:PRO:HG2   | 2.21                     | 0.40              |
| 1:C:39:LEU:HD12  | 1:C:39:LEU:N     | 2.36                     | 0.40              |
| 1:C:132:ASN:O    | 1:C:170:HIS:ND1  | 2.54                     | 0.40              |
| 1:C:197:TYR:CE1  | 2:D:143:LYS:HA   | 2.56                     | 0.40              |
| 1:C:219:MET:CB   | 1:C:256:ASN:ND2  | 2.72                     | 0.40              |
| 2:D:65:PHE:HB3   | 2:D:66:LEU:H     | 1.67                     | 0.40              |
| 2:D:86:ILE:HG13  | 2:D:91:VAL:HG22  | 2.02                     | 0.40              |
| 1:A:33:ASN:HA    | 1:A:34:PRO:HD3   | 1.74                     | 0.40              |
| 1:C:135:PRO:HG2  | 1:C:136:THR:N    | 2.35                     | 0.40              |
| 1:C:189:PRO:HD2  | 1:C:192:LEU:HD12 | 2.02                     | 0.40              |
| 1:C:250:ARG:O    | 1:C:252:SER:N    | 2.54                     | 0.40              |
| 1:C:264:LEU:CA   | 1:C:288:GLN:OE1  | 2.70                     | 0.40              |
| 1:C:271:ASP:O    | 1:C:272:GLU:C    | 2.59                     | 0.40              |
| 1:A:12:ILE:HD11  | 1:A:135:PRO:HA   | 2.04                     | 0.40              |
| 1:A:160:VAL:O    | 1:A:227:MET:HA   | 2.21                     | 0.40              |
| 1:A:229:ARG:HA   | 1:A:272:GLU:OE2  | 2.21                     | 0.40              |
| 1:A:277:VAL:HG12 | 1:A:285:TYR:OH   | 2.21                     | 0.40              |
| 1:C:164:LYS:HG3  | 1:C:195:PRO:HD3  | 2.02                     | 0.40              |
| 2:D:34:LYS:HD3   | 2:D:37:GLU:CD    | 2.42                     | 0.40              |
| 2:B:46:LEU:HD12  | 2:D:42:ILE:CD1   | 2.52                     | 0.40              |
| 2:B:117:HIS:ND1  | 2:B:117:HIS:N    | 2.69                     | 0.40              |
| 1:C:31:LYS:NZ    | 1:C:143:PHE:CE2  | 2.80                     | 0.40              |
| 1:C:246:GLN:HA   | 5:C:314:HOH:O    | 2.20                     | 0.40              |
| 2:D:30:LEU:HD13  | 2:D:30:LEU:N     | 2.34                     | 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 X-ray entries followed by that with respect to entries of similar resolution.

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   | A     | 308/310 (99%) | 200 (65%) | 73 (24%)  | 35 (11%)  | 0           | 1 |
| 1   | C     | 308/310 (99%) | 187 (61%) | 70 (23%)  | 51 (17%)  | 0           | 0 |
| 2   | B     | 144/153 (94%) | 82 (57%)  | 44 (31%)  | 18 (12%)  | 0           | 0 |
| 2   | D     | 144/153 (94%) | 88 (61%)  | 34 (24%)  | 22 (15%)  | 0           | 0 |
| All | All   | 904/926 (98%) | 557 (62%) | 221 (24%) | 126 (14%) | 0           | 0 |

All (126) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | GLN  |
| 1   | A     | 21  | ASN  |
| 1   | A     | 192 | LEU  |
| 1   | A     | 231 | GLN  |
| 1   | A     | 244 | LYS  |
| 1   | A     | 302 | LEU  |
| 2   | B     | 10  | GLU  |
| 2   | B     | 85  | ARG  |
| 2   | B     | 106 | VAL  |
| 2   | B     | 142 | GLU  |
| 1   | C     | 32  | ALA  |
| 1   | C     | 37  | GLU  |
| 1   | C     | 68  | ALA  |
| 1   | C     | 97  | THR  |
| 1   | C     | 98  | TYR  |
| 1   | C     | 190 | ASP  |
| 1   | C     | 209 | TRP  |
| 1   | C     | 213 | SER  |
| 1   | C     | 231 | GLN  |
| 1   | C     | 235 | LEU  |
| 1   | C     | 258 | LYS  |
| 1   | C     | 283 | ALA  |
| 1   | C     | 293 | ILE  |
| 1   | C     | 295 | ALA  |
| 1   | C     | 296 | ARG  |
| 2   | D     | 75  | ALA  |
| 2   | D     | 105 | ASN  |
| 2   | D     | 106 | VAL  |
| 2   | D     | 115 | ILE  |
| 2   | D     | 127 | VAL  |
| 1   | A     | 37  | GLU  |
| 1   | A     | 38  | LEU  |
| 1   | A     | 42  | LYS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 89  | ALA  |
| 1   | A     | 93  | SER  |
| 1   | A     | 132 | ASN  |
| 1   | A     | 150 | GLY  |
| 1   | A     | 197 | TYR  |
| 1   | A     | 201 | MET  |
| 1   | A     | 252 | SER  |
| 1   | A     | 267 | LEU  |
| 1   | A     | 309 | VAL  |
| 2   | B     | 41  | ARG  |
| 2   | B     | 67  | SER  |
| 2   | B     | 77  | TYR  |
| 2   | B     | 101 | GLU  |
| 2   | B     | 105 | ASN  |
| 2   | B     | 118 | ALA  |
| 1   | C     | 14  | ASP  |
| 1   | C     | 42  | LYS  |
| 1   | C     | 113 | ARG  |
| 1   | C     | 153 | ASP  |
| 1   | C     | 154 | ASN  |
| 1   | C     | 166 | GLY  |
| 1   | C     | 193 | ALA  |
| 1   | C     | 238 | SER  |
| 1   | C     | 255 | HIS  |
| 1   | C     | 306 | ARG  |
| 2   | D     | 29  | LEU  |
| 2   | D     | 114 | CYS  |
| 2   | D     | 123 | SER  |
| 2   | D     | 135 | ALA  |
| 2   | D     | 142 | GLU  |
| 1   | A     | 16  | SER  |
| 1   | A     | 52  | SER  |
| 1   | A     | 78  | ASN  |
| 1   | A     | 205 | LYS  |
| 1   | A     | 283 | ALA  |
| 2   | B     | 9   | VAL  |
| 2   | B     | 47  | ASN  |
| 2   | B     | 63  | ASN  |
| 2   | B     | 88  | ASN  |
| 1   | C     | 18  | ASP  |
| 1   | C     | 40  | LYS  |
| 1   | C     | 54  | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 55  | THR  |
| 1   | C     | 135 | PRO  |
| 1   | C     | 151 | ARG  |
| 1   | C     | 157 | VAL  |
| 1   | C     | 158 | ALA  |
| 1   | C     | 172 | LEU  |
| 1   | C     | 194 | MET  |
| 1   | C     | 292 | GLY  |
| 2   | D     | 10  | GLU  |
| 2   | D     | 112 | SER  |
| 2   | D     | 131 | ALA  |
| 2   | D     | 147 | HIS  |
| 1   | A     | 167 | ARG  |
| 1   | A     | 219 | MET  |
| 1   | A     | 255 | HIS  |
| 2   | B     | 124 | SER  |
| 1   | C     | 67  | GLY  |
| 1   | C     | 246 | GLN  |
| 2   | D     | 42  | ILE  |
| 2   | D     | 67  | SER  |
| 2   | D     | 116 | SER  |
| 1   | A     | 3   | PRO  |
| 1   | A     | 271 | ASP  |
| 2   | B     | 73  | GLN  |
| 2   | B     | 130 | ARG  |
| 1   | C     | 36  | PRO  |
| 1   | C     | 71  | VAL  |
| 1   | C     | 83  | LYS  |
| 1   | C     | 84  | LYS  |
| 1   | C     | 242 | ASN  |
| 1   | C     | 302 | LEU  |
| 2   | D     | 95  | SER  |
| 1   | A     | 144 | THR  |
| 1   | A     | 168 | THR  |
| 1   | A     | 218 | VAL  |
| 1   | C     | 66  | LEU  |
| 1   | C     | 76  | SER  |
| 1   | C     | 267 | LEU  |
| 2   | D     | 12  | ILE  |
| 1   | A     | 206 | GLY  |
| 1   | A     | 222 | VAL  |
| 2   | D     | 45  | GLY  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 134 | ILE  |
| 1   | A     | 293 | ILE  |
| 1   | C     | 10  | ILE  |
| 1   | A     | 189 | PRO  |
| 2   | B     | 92  | VAL  |
| 1   | C     | 270 | VAL  |
| 2   | D     | 121 | VAL  |
| 1   | C     | 187 | ILE  |
| 1   | C     | 207 | ILE  |

### 5.3.2 Protein sidechains [\(i\)](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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   | A     | 260/260 (100%) | 209 (80%) | 51 (20%)  | 1   4       |
| 1   | C     | 260/260 (100%) | 218 (84%) | 42 (16%)  | 2   7       |
| 2   | B     | 129/137 (94%)  | 112 (87%) | 17 (13%)  | 4   12      |
| 2   | D     | 129/137 (94%)  | 112 (87%) | 17 (13%)  | 4   12      |
| All | All   | 778/794 (98%)  | 651 (84%) | 127 (16%) | 2   7       |

All (127) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | ASP  |
| 1   | A     | 18  | ASP  |
| 1   | A     | 19  | ASP  |
| 1   | A     | 21  | ASN  |
| 1   | A     | 35  | GLN  |
| 1   | A     | 37  | GLU  |
| 1   | A     | 47  | CYS  |
| 1   | A     | 59  | PHE  |
| 1   | A     | 62  | SER  |
| 1   | A     | 70  | VAL  |
| 1   | A     | 74  | SER  |
| 1   | A     | 79  | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 91  | THR  |
| 1   | A     | 92  | ILE  |
| 1   | A     | 97  | THR  |
| 1   | A     | 100 | ASP  |
| 1   | A     | 104 | MET  |
| 1   | A     | 109 | GLU  |
| 1   | A     | 113 | ARG  |
| 1   | A     | 114 | LEU  |
| 1   | A     | 125 | LEU  |
| 1   | A     | 134 | HIS  |
| 1   | A     | 137 | GLN  |
| 1   | A     | 143 | PHE  |
| 1   | A     | 144 | THR  |
| 1   | A     | 145 | ILE  |
| 1   | A     | 146 | GLN  |
| 1   | A     | 152 | LEU  |
| 1   | A     | 156 | HIS  |
| 1   | A     | 176 | LEU  |
| 1   | A     | 180 | ASP  |
| 1   | A     | 194 | MET  |
| 1   | A     | 196 | GLN  |
| 1   | A     | 219 | MET  |
| 1   | A     | 225 | LEU  |
| 1   | A     | 233 | GLU  |
| 1   | A     | 250 | ARG  |
| 1   | A     | 253 | ASP  |
| 1   | A     | 255 | HIS  |
| 1   | A     | 267 | LEU  |
| 1   | A     | 269 | ARG  |
| 1   | A     | 275 | THR  |
| 1   | A     | 278 | ASP  |
| 1   | A     | 282 | HIS  |
| 1   | A     | 285 | TYR  |
| 1   | A     | 287 | GLN  |
| 1   | A     | 291 | ASN  |
| 1   | A     | 302 | LEU  |
| 1   | A     | 303 | VAL  |
| 1   | A     | 305 | ASN  |
| 1   | A     | 306 | ARG  |
| 2   | B     | 36  | THR  |
| 2   | B     | 37  | GLU  |
| 2   | B     | 38  | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 44  | ILE  |
| 2   | B     | 46  | LEU  |
| 2   | B     | 47  | ASN  |
| 2   | B     | 53  | MET  |
| 2   | B     | 70  | GLN  |
| 2   | B     | 76  | LEU  |
| 2   | B     | 102 | ARG  |
| 2   | B     | 106 | VAL  |
| 2   | B     | 113 | ASN  |
| 2   | B     | 117 | HIS  |
| 2   | B     | 129 | LYS  |
| 2   | B     | 134 | ILE  |
| 2   | B     | 151 | LEU  |
| 2   | B     | 153 | ASN  |
| 1   | C     | 14  | ASP  |
| 1   | C     | 15  | LEU  |
| 1   | C     | 18  | ASP  |
| 1   | C     | 23  | VAL  |
| 1   | C     | 37  | GLU  |
| 1   | C     | 38  | LEU  |
| 1   | C     | 48  | PHE  |
| 1   | C     | 49  | PHE  |
| 1   | C     | 56  | ARG  |
| 1   | C     | 59  | PHE  |
| 1   | C     | 70  | VAL  |
| 1   | C     | 98  | TYR  |
| 1   | C     | 100 | ASP  |
| 1   | C     | 102 | ILE  |
| 1   | C     | 106 | HIS  |
| 1   | C     | 109 | GLU  |
| 1   | C     | 121 | ASN  |
| 1   | C     | 140 | LEU  |
| 1   | C     | 146 | GLN  |
| 1   | C     | 147 | GLU  |
| 1   | C     | 149 | GLN  |
| 1   | C     | 151 | ARG  |
| 1   | C     | 152 | LEU  |
| 1   | C     | 174 | GLN  |
| 1   | C     | 180 | ASP  |
| 1   | C     | 183 | ARG  |
| 1   | C     | 196 | GLN  |
| 1   | C     | 202 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 204 | GLU  |
| 1   | C     | 205 | LYS  |
| 1   | C     | 216 | GLU  |
| 1   | C     | 233 | GLU  |
| 1   | C     | 235 | LEU  |
| 1   | C     | 242 | ASN  |
| 1   | C     | 243 | VAL  |
| 1   | C     | 247 | PHE  |
| 1   | C     | 278 | ASP  |
| 1   | C     | 293 | ILE  |
| 1   | C     | 294 | PHE  |
| 1   | C     | 306 | ARG  |
| 1   | C     | 308 | LEU  |
| 1   | C     | 310 | LEU  |
| 2   | D     | 12  | ILE  |
| 2   | D     | 27  | PHE  |
| 2   | D     | 30  | LEU  |
| 2   | D     | 36  | THR  |
| 2   | D     | 39  | ASP  |
| 2   | D     | 44  | ILE  |
| 2   | D     | 52  | GLU  |
| 2   | D     | 57  | ASP  |
| 2   | D     | 58  | LEU  |
| 2   | D     | 72  | ASP  |
| 2   | D     | 76  | LEU  |
| 2   | D     | 77  | TYR  |
| 2   | D     | 99  | LEU  |
| 2   | D     | 106 | VAL  |
| 2   | D     | 114 | CYS  |
| 2   | D     | 125 | PHE  |
| 2   | D     | 136 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 33  | ASN  |
| 1   | A     | 35  | GLN  |
| 1   | A     | 78  | ASN  |
| 1   | A     | 126 | ASN  |
| 1   | A     | 146 | GLN  |
| 1   | A     | 149 | GLN  |
| 1   | A     | 231 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 242 | ASN  |
| 1   | A     | 287 | GLN  |
| 1   | A     | 291 | ASN  |
| 2   | B     | 63  | ASN  |
| 2   | B     | 70  | GLN  |
| 2   | B     | 105 | ASN  |
| 2   | B     | 132 | ASN  |
| 1   | C     | 33  | ASN  |
| 1   | C     | 64  | HIS  |
| 1   | C     | 121 | ASN  |
| 1   | C     | 231 | GLN  |
| 1   | C     | 256 | ASN  |
| 1   | C     | 287 | GLN  |
| 2   | D     | 24  | GLN  |
| 2   | D     | 63  | ASN  |
| 2   | D     | 111 | ASN  |
| 2   | D     | 132 | ASN  |
| 2   | D     | 148 | ASN  |

### 5.3.3 RNA [\(i\)](#)

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 monosaccharides in this entry.

### 5.6 Ligand geometry [\(i\)](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | PCT  | A     | 1311 | -    | 7,7,7        | 2.81 | 3 (42%)  | 9,10,10     | 0.93 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|-------|
| 3   | PCT  | A     | 1311 | -    | -       | 1/4/5/5  | -     |

All (3) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | A     | 1311 | PCT  | P-O1P | 5.41  | 1.61        | 1.50     |
| 3   | A     | 1311 | PCT  | P-O2P | -3.47 | 1.47        | 1.54     |
| 3   | A     | 1311 | PCT  | P-O3P | 2.97  | 1.61        | 1.54     |

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 3   | A     | 1311 | PCT  | O1-C1-C1P-P |

There are no ring outliers.

1 monomer is involved in 3 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | A     | 1311 | PCT  | 3       | 0            |

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 1   | A     | 310/310 (100%) | -0.63  | 0 100 100    | 13, 49, 72, 89        | 0     |
| 1   | C     | 310/310 (100%) | -0.50  | 3 (0%) 82 82 | 60, 90, 112, 137      | 0     |
| 2   | B     | 146/153 (95%)  | -0.48  | 1 (0%) 87 87 | 41, 78, 98, 102       | 0     |
| 2   | D     | 146/153 (95%)  | -0.24  | 5 (3%) 45 40 | 84, 104, 121, 127     | 0     |
| All | All   | 912/926 (98%)  | -0.50  | 9 (0%) 82 82 | 13, 82, 115, 137      | 0     |

All (9) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | D     | 18  | ILE  | 5.2  |
| 2   | D     | 58  | LEU  | 5.0  |
| 2   | D     | 59  | ILE  | 4.1  |
| 1   | C     | 173 | THR  | 3.9  |
| 2   | B     | 9   | VAL  | 2.8  |
| 2   | D     | 56  | LYS  | 2.7  |
| 1   | C     | 186 | PHE  | 2.5  |
| 2   | D     | 21  | ILE  | 2.3  |
| 1   | C     | 40  | LYS  | 2.1  |

### 6.2 Non-standard residues in protein, DNA, RNA chains i

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

### 6.3 Carbohydrates i

There are no monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 3   | PCT  | A     | 1311 | 8/8   | 0.96 | 0.15 | 32,36,38,39                | 0     |
| 4   | ZN   | D     | 154  | 1/1   | 0.98 | 0.07 | 47,47,47,47                | 0     |
| 4   | ZN   | B     | 154  | 1/1   | 0.99 | 0.16 | 45,45,45,45                | 0     |

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.