



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 12:24 PM JST

PDB ID : 5IZ7
EMDB ID : EMD-8139
Title : Cryo-EM structure of thermally stable Zika virus strain H/PF/2013
Authors : Kostyuchenko, V.A.; Zhang, S.; Fibriansah, G.; Lok, S.M.
Deposited on : 2016-03-25
Resolution : 3.70 Å(reported)
Based on initial model : 3J27

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

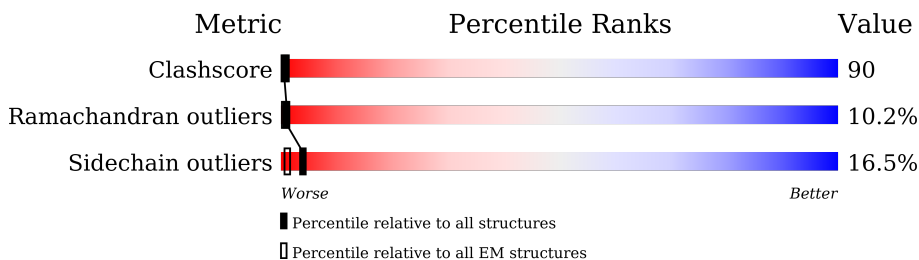
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 504 | <div> <div>36%</div> <div>18% 62% 18%</div> </div> |
| 1 | B | 504 | <div> <div>32%</div> <div>19% 59% 20%</div> </div> |
| 1 | C | 504 | <div> <div>44%</div> <div>22% 61% 15%</div> </div> |
| 2 | D | 75 | <div> <div>53%</div> <div>11% 67% 19%</div> </div> |
| 2 | E | 75 | <div> <div>64%</div> <div>19% 64% 17%</div> </div> |
| 2 | F | 75 | <div> <div>56%</div> <div>23% 60% 16%</div> </div> |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13268 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called structural protein E.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 504 | Total | C | N | O | S | 0 | 0 |
| | | | 3809 | 2395 | 660 | 723 | 31 | | |
| 1 | C | 504 | Total | C | N | O | S | 0 | 0 |
| | | | 3808 | 2395 | 660 | 722 | 31 | | |
| 1 | B | 504 | Total | C | N | O | S | 0 | 0 |
| | | | 3809 | 2395 | 660 | 723 | 31 | | |

- Molecule 2 is a protein called structural protein M.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | D | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 600 | 391 | 105 | 103 | 1 | | |
| 2 | E | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 600 | 391 | 105 | 103 | 1 | | |
| 2 | F | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 600 | 391 | 105 | 103 | 1 | | |

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

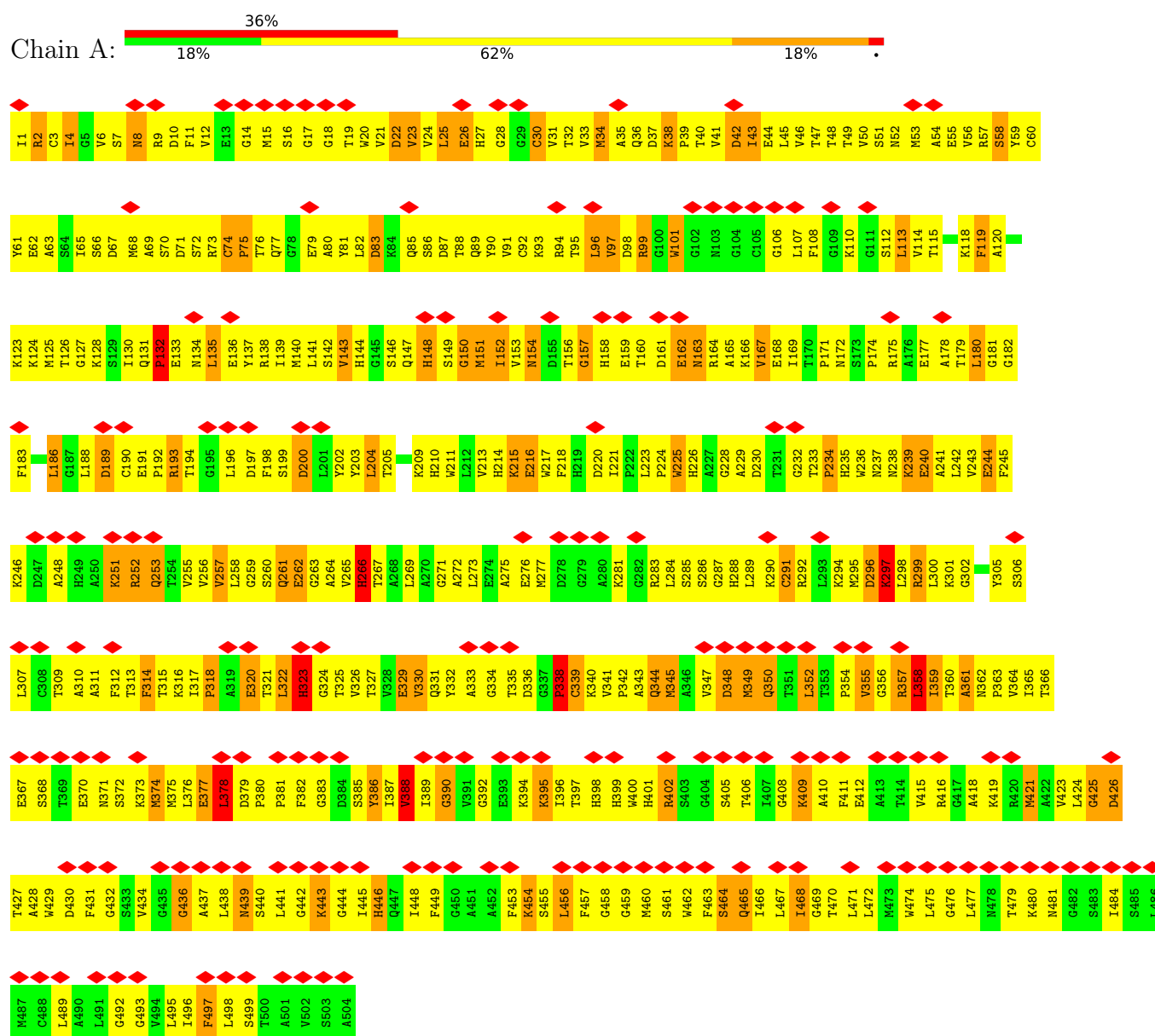


| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 3 | A | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 3 | C | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 3 | B | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |

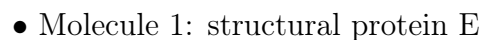
3 Residue-property plots

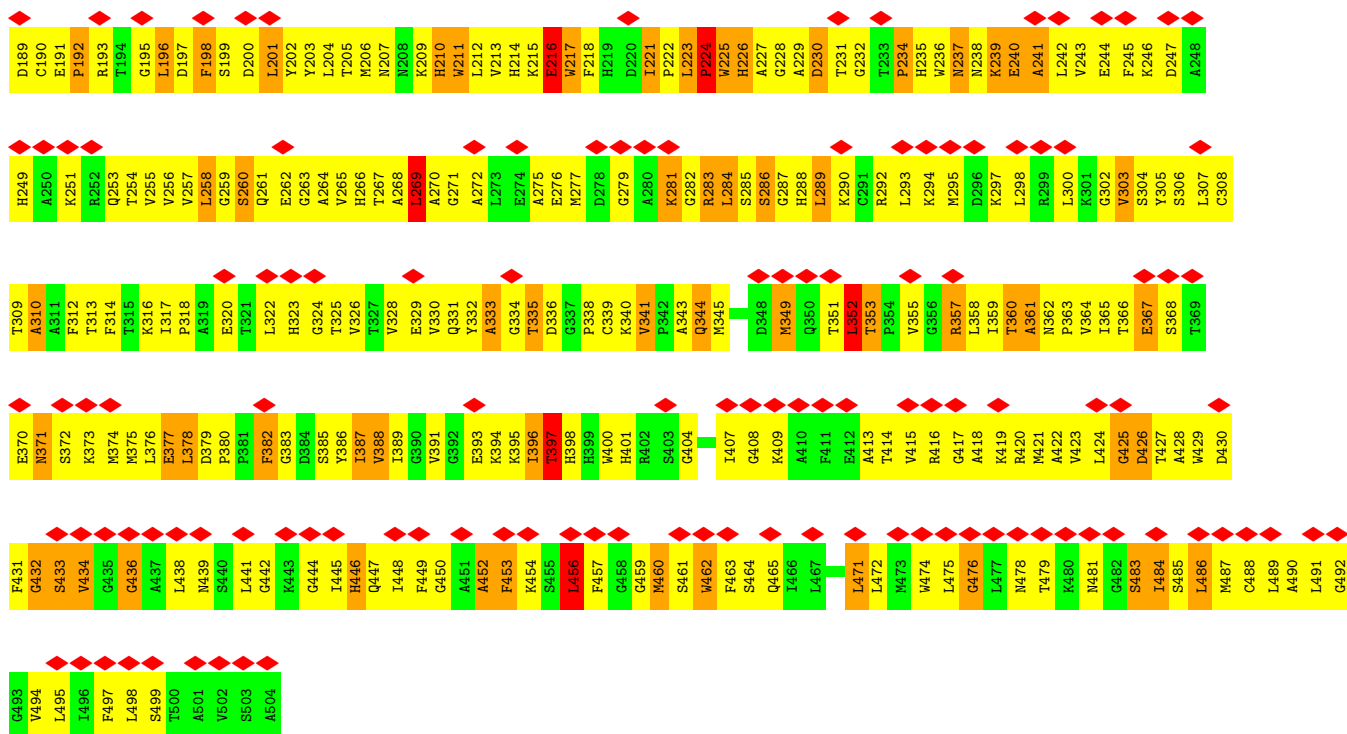
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: structural protein E

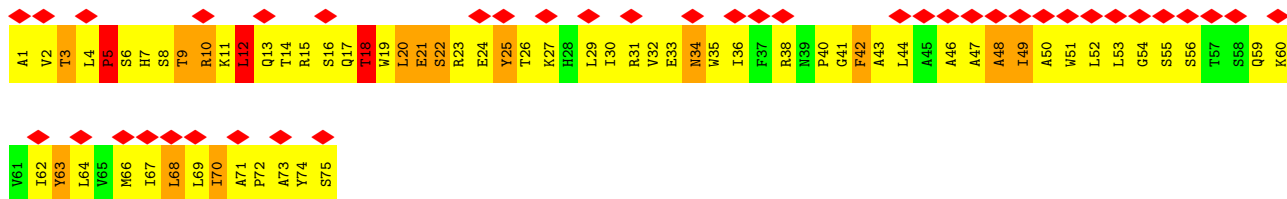
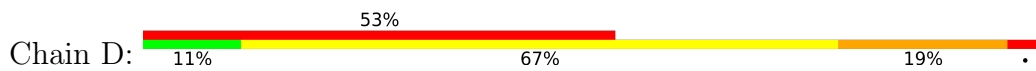


• Molecule 1: structural protein E

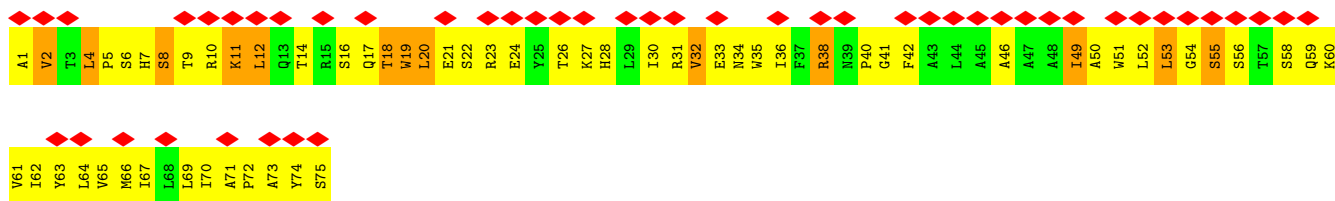




• Molecule 2: structural protein M



• Molecule 2: structural protein M



• Molecule 2: structural protein M



| | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Y61 | Y62 | Y63 | Y64 | Y65 | Y66 | Y67 | Y68 | Y69 | Y70 | Y71 | Y72 | Y73 | Y74 | Y75 |
| | | | | | | | | | | | | | | |

4 Experimental information

| Property | Value | Source |
|--------------------------------------|--|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, I | Depositor |
| Number of particles used | 7180 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION; correction for astigmatism included | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON II (4k x 4k) | Depositor |
| Maximum map value | 11.108 | Depositor |
| Minimum map value | -6.234 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 1.000 | Depositor |
| Recommended contour level | 3.5 | Depositor |
| Map size (\AA) | 536.0, 536.0, 536.0 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.34, 1.34, 1.34 | Depositor |

5 Model quality

5.1 Standard geometry

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

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 | 0.60 | 0/3888 | 0.87 | 5/5261 (0.1%) |
| 1 | B | 0.65 | 0/3888 | 0.93 | 9/5261 (0.2%) |
| 1 | C | 0.66 | 1/3887 (0.0%) | 0.91 | 8/5261 (0.2%) |
| 2 | D | 0.61 | 0/615 | 0.82 | 1/838 (0.1%) |
| 2 | E | 0.77 | 0/615 | 0.86 | 0/838 |
| 2 | F | 0.66 | 0/615 | 0.85 | 1/838 (0.1%) |
| All | All | 0.64 | 1/13508 (0.0%) | 0.90 | 24/18297 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | F | 0 | 1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | C | 225 | TRP | CB-CG | -8.14 | 1.35 | 1.50 |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | C | 334 | GLY | N-CA-C | 6.91 | 130.37 | 113.10 |
| 1 | B | 224 | PRO | N-CA-C | -6.73 | 94.61 | 112.10 |
| 1 | B | 82 | LEU | N-CA-C | 6.66 | 128.98 | 111.00 |
| 1 | C | 348 | ASP | N-CA-C | 6.48 | 128.49 | 111.00 |
| 1 | B | 456 | LEU | CA-CB-CG | 6.47 | 130.18 | 115.30 |
| 1 | B | 438 | LEU | CA-CB-CG | 6.42 | 130.06 | 115.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | B | 378 | LEU | CA-CB-CG | 6.17 | 129.49 | 115.30 |
| 1 | C | 204 | LEU | CA-CB-CG | -5.84 | 101.86 | 115.30 |
| 1 | C | 392 | GLY | N-CA-C | 5.81 | 127.63 | 113.10 |
| 2 | D | 5 | PRO | N-CA-C | 5.78 | 127.13 | 112.10 |
| 1 | A | 458 | GLY | N-CA-C | -5.74 | 98.75 | 113.10 |
| 1 | A | 358 | LEU | N-CA-C | 5.73 | 126.46 | 111.00 |
| 1 | A | 310 | ALA | N-CA-C | 5.59 | 126.10 | 111.00 |
| 1 | B | 230 | ASP | N-CA-C | -5.54 | 96.03 | 111.00 |
| 1 | A | 251 | LYS | N-CA-C | 5.52 | 125.91 | 111.00 |
| 1 | C | 3 | CYS | CA-CB-SG | -5.50 | 104.11 | 114.00 |
| 1 | B | 308 | CYS | CA-CB-SG | 5.38 | 123.69 | 114.00 |
| 2 | F | 54 | GLY | N-CA-C | -5.37 | 99.67 | 113.10 |
| 1 | B | 228 | GLY | N-CA-C | -5.29 | 99.87 | 113.10 |
| 1 | C | 226 | HIS | N-CA-C | -5.27 | 96.78 | 111.00 |
| 1 | A | 309 | THR | N-CA-C | 5.21 | 125.05 | 111.00 |
| 1 | C | 348 | ASP | CB-CG-OD2 | -5.20 | 113.62 | 118.30 |
| 1 | B | 27 | HIS | N-CA-C | -5.12 | 97.18 | 111.00 |
| 1 | C | 310 | ALA | N-CA-C | -5.09 | 97.25 | 111.00 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | F | 74 | 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 | 3809 | 0 | 3761 | 684 | 0 |
| 1 | B | 3809 | 0 | 3760 | 770 | 0 |
| 1 | C | 3808 | 0 | 3760 | 682 | 0 |
| 2 | D | 600 | 0 | 624 | 165 | 0 |
| 2 | E | 600 | 0 | 624 | 119 | 0 |
| 2 | F | 600 | 0 | 624 | 124 | 0 |
| 3 | A | 14 | 0 | 13 | 4 | 0 |
| 3 | B | 14 | 0 | 13 | 1 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | C | 14 | 0 | 13 | 5 | 0 |
| All | All | 13268 | 0 | 13192 | 2386 | 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 90.

All (2386) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:68:MET:SD | 1:C:255:VAL:HB | 1.79 | 1.21 |
| 1:B:345:MET:HE3 | 1:B:380:PRO:HA | 1.23 | 1.16 |
| 1:C:178:ALA:HB3 | 1:C:186:LEU:H | 1.08 | 1.15 |
| 1:A:158:HIS:HB3 | 1:A:166:LYS:HE3 | 1.20 | 1.15 |
| 1:B:60:CYS:HB3 | 1:B:224:PRO:HG2 | 1.21 | 1.14 |
| 1:B:271:GLY:HA3 | 2:E:7:HIS:CD2 | 1.83 | 1.14 |
| 1:A:50:VAL:HG11 | 1:A:130:ILE:HD12 | 1.15 | 1.14 |
| 1:A:332:TYR:HB3 | 1:A:335:THR:HG21 | 1.20 | 1.14 |
| 2:E:55:SER:HA | 2:E:60:LYS:HG3 | 1.29 | 1.13 |
| 1:C:34:MET:HE1 | 1:C:359:ILE:HG23 | 1.15 | 1.13 |
| 1:B:286:SER:HB3 | 2:E:16:SER:HB3 | 1.31 | 1.12 |
| 1:A:73:ARG:NH2 | 1:A:77:GLN:HB3 | 1.63 | 1.12 |
| 1:C:65:ILE:HD11 | 1:C:243:VAL:HG22 | 1.30 | 1.10 |
| 2:E:56:SER:HB3 | 2:E:59:GLN:HB2 | 1.35 | 1.09 |
| 1:B:71:ASP:HB2 | 1:B:82:LEU:HD13 | 1.30 | 1.09 |
| 1:B:95:THR:HG22 | 1:B:96:LEU:H | 1.01 | 1.08 |
| 1:C:12:VAL:HG13 | 1:C:33:VAL:HG13 | 1.31 | 1.08 |
| 1:C:93:LYS:HB2 | 1:C:245:PHE:HE1 | 1.12 | 1.08 |
| 1:C:211:TRP:HE1 | 1:C:269:LEU:HD13 | 1.04 | 1.08 |
| 1:B:1:ILE:HG21 | 1:B:147:GLN:HB2 | 1.36 | 1.08 |
| 2:D:56:SER:HB3 | 2:D:59:GLN:HG2 | 1.08 | 1.06 |
| 1:B:41:VAL:HG22 | 1:B:143:VAL:HG22 | 1.31 | 1.06 |
| 1:A:152:ILE:HG12 | 1:A:153:VAL:H | 1.17 | 1.05 |
| 1:A:479:THR:HG22 | 1:A:480:LYS:H | 1.19 | 1.05 |
| 1:A:332:TYR:HB3 | 1:A:335:THR:CG2 | 1.86 | 1.05 |
| 1:A:263:GLY:O | 1:A:267:THR:HG23 | 1.54 | 1.05 |
| 1:C:25:LEU:HD23 | 1:C:43:ILE:HD12 | 1.38 | 1.04 |
| 1:B:21:VAL:HG11 | 1:B:293:LEU:HB3 | 1.37 | 1.04 |
| 1:B:100:GLY:HA3 | 1:B:108:PHE:CE1 | 1.91 | 1.04 |
| 1:C:300:LEU:HD23 | 1:C:301:LYS:H | 1.16 | 1.04 |
| 1:C:337:GLY:HA2 | 1:C:368:SER:HA | 1.04 | 1.03 |
| 2:D:32:VAL:HG23 | 2:D:72:PRO:HG3 | 1.38 | 1.03 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:67:ILE:HA | 2:D:70:ILE:HG22 | 1.41 | 1.03 |
| 1:C:245:PHE:HB3 | 1:C:255:VAL:HA | 1.41 | 1.02 |
| 2:D:55:SER:HA | 2:D:60:LYS:HE2 | 1.39 | 1.01 |
| 1:B:21:VAL:HG13 | 1:B:293:LEU:H | 1.23 | 1.01 |
| 1:A:46:VAL:HG12 | 1:A:47:THR:HG23 | 1.42 | 1.01 |
| 2:D:18:THR:HG23 | 2:D:21:GLU:HB2 | 1.39 | 1.00 |
| 1:A:299:ARG:HB2 | 1:A:299:ARG:NH1 | 1.77 | 1.00 |
| 1:B:180:LEU:H | 1:B:180:LEU:HD12 | 1.24 | 1.00 |
| 1:B:223:LEU:HB2 | 1:B:224:PRO:HD3 | 1.44 | 1.00 |
| 1:A:152:ILE:HG12 | 1:A:153:VAL:N | 1.70 | 1.00 |
| 1:B:43:ILE:HG23 | 1:B:141:LEU:HB3 | 1.41 | 1.00 |
| 1:A:359:ILE:HD11 | 1:A:377:GLU:HG2 | 1.42 | 0.99 |
| 1:C:2:ARG:HD2 | 1:C:44:GLU:OE1 | 1.61 | 0.99 |
| 1:B:25:LEU:HD13 | 1:B:139:ILE:HG21 | 1.40 | 0.99 |
| 1:B:221:ILE:HD12 | 2:E:4:LEU:HA | 1.41 | 0.98 |
| 1:C:59:TYR:O | 1:C:124:LYS:HB2 | 1.64 | 0.98 |
| 1:B:32:THR:HA | 1:B:42:ASP:HB3 | 1.44 | 0.98 |
| 1:B:57:ARG:HA | 1:B:227:ALA:CB | 1.94 | 0.98 |
| 1:C:20:TRP:HA | 1:C:293:LEU:O | 1.63 | 0.97 |
| 1:A:175:ARG:HG2 | 1:A:189:ASP:HB3 | 1.46 | 0.97 |
| 1:B:20:TRP:O | 1:B:433:SER:HB3 | 1.63 | 0.97 |
| 1:B:4:ILE:H | 1:B:151:MET:HE3 | 1.29 | 0.96 |
| 1:C:345:MET:HB2 | 1:C:355:VAL:O | 1.63 | 0.96 |
| 2:D:23:ARG:HB3 | 2:D:27:LYS:HE3 | 1.47 | 0.96 |
| 2:D:56:SER:CB | 2:D:59:GLN:HG2 | 1.95 | 0.96 |
| 1:C:27:HIS:CE1 | 1:C:48:THR:HG22 | 2.01 | 0.96 |
| 1:B:137:TYR:HD2 | 1:B:289:LEU:HD22 | 1.29 | 0.96 |
| 1:C:55:GLU:HA | 1:C:128:LYS:HA | 1.46 | 0.96 |
| 1:B:272:ALA:HB2 | 2:E:18:THR:HG22 | 1.45 | 0.96 |
| 1:C:100:GLY:HA3 | 1:C:108:PHE:CE1 | 2.00 | 0.96 |
| 1:A:265:VAL:HG23 | 2:D:4:LEU:HD13 | 1.47 | 0.95 |
| 1:A:37:ASP:O | 1:A:300:LEU:HD11 | 1.65 | 0.95 |
| 2:E:56:SER:HB3 | 2:E:59:GLN:CB | 1.96 | 0.95 |
| 1:A:204:LEU:HD23 | 1:A:204:LEU:H | 1.29 | 0.95 |
| 1:B:236:TRP:HB2 | 1:B:239:LYS:HE3 | 1.44 | 0.95 |
| 1:C:331:GLN:OE1 | 1:C:371:ASN:HB2 | 1.65 | 0.95 |
| 1:A:1:ILE:HD13 | 1:A:144:HIS:HA | 1.48 | 0.95 |
| 1:A:302:GLY:HA3 | 1:A:305:TYR:CD2 | 2.01 | 0.95 |
| 1:B:1:ILE:HG21 | 1:B:147:GLN:CB | 1.97 | 0.95 |
| 1:A:150:GLY:C | 1:A:152:ILE:H | 1.69 | 0.94 |
| 1:A:20:TRP:CE3 | 1:A:434:VAL:HG12 | 2.02 | 0.94 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:305:TYR:HB2 | 1:A:340:LYS:HG3 | 1.50 | 0.94 |
| 1:C:65:ILE:HD13 | 1:C:257:VAL:HG12 | 1.49 | 0.94 |
| 1:B:30:CYS:SG | 1:B:31:VAL:N | 2.39 | 0.94 |
| 1:B:95:THR:HG22 | 1:B:96:LEU:N | 1.80 | 0.94 |
| 1:B:272:ALA:CB | 2:E:18:THR:HG22 | 1.98 | 0.93 |
| 1:C:39:PRO:HD2 | 1:C:298:LEU:HD11 | 1.49 | 0.93 |
| 1:C:93:LYS:HB2 | 1:C:245:PHE:CE1 | 2.04 | 0.93 |
| 1:C:315:THR:HG21 | 1:C:373:LYS:HE2 | 1.49 | 0.93 |
| 1:C:389:ILE:HD11 | 1:C:396:ILE:HG23 | 1.49 | 0.92 |
| 1:B:170:THR:HG22 | 1:B:171:PRO:HD2 | 1.52 | 0.92 |
| 1:A:312:PHE:HB3 | 1:A:396:ILE:HD13 | 1.51 | 0.91 |
| 1:A:38:LYS:HA | 1:A:38:LYS:HE3 | 1.53 | 0.91 |
| 1:A:331:GLN:HG3 | 1:A:373:LYS:HG2 | 1.53 | 0.91 |
| 1:C:211:TRP:NE1 | 1:C:269:LEU:HD13 | 1.86 | 0.91 |
| 1:C:154:ASN:HB2 | 3:C:601:NAG:H82 | 1.51 | 0.91 |
| 1:B:95:THR:CG2 | 1:B:96:LEU:H | 1.84 | 0.90 |
| 1:B:21:VAL:CG1 | 1:B:293:LEU:HB3 | 2.02 | 0.90 |
| 1:A:56:VAL:HG23 | 1:B:78:GLY:HA3 | 1.52 | 0.90 |
| 1:A:358:LEU:O | 1:A:359:ILE:HG12 | 1.71 | 0.90 |
| 1:C:217:TRP:NE1 | 2:F:5:PRO:HB2 | 1.87 | 0.90 |
| 2:D:23:ARG:CB | 2:D:27:LYS:HE3 | 2.02 | 0.90 |
| 1:C:13:GLU:HG2 | 1:C:34:MET:HG3 | 1.52 | 0.90 |
| 1:C:300:LEU:HD23 | 1:C:301:LYS:N | 1.87 | 0.90 |
| 1:B:48:THR:HG23 | 1:B:284:LEU:HG | 1.50 | 0.90 |
| 1:A:47:THR:OG1 | 1:A:138:ARG:HD3 | 1.72 | 0.89 |
| 1:C:65:ILE:HD11 | 1:C:243:VAL:CG2 | 2.02 | 0.89 |
| 2:D:1:ALA:CB | 2:F:23:ARG:HD2 | 2.02 | 0.89 |
| 1:A:314:PHE:HD1 | 1:A:314:PHE:H | 1.21 | 0.89 |
| 1:A:392:GLY:C | 1:A:394:LYS:H | 1.75 | 0.89 |
| 1:A:305:TYR:CB | 1:A:340:LYS:HG3 | 2.02 | 0.89 |
| 1:B:486:LEU:HD23 | 1:B:487:MET:H | 1.36 | 0.89 |
| 1:B:345:MET:HG2 | 1:B:378:LEU:HD23 | 1.55 | 0.88 |
| 1:A:171:PRO:HA | 1:A:192:PRO:CG | 2.03 | 0.88 |
| 1:A:169:ILE:HD11 | 1:A:289:LEU:HD21 | 1.54 | 0.88 |
| 1:C:337:GLY:HA2 | 1:C:368:SER:CA | 2.00 | 0.88 |
| 1:C:41:VAL:HG23 | 1:C:143:VAL:HG22 | 1.55 | 0.88 |
| 1:B:175:ARG:HA | 1:B:188:LEU:O | 1.72 | 0.88 |
| 1:C:420:ARG:HD2 | 1:C:431:PHE:CD2 | 2.09 | 0.88 |
| 1:B:375:MET:C | 1:B:376:LEU:HG | 1.92 | 0.88 |
| 1:A:76:THR:HG21 | 1:A:107:LEU:HD12 | 1.55 | 0.88 |
| 1:B:23:VAL:HG21 | 1:B:31:VAL:HG11 | 1.56 | 0.88 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:405:SER:HB2 | 1:A:408:GLY:HA3 | 1.55 | 0.87 |
| 2:E:71:ALA:N | 2:E:72:PRO:HD2 | 1.88 | 0.87 |
| 1:C:337:GLY:CA | 1:C:368:SER:HA | 2.00 | 0.87 |
| 1:A:65:ILE:HD12 | 1:A:257:VAL:HG22 | 1.55 | 0.87 |
| 1:A:171:PRO:HA | 1:A:192:PRO:HG2 | 1.56 | 0.87 |
| 1:C:28:GLY:HA3 | 2:F:15:ARG:HG3 | 1.55 | 0.87 |
| 1:B:71:ASP:O | 1:B:113:LEU:HB2 | 1.75 | 0.86 |
| 1:A:352:LEU:H | 1:A:352:LEU:HD12 | 1.40 | 0.86 |
| 1:C:457:PHE:O | 1:C:460:MET:HG2 | 1.75 | 0.86 |
| 1:B:269:LEU:O | 2:E:19:TRP:HD1 | 1.59 | 0.86 |
| 1:A:302:GLY:HA3 | 1:A:305:TYR:CE2 | 2.09 | 0.86 |
| 1:C:133:GLU:O | 1:C:134:ASN:HB2 | 1.73 | 0.86 |
| 1:B:40:THR:HG23 | 1:B:144:HIS:HD2 | 1.39 | 0.86 |
| 2:D:1:ALA:N | 2:F:27:LYS:HD3 | 1.91 | 0.86 |
| 1:C:154:ASN:CB | 3:C:601:NAG:H82 | 2.06 | 0.86 |
| 1:A:2:ARG:HB2 | 1:A:142:SER:CB | 2.06 | 0.85 |
| 1:A:460:MET:HG3 | 1:A:464:SER:HB2 | 1.57 | 0.85 |
| 1:B:320:GLU:HB2 | 1:B:400:TRP:HZ2 | 1.41 | 0.85 |
| 1:A:97:VAL:O | 1:A:110:LYS:HG3 | 1.77 | 0.85 |
| 2:F:4:LEU:HD23 | 2:F:5:PRO:HD3 | 1.59 | 0.85 |
| 1:B:486:LEU:HD23 | 1:B:487:MET:N | 1.91 | 0.85 |
| 1:C:389:ILE:HD11 | 1:C:396:ILE:CG2 | 2.06 | 0.85 |
| 1:A:493:GLY:HA2 | 1:A:496:ILE:HD12 | 1.59 | 0.85 |
| 1:A:341:VAL:HG22 | 1:A:365:ILE:HG13 | 1.56 | 0.85 |
| 2:D:49:ILE:HA | 2:D:52:LEU:HD22 | 1.57 | 0.84 |
| 1:C:426:ASP:HB3 | 1:C:446:HIS:CB | 2.06 | 0.84 |
| 1:B:137:TYR:CD2 | 1:B:289:LEU:HD22 | 2.12 | 0.84 |
| 1:A:115:THR:HG22 | 1:A:253:GLN:NE2 | 1.92 | 0.84 |
| 1:A:332:TYR:CB | 1:A:335:THR:HG21 | 2.07 | 0.84 |
| 1:B:60:CYS:H | 1:B:224:PRO:HD2 | 1.42 | 0.84 |
| 1:C:439:ASN:C | 1:C:441:LEU:H | 1.80 | 0.84 |
| 1:B:66:SER:OG | 1:B:118:LYS:HB3 | 1.77 | 0.84 |
| 2:F:27:LYS:HG3 | 2:F:28:HIS:H | 1.42 | 0.84 |
| 1:C:273:LEU:N | 2:F:12:LEU:HD21 | 1.93 | 0.84 |
| 1:A:138:ARG:HH21 | 1:A:140:MET:HE2 | 1.43 | 0.84 |
| 1:C:184:GLY:HA3 | 1:C:297:LYS:O | 1.76 | 0.84 |
| 1:B:262:GLU:O | 1:B:265:VAL:HG12 | 1.77 | 0.84 |
| 1:A:46:VAL:HG21 | 1:A:140:MET:HG2 | 1.60 | 0.83 |
| 1:C:178:ALA:O | 1:C:185:SER:HB3 | 1.78 | 0.83 |
| 2:D:73:ALA:HB2 | 2:F:74:TYR:CE2 | 2.13 | 0.83 |
| 1:B:97:VAL:HG13 | 1:B:251:LYS:HA | 1.58 | 0.83 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:151:MET:O | 1:B:153:VAL:HG22 | 1.78 | 0.83 |
| 1:A:312:PHE:HD2 | 1:A:396:ILE:HB | 1.40 | 0.83 |
| 1:B:21:VAL:HG13 | 1:B:293:LEU:N | 1.93 | 0.83 |
| 1:A:261:GLN:CA | 1:A:261:GLN:HE21 | 1.90 | 0.83 |
| 1:C:429:TRP:HB3 | 1:C:442:GLY:O | 1.77 | 0.83 |
| 1:B:21:VAL:HG11 | 1:B:293:LEU:CB | 2.08 | 0.83 |
| 1:B:33:VAL:HG22 | 1:B:41:VAL:O | 1.77 | 0.83 |
| 1:B:57:ARG:HA | 1:B:227:ALA:HB2 | 1.61 | 0.83 |
| 1:C:475:LEU:HD13 | 2:D:52:LEU:HD23 | 1.60 | 0.83 |
| 1:A:20:TRP:HE3 | 1:A:434:VAL:HG12 | 1.42 | 0.83 |
| 1:C:238:ASN:HA | 1:C:240:GLU:OE1 | 1.77 | 0.83 |
| 1:B:313:THR:HA | 1:B:396:ILE:HD12 | 1.60 | 0.83 |
| 1:B:25:LEU:CD1 | 1:B:139:ILE:HG21 | 2.08 | 0.83 |
| 1:C:115:THR:HG21 | 1:C:253:GLN:HB3 | 1.59 | 0.83 |
| 1:C:34:MET:CE | 1:C:359:ILE:HG23 | 2.03 | 0.83 |
| 1:C:137:TYR:CD2 | 1:C:289:LEU:HD22 | 2.12 | 0.83 |
| 1:C:419:LYS:HB3 | 2:F:15:ARG:HH22 | 1.41 | 0.83 |
| 1:B:1:ILE:HD11 | 1:B:142:SER:OG | 1.79 | 0.83 |
| 1:A:65:ILE:HB | 1:A:257:VAL:HG21 | 1.59 | 0.82 |
| 1:C:210:HIS:CD2 | 1:C:277:MET:H | 1.97 | 0.82 |
| 1:B:99:ARG:HH21 | 1:B:103:ASN:HB3 | 1.45 | 0.82 |
| 1:B:396:ILE:O | 1:B:396:ILE:HG12 | 1.77 | 0.82 |
| 1:A:118:LYS:HG2 | 1:A:119:PHE:H | 1.42 | 0.82 |
| 1:B:223:LEU:CB | 1:B:224:PRO:HD3 | 2.07 | 0.82 |
| 1:A:332:TYR:HD2 | 1:A:335:THR:HB | 1.43 | 0.82 |
| 1:B:107:LEU:HD12 | 1:B:107:LEU:H | 1.43 | 0.82 |
| 1:B:107:LEU:HD12 | 1:B:107:LEU:N | 1.94 | 0.82 |
| 1:B:260:SER:O | 1:B:261:GLN:HB2 | 1.78 | 0.82 |
| 1:B:73:ARG:HB3 | 1:B:77:GLN:HE21 | 1.44 | 0.82 |
| 1:A:252:ARG:HB2 | 1:A:252:ARG:NH1 | 1.94 | 0.82 |
| 1:B:181:GLY:C | 1:B:183:PHE:H | 1.79 | 0.82 |
| 1:B:434:VAL:HG13 | 1:B:436:GLY:H | 1.43 | 0.82 |
| 1:B:382:PHE:HB3 | 1:B:404:GLY:O | 1.80 | 0.82 |
| 1:A:50:VAL:HG11 | 1:A:130:ILE:CD1 | 2.04 | 0.82 |
| 1:C:97:VAL:O | 1:C:99:ARG:HD2 | 1.79 | 0.82 |
| 1:B:49:THR:HG22 | 1:B:283:ARG:HG2 | 1.60 | 0.82 |
| 1:A:43:ILE:HG23 | 1:A:141:LEU:HD21 | 1.62 | 0.81 |
| 1:A:305:TYR:HE1 | 1:A:338:PRO:HG2 | 1.45 | 0.81 |
| 1:A:314:PHE:CE2 | 1:A:318:PRO:HD3 | 2.15 | 0.81 |
| 1:C:68:MET:SD | 1:C:255:VAL:CB | 2.68 | 0.81 |
| 1:B:12:VAL:CG1 | 1:B:33:VAL:HG12 | 2.10 | 0.81 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:40:THR:HG23 | 1:B:144:HIS:CD2 | 2.15 | 0.81 |
| 1:B:137:TYR:CE2 | 1:B:289:LEU:HD13 | 2.14 | 0.81 |
| 1:A:240:GLU:HA | 1:A:243:VAL:HG22 | 1.61 | 0.81 |
| 1:B:481:ASN:ND2 | 1:B:483:SER:HB3 | 1.95 | 0.81 |
| 1:A:1:ILE:O | 1:A:4:ILE:HG13 | 1.81 | 0.81 |
| 1:C:462:TRP:CZ3 | 1:C:499:SER:HB2 | 2.15 | 0.81 |
| 2:F:27:LYS:HG3 | 2:F:28:HIS:N | 1.96 | 0.81 |
| 1:B:365:ILE:HG22 | 1:B:366:THR:O | 1.81 | 0.81 |
| 1:C:137:TYR:HE2 | 1:C:289:LEU:HB2 | 1.46 | 0.81 |
| 1:C:273:LEU:HD21 | 1:C:286:SER:HB2 | 1.60 | 0.81 |
| 1:C:344:GLN:HE21 | 1:C:354:PRO:HB3 | 1.44 | 0.81 |
| 2:D:10:ARG:HH21 | 2:D:10:ARG:HG2 | 1.45 | 0.81 |
| 2:D:11:LYS:HD2 | 2:D:18:THR:HG21 | 1.61 | 0.81 |
| 2:E:62:ILE:O | 2:E:65:VAL:HG12 | 1.81 | 0.81 |
| 1:B:204:LEU:O | 1:B:210:HIS:HB3 | 1.80 | 0.81 |
| 1:A:2:ARG:HB2 | 1:A:142:SER:HB3 | 1.63 | 0.80 |
| 1:C:491:LEU:O | 1:C:495:LEU:HG | 1.81 | 0.80 |
| 1:A:322:LEU:HG | 1:A:323:HIS:H | 1.46 | 0.80 |
| 2:D:31:ARG:HG2 | 2:F:4:LEU:HB2 | 1.63 | 0.80 |
| 2:D:50:ALA:HB1 | 2:D:60:LYS:HB3 | 1.63 | 0.80 |
| 1:B:27:HIS:CD2 | 1:B:45:LEU:HD22 | 2.16 | 0.80 |
| 1:A:2:ARG:HG2 | 1:A:44:GLU:OE1 | 1.80 | 0.80 |
| 1:B:198:PHE:HA | 1:B:201:LEU:HB2 | 1.62 | 0.80 |
| 1:B:485:SER:HA | 1:B:488:CYS:SG | 2.22 | 0.80 |
| 1:C:98:ASP:OD1 | 1:C:110:LYS:HG3 | 1.82 | 0.80 |
| 1:C:171:PRO:HB2 | 1:C:193:ARG:HD2 | 1.62 | 0.80 |
| 1:A:344:GLN:O | 1:A:388:VAL:HG23 | 1.82 | 0.80 |
| 1:A:373:LYS:O | 1:A:374:MET:HB3 | 1.82 | 0.80 |
| 1:C:423:VAL:HG22 | 1:C:502:VAL:HG21 | 1.62 | 0.80 |
| 1:C:178:ALA:HB3 | 1:C:186:LEU:N | 1.92 | 0.80 |
| 1:B:171:PRO:HA | 1:B:192:PRO:HB2 | 1.62 | 0.79 |
| 1:A:139:ILE:HB | 1:A:167:VAL:HG23 | 1.63 | 0.79 |
| 1:C:89:GLN:HA | 1:C:239:LYS:NZ | 1.97 | 0.79 |
| 1:B:175:ARG:CZ | 1:B:175:ARG:HB2 | 2.12 | 0.79 |
| 1:C:34:MET:HE1 | 1:C:359:ILE:CG2 | 2.08 | 0.79 |
| 1:C:422:ALA:HB1 | 1:C:498:LEU:CD1 | 2.12 | 0.79 |
| 1:B:12:VAL:HG11 | 1:B:33:VAL:HG12 | 1.65 | 0.79 |
| 1:B:158:HIS:HB3 | 1:B:164:ARG:HD3 | 1.64 | 0.79 |
| 1:A:12:VAL:HG11 | 1:A:432:GLY:HA3 | 1.65 | 0.79 |
| 1:C:9:ARG:HH11 | 1:C:32:THR:HG21 | 1.47 | 0.79 |
| 2:D:67:ILE:HA | 2:D:70:ILE:CG2 | 2.12 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:66:MET:O | 2:E:70:ILE:HG22 | 1.83 | 0.79 |
| 1:B:133:GLU:O | 1:B:134:ASN:HB3 | 1.83 | 0.79 |
| 1:B:357:ARG:HB2 | 1:B:357:ARG:HH11 | 1.47 | 0.79 |
| 1:C:423:VAL:CG2 | 1:C:502:VAL:HG11 | 2.13 | 0.79 |
| 1:B:223:LEU:HB2 | 1:B:224:PRO:CD | 2.12 | 0.79 |
| 1:B:4:ILE:HA | 1:B:9:ARG:HE | 1.48 | 0.79 |
| 1:A:360:THR:CG2 | 1:A:377:GLU:H | 1.95 | 0.78 |
| 2:D:67:ILE:HD12 | 2:D:70:ILE:HG21 | 1.65 | 0.78 |
| 1:B:27:HIS:CE1 | 1:B:285:SER:HA | 2.18 | 0.78 |
| 1:A:154:ASN:HB2 | 3:A:601:NAG:H82 | 1.65 | 0.78 |
| 1:A:336:ASP:HA | 1:A:368:SER:O | 1.82 | 0.78 |
| 1:A:356:GLY:O | 1:A:357:ARG:HB3 | 1.83 | 0.78 |
| 1:B:261:GLN:HE21 | 2:E:1:ALA:N | 1.82 | 0.78 |
| 1:C:15:MET:SD | 1:C:36:GLN:HB2 | 2.23 | 0.78 |
| 1:C:74:CYS:HB3 | 1:C:75:PRO:HD2 | 1.65 | 0.78 |
| 1:B:386:TYR:O | 1:B:388:VAL:HG13 | 1.83 | 0.78 |
| 1:A:95:THR:HG23 | 1:A:96:LEU:HD12 | 1.65 | 0.78 |
| 1:A:307:LEU:HD22 | 1:A:307:LEU:N | 1.99 | 0.78 |
| 1:A:409:LYS:NZ | 1:A:409:LYS:HB3 | 1.98 | 0.78 |
| 1:C:300:LEU:HD22 | 1:C:303:VAL:HG23 | 1.63 | 0.78 |
| 2:D:35:TRP:HE3 | 2:D:36:ILE:HD12 | 1.47 | 0.78 |
| 1:C:273:LEU:H | 2:F:12:LEU:HD21 | 1.48 | 0.78 |
| 2:D:41:GLY:C | 2:D:43:ALA:H | 1.87 | 0.78 |
| 1:B:360:THR:OG1 | 1:B:376:LEU:HB3 | 1.83 | 0.78 |
| 1:B:32:THR:CA | 1:B:42:ASP:HB3 | 2.14 | 0.78 |
| 1:C:24:VAL:HG11 | 1:C:424:LEU:HD13 | 1.65 | 0.78 |
| 1:C:426:ASP:HB3 | 1:C:446:HIS:HB2 | 1.63 | 0.78 |
| 1:C:475:LEU:HD11 | 2:D:52:LEU:HB3 | 1.66 | 0.78 |
| 1:B:19:THR:HB | 1:B:295:MET:HB2 | 1.66 | 0.78 |
| 1:A:51:SER:OG | 1:A:281:LYS:HE3 | 1.84 | 0.78 |
| 1:A:65:ILE:HB | 1:A:257:VAL:CG2 | 2.12 | 0.78 |
| 1:C:164:ARG:HG2 | 1:C:164:ARG:HH11 | 1.46 | 0.78 |
| 1:C:167:VAL:HG22 | 1:C:168:GLU:H | 1.47 | 0.77 |
| 2:D:9:THR:HG22 | 2:D:10:ARG:N | 1.97 | 0.77 |
| 1:B:138:ARG:NH1 | 1:B:138:ARG:HB2 | 1.98 | 0.77 |
| 1:B:269:LEU:O | 2:E:19:TRP:CD1 | 2.37 | 0.77 |
| 2:D:12:LEU:H | 2:D:12:LEU:HD12 | 1.49 | 0.77 |
| 1:B:38:LYS:HA | 1:B:300:LEU:HD11 | 1.64 | 0.77 |
| 1:B:38:LYS:HG2 | 1:B:39:PRO:CD | 2.14 | 0.77 |
| 1:B:426:ASP:C | 1:B:428:ALA:H | 1.84 | 0.77 |
| 1:B:320:GLU:HB2 | 1:B:400:TRP:CZ2 | 2.19 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:138:ARG:HB2 | 1:B:138:ARG:HH11 | 1.48 | 0.77 |
| 1:B:222:PRO:O | 1:B:223:LEU:HG | 1.84 | 0.77 |
| 1:A:46:VAL:CG1 | 1:A:47:THR:HG23 | 2.15 | 0.77 |
| 1:C:50:VAL:HG11 | 1:C:130:ILE:HG21 | 1.65 | 0.77 |
| 2:E:51:TRP:HD1 | 2:E:60:LYS:HZ2 | 1.29 | 0.77 |
| 1:C:1:ILE:HD12 | 1:C:1:ILE:H1 | 1.50 | 0.77 |
| 1:C:329:GLU:HG3 | 1:C:375:MET:HB3 | 1.66 | 0.77 |
| 1:C:374:MET:C | 1:C:375:MET:HE3 | 2.04 | 0.77 |
| 2:D:53:LEU:HD13 | 2:F:62:ILE:HG21 | 1.67 | 0.76 |
| 1:A:443:LYS:NZ | 1:A:443:LYS:HB3 | 1.99 | 0.76 |
| 1:B:74:CYS:O | 1:B:76:THR:N | 2.16 | 0.76 |
| 1:B:154:ASN:HB2 | 1:B:158:HIS:CE1 | 2.20 | 0.76 |
| 1:B:323:HIS:CD2 | 1:B:416:ARG:HH12 | 2.02 | 0.76 |
| 1:B:365:ILE:HA | 1:B:374:MET:SD | 2.25 | 0.76 |
| 1:C:143:VAL:HB | 1:C:163:ASN:ND2 | 2.00 | 0.76 |
| 1:A:347:VAL:HG23 | 1:A:355:VAL:HB | 1.67 | 0.76 |
| 1:A:448:ILE:HG13 | 1:A:449:PHE:HD1 | 1.50 | 0.76 |
| 1:C:139:ILE:HB | 1:C:167:VAL:CG1 | 2.16 | 0.76 |
| 1:C:374:MET:O | 1:C:374:MET:SD | 2.43 | 0.76 |
| 1:C:223:LEU:HD22 | 1:C:242:LEU:HD21 | 1.67 | 0.76 |
| 1:A:203:TYR:HE2 | 1:A:277:MET:CE | 1.99 | 0.76 |
| 1:B:330:VAL:O | 1:B:373:LYS:HA | 1.86 | 0.76 |
| 1:A:476:GLY:HA3 | 1:A:489:LEU:HG | 1.68 | 0.76 |
| 1:B:1:ILE:HD12 | 1:B:2:ARG:N | 2.01 | 0.76 |
| 1:B:74:CYS:SG | 1:B:99:ARG:HB3 | 2.26 | 0.75 |
| 1:B:393:GLU:HG3 | 1:B:394:LYS:H | 1.50 | 0.75 |
| 1:A:154:ASN:CB | 3:A:601:NAG:H82 | 2.16 | 0.75 |
| 1:B:373:LYS:HG3 | 1:B:373:LYS:O | 1.87 | 0.75 |
| 2:D:44:LEU:O | 2:D:48:ALA:HB2 | 1.84 | 0.75 |
| 1:B:41:VAL:HG22 | 1:B:143:VAL:CG2 | 2.15 | 0.75 |
| 1:A:131:GLN:O | 1:A:133:GLU:N | 2.19 | 0.75 |
| 2:D:49:ILE:HD11 | 2:D:67:ILE:HG21 | 1.68 | 0.75 |
| 1:B:238:ASN:O | 1:B:239:LYS:HB2 | 1.86 | 0.75 |
| 1:A:174:PRO:O | 1:A:189:ASP:HA | 1.86 | 0.75 |
| 1:C:307:LEU:HG | 1:C:340:LYS:HD2 | 1.69 | 0.75 |
| 1:B:271:GLY:CA | 2:E:7:HIS:CD2 | 2.67 | 0.75 |
| 1:C:139:ILE:HB | 1:C:167:VAL:HG11 | 1.66 | 0.75 |
| 1:C:344:GLN:NE2 | 1:C:354:PRO:HB3 | 2.02 | 0.75 |
| 1:B:479:THR:HG21 | 1:B:485:SER:CB | 2.17 | 0.75 |
| 1:A:154:ASN:CG | 3:A:601:NAG:H82 | 2.06 | 0.75 |
| 1:A:479:THR:HG22 | 1:A:480:LYS:N | 2.00 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:39:PRO:HG2 | 1:C:183:PHE:HE2 | 1.52 | 0.75 |
| 1:C:97:VAL:HG21 | 1:C:113:LEU:HD23 | 1.67 | 0.75 |
| 1:B:21:VAL:O | 1:B:21:VAL:HG22 | 1.85 | 0.75 |
| 1:B:60:CYS:CB | 1:B:224:PRO:HG2 | 2.10 | 0.75 |
| 1:A:169:ILE:HD12 | 1:A:190:CYS:HB2 | 1.69 | 0.75 |
| 1:C:26:GLU:HB3 | 1:C:288:HIS:HA | 1.69 | 0.75 |
| 1:C:39:PRO:HG2 | 1:C:183:PHE:CE2 | 2.22 | 0.75 |
| 1:C:50:VAL:HG11 | 1:C:130:ILE:CG2 | 2.17 | 0.75 |
| 1:B:73:ARG:CB | 1:B:77:GLN:HE21 | 2.00 | 0.75 |
| 1:B:141:LEU:CD1 | 1:B:165:ALA:HB3 | 2.16 | 0.75 |
| 1:A:73:ARG:HG3 | 1:A:79:GLU:O | 1.87 | 0.74 |
| 1:B:82:LEU:HG | 1:B:82:LEU:O | 1.86 | 0.74 |
| 1:B:212:LEU:HD12 | 1:B:275:ALA:HB2 | 1.69 | 0.74 |
| 1:A:307:LEU:HD22 | 1:A:307:LEU:H | 1.51 | 0.74 |
| 1:A:360:THR:HG21 | 1:A:377:GLU:H | 1.52 | 0.74 |
| 1:C:273:LEU:HD12 | 1:C:274:GLU:N | 2.02 | 0.74 |
| 1:C:276:GLU:OE1 | 1:C:276:GLU:N | 2.20 | 0.74 |
| 2:F:32:VAL:O | 2:F:36:ILE:HG12 | 1.86 | 0.74 |
| 1:A:204:LEU:H | 1:A:204:LEU:CD2 | 2.01 | 0.74 |
| 1:C:137:TYR:CE2 | 1:C:289:LEU:HB2 | 2.21 | 0.74 |
| 1:B:57:ARG:NH1 | 1:B:225:TRP:NE1 | 2.34 | 0.74 |
| 1:B:261:GLN:NE2 | 2:E:1:ALA:N | 2.34 | 0.74 |
| 1:A:44:GLU:HG3 | 1:A:46:VAL:HG23 | 1.70 | 0.74 |
| 1:B:27:HIS:HD2 | 1:B:45:LEU:HD22 | 1.50 | 0.74 |
| 1:B:38:LYS:HG2 | 1:B:39:PRO:HD2 | 1.69 | 0.74 |
| 1:B:246:LYS:O | 1:B:254:THR:HG22 | 1.87 | 0.74 |
| 1:B:345:MET:HE3 | 1:B:380:PRO:CA | 2.11 | 0.74 |
| 1:B:141:LEU:HD11 | 1:B:165:ALA:HB3 | 1.69 | 0.74 |
| 1:C:114:VAL:O | 1:C:114:VAL:HG13 | 1.88 | 0.74 |
| 1:C:133:GLU:HB2 | 1:C:193:ARG:HH12 | 1.52 | 0.74 |
| 1:A:314:PHE:HE2 | 1:A:318:PRO:HD3 | 1.51 | 0.74 |
| 1:A:290:LYS:HD2 | 1:A:427:THR:HG23 | 1.68 | 0.74 |
| 1:A:329:GLU:HB2 | 1:C:101:TRP:CZ3 | 2.23 | 0.74 |
| 1:A:397:THR:HG22 | 1:A:397:THR:O | 1.87 | 0.74 |
| 1:B:225:TRP:CZ3 | 1:B:226:HIS:HA | 2.22 | 0.74 |
| 1:B:445:ILE:HG23 | 1:B:446:HIS:H | 1.52 | 0.74 |
| 1:A:305:TYR:CE1 | 1:A:338:PRO:HG2 | 2.22 | 0.74 |
| 1:A:461:SER:OG | 2:D:8:SER:HB3 | 1.88 | 0.73 |
| 1:C:326:VAL:HG21 | 1:C:380:PRO:HG2 | 1.69 | 0.73 |
| 1:B:227:ALA:C | 1:B:229:ALA:N | 2.36 | 0.73 |
| 2:E:51:TRP:HD1 | 2:E:60:LYS:NZ | 1.85 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:455:SER:O | 2:F:41:GLY:HA3 | 1.88 | 0.73 |
| 1:C:41:VAL:HG23 | 1:C:143:VAL:CG2 | 2.17 | 0.73 |
| 1:C:422:ALA:HB1 | 1:C:498:LEU:HD13 | 1.68 | 0.73 |
| 1:B:494:VAL:O | 1:B:498:LEU:HG | 1.88 | 0.73 |
| 1:B:297:LYS:O | 1:B:298:LEU:HG | 1.86 | 0.73 |
| 1:A:23:VAL:HG13 | 1:A:25:LEU:HD23 | 1.70 | 0.73 |
| 1:A:39:PRO:HD3 | 1:A:300:LEU:HD12 | 1.71 | 0.73 |
| 1:C:347:VAL:O | 1:C:348:ASP:HB2 | 1.88 | 0.73 |
| 1:A:31:VAL:HB | 1:A:43:ILE:HD11 | 1.70 | 0.73 |
| 1:A:141:LEU:HB2 | 1:A:165:ALA:HB3 | 1.71 | 0.73 |
| 1:B:268:ALA:HA | 2:E:4:LEU:HD21 | 1.69 | 0.73 |
| 1:C:332:TYR:O | 1:C:371:ASN:HA | 1.87 | 0.73 |
| 1:B:197:ASP:C | 1:B:199:SER:H | 1.91 | 0.73 |
| 1:A:1:ILE:HG23 | 1:A:152:ILE:HG22 | 1.70 | 0.73 |
| 1:C:312:PHE:O | 1:C:396:ILE:HG21 | 1.88 | 0.73 |
| 1:A:252:ARG:HB2 | 1:A:252:ARG:CZ | 2.19 | 0.73 |
| 1:A:312:PHE:CG | 1:A:389:ILE:HB | 2.23 | 0.73 |
| 1:B:186:LEU:HD23 | 1:B:293:LEU:HD11 | 1.70 | 0.73 |
| 1:B:40:THR:CG2 | 1:B:144:HIS:HD2 | 2.02 | 0.72 |
| 1:B:113:LEU:HD22 | 1:B:114:VAL:N | 2.04 | 0.72 |
| 1:A:157:GLY:C | 1:A:159:GLU:H | 1.92 | 0.72 |
| 1:C:196:LEU:HD13 | 1:C:288:HIS:HB3 | 1.69 | 0.72 |
| 1:C:170:THR:HB | 1:C:171:PRO:HD2 | 1.70 | 0.72 |
| 1:C:300:LEU:HD22 | 1:C:303:VAL:CG2 | 2.18 | 0.72 |
| 1:C:445:ILE:HD13 | 1:C:448:ILE:HD12 | 1.70 | 0.72 |
| 1:B:442:GLY:HA2 | 1:B:445:ILE:HG22 | 1.69 | 0.72 |
| 2:F:56:SER:HB3 | 2:F:59:GLN:HB2 | 1.71 | 0.72 |
| 1:A:43:ILE:HG23 | 1:A:141:LEU:CD2 | 2.19 | 0.72 |
| 1:A:342:PRO:HG2 | 1:A:389:ILE:HG13 | 1.69 | 0.72 |
| 1:C:36:GLN:O | 1:C:38:LYS:N | 2.23 | 0.72 |
| 1:A:300:LEU:HD12 | 1:A:300:LEU:N | 2.04 | 0.72 |
| 1:C:70:SER:HB2 | 1:C:115:THR:HA | 1.70 | 0.72 |
| 1:C:389:ILE:O | 1:C:389:ILE:HD12 | 1.89 | 0.72 |
| 1:C:460:MET:HE2 | 1:C:468:ILE:HD12 | 1.72 | 0.72 |
| 1:C:319:ALA:O | 1:C:326:VAL:HG13 | 1.90 | 0.72 |
| 1:C:327:THR:HB | 1:C:329:GLU:OE2 | 1.89 | 0.72 |
| 1:B:359:ILE:HB | 1:B:377:GLU:HB3 | 1.70 | 0.72 |
| 1:A:7:SER:O | 1:A:8:ASN:HB2 | 1.89 | 0.72 |
| 1:A:130:ILE:HG21 | 1:A:198:PHE:HD2 | 1.54 | 0.72 |
| 1:B:222:PRO:C | 1:B:223:LEU:HD12 | 2.09 | 0.72 |
| 1:A:135:LEU:N | 1:A:135:LEU:HD23 | 2.05 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:73:ARG:HG3 | 1:B:79:GLU:O | 1.89 | 0.72 |
| 1:C:100:GLY:HA3 | 1:C:108:PHE:CD1 | 2.24 | 0.72 |
| 2:D:55:SER:CA | 2:D:60:LYS:HE2 | 2.15 | 0.72 |
| 2:D:1:ALA:H2 | 2:F:27:LYS:HD3 | 1.51 | 0.71 |
| 1:B:38:LYS:HG3 | 1:B:298:LEU:CB | 2.20 | 0.71 |
| 2:F:9:THR:HG22 | 2:F:10:ARG:NH2 | 2.04 | 0.71 |
| 1:A:28:GLY:HA3 | 2:D:15:ARG:HG3 | 1.72 | 0.71 |
| 1:C:204:LEU:O | 1:C:210:HIS:HB3 | 1.89 | 0.71 |
| 2:D:71:ALA:HB3 | 2:D:72:PRO:CD | 2.20 | 0.71 |
| 1:C:467:LEU:HD13 | 2:F:69:LEU:HD21 | 1.72 | 0.71 |
| 1:B:53:MET:HB2 | 1:B:128:LYS:HD3 | 1.72 | 0.71 |
| 1:A:85:GLN:HE22 | 1:A:94:ARG:HH22 | 1.34 | 0.71 |
| 1:A:144:HIS:ND1 | 1:A:360:THR:HG22 | 2.04 | 0.71 |
| 1:A:158:HIS:CB | 1:A:166:LYS:HE3 | 2.12 | 0.71 |
| 1:B:261:GLN:NE2 | 2:E:1:ALA:H1 | 1.88 | 0.71 |
| 1:C:92:CYS:HB3 | 1:C:115:THR:O | 1.91 | 0.71 |
| 1:C:284:LEU:HD22 | 1:C:285:SER:O | 1.91 | 0.71 |
| 1:B:23:VAL:CG2 | 1:B:31:VAL:HG11 | 2.20 | 0.71 |
| 1:A:25:LEU:O | 1:A:45:LEU:HB2 | 1.89 | 0.71 |
| 1:C:320:GLU:OE2 | 1:C:402:ARG:HG3 | 1.90 | 0.71 |
| 1:A:261:GLN:HE21 | 1:A:261:GLN:HA | 1.55 | 0.71 |
| 1:A:377:GLU:O | 1:A:378:LEU:HB2 | 1.90 | 0.71 |
| 1:C:347:VAL:O | 1:C:347:VAL:HG13 | 1.89 | 0.71 |
| 1:C:384:ASP:O | 1:C:385:SER:HB3 | 1.90 | 0.71 |
| 1:C:460:MET:CE | 1:C:468:ILE:HD12 | 2.19 | 0.71 |
| 1:B:12:VAL:HG13 | 1:B:12:VAL:O | 1.89 | 0.71 |
| 1:B:31:VAL:O | 1:B:43:ILE:HD12 | 1.90 | 0.71 |
| 1:B:91:VAL:HG13 | 1:B:91:VAL:O | 1.90 | 0.71 |
| 1:C:184:GLY:HA3 | 1:C:297:LYS:C | 2.11 | 0.71 |
| 1:C:295:MET:CE | 1:C:298:LEU:HB3 | 2.21 | 0.71 |
| 1:C:426:ASP:HB3 | 1:C:446:HIS:HB3 | 1.71 | 0.71 |
| 2:D:1:ALA:HB2 | 2:F:23:ARG:HD2 | 1.72 | 0.71 |
| 2:E:6:SER:HB2 | 2:E:8:SER:HB2 | 1.73 | 0.71 |
| 2:D:29:LEU:HD23 | 2:D:29:LEU:O | 1.91 | 0.70 |
| 1:B:57:ARG:NH1 | 1:B:225:TRP:HE1 | 1.88 | 0.70 |
| 1:B:305:TYR:HB3 | 1:B:339:CYS:HA | 1.73 | 0.70 |
| 1:B:377:GLU:O | 1:B:378:LEU:HD12 | 1.91 | 0.70 |
| 2:E:28:HIS:O | 2:E:32:VAL:HG22 | 1.91 | 0.70 |
| 1:A:118:LYS:HG2 | 1:A:119:PHE:N | 2.05 | 0.70 |
| 1:A:307:LEU:H | 1:A:307:LEU:CD2 | 2.04 | 0.70 |
| 2:E:4:LEU:HD23 | 2:E:4:LEU:C | 2.11 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:71:ALA:HB3 | 2:F:72:PRO:HD3 | 1.74 | 0.70 |
| 1:B:357:ARG:HB2 | 1:B:357:ARG:NH1 | 2.06 | 0.70 |
| 1:B:316:LYS:HB2 | 1:B:329:GLU:HB2 | 1.71 | 0.70 |
| 1:A:150:GLY:HA2 | 1:A:152:ILE:HG23 | 1.74 | 0.70 |
| 1:A:299:ARG:HB2 | 1:A:299:ARG:CZ | 2.22 | 0.70 |
| 1:B:38:LYS:HG3 | 1:B:298:LEU:HB3 | 1.74 | 0.70 |
| 1:B:432:GLY:HA3 | 1:B:439:ASN:HD22 | 1.56 | 0.70 |
| 1:B:6:VAL:C | 1:B:8:ASN:H | 1.95 | 0.70 |
| 1:B:261:GLN:HE21 | 2:E:1:ALA:H1 | 1.38 | 0.70 |
| 1:A:295:MET:HE2 | 1:A:295:MET:HA | 1.71 | 0.70 |
| 1:A:27:HIS:CD2 | 1:A:285:SER:HA | 2.27 | 0.70 |
| 1:C:171:PRO:HA | 1:C:192:PRO:HB2 | 1.74 | 0.70 |
| 1:B:138:ARG:HG2 | 1:B:138:ARG:O | 1.91 | 0.70 |
| 1:A:65:ILE:CG2 | 1:A:66:SER:N | 2.54 | 0.70 |
| 1:A:150:GLY:C | 1:A:152:ILE:N | 2.42 | 0.70 |
| 1:A:204:LEU:HD23 | 1:A:204:LEU:N | 2.06 | 0.70 |
| 1:C:39:PRO:HD2 | 1:C:298:LEU:CD1 | 2.22 | 0.70 |
| 1:C:300:LEU:HD11 | 1:C:362:ASN:HB2 | 1.73 | 0.70 |
| 1:C:329:GLU:HB3 | 1:C:373:LYS:NZ | 2.07 | 0.70 |
| 1:B:187:GLY:O | 1:B:293:LEU:HA | 1.92 | 0.70 |
| 1:C:475:LEU:CD1 | 2:D:52:LEU:HD23 | 2.22 | 0.69 |
| 1:B:197:ASP:O | 1:B:199:SER:N | 2.24 | 0.69 |
| 1:B:309:THR:HA | 1:B:391:VAL:HG22 | 1.72 | 0.69 |
| 2:E:52:LEU:O | 2:E:53:LEU:HD13 | 1.91 | 0.69 |
| 1:C:329:GLU:HB3 | 1:C:373:LYS:HZ1 | 1.56 | 0.69 |
| 1:B:357:ARG:HD3 | 1:B:359:ILE:HD13 | 1.74 | 0.69 |
| 1:A:360:THR:HG21 | 1:A:376:LEU:HA | 1.75 | 0.69 |
| 1:C:315:THR:CG2 | 1:C:373:LYS:HE2 | 2.23 | 0.69 |
| 1:A:34:MET:HB3 | 1:A:40:THR:HG23 | 1.75 | 0.69 |
| 1:B:286:SER:HB3 | 2:E:16:SER:CB | 2.18 | 0.69 |
| 2:E:46:ALA:O | 2:E:49:ILE:HG23 | 1.92 | 0.69 |
| 1:A:151:MET:O | 1:A:151:MET:HG2 | 1.92 | 0.69 |
| 1:A:169:ILE:HG13 | 1:A:169:ILE:O | 1.90 | 0.69 |
| 1:C:273:LEU:HB2 | 2:F:12:LEU:CD1 | 2.23 | 0.69 |
| 2:D:3:THR:OG1 | 2:F:31:ARG:HD3 | 1.92 | 0.69 |
| 1:A:299:ARG:HB2 | 1:A:299:ARG:HH11 | 1.52 | 0.69 |
| 1:A:341:VAL:HG22 | 1:A:365:ILE:CG1 | 2.21 | 0.69 |
| 1:B:3:CYS:O | 1:B:9:ARG:NE | 2.26 | 0.69 |
| 1:A:175:ARG:HG2 | 1:A:189:ASP:CB | 2.21 | 0.69 |
| 1:B:6:VAL:O | 1:B:8:ASN:N | 2.26 | 0.69 |
| 1:B:138:ARG:HH11 | 1:B:138:ARG:CB | 2.05 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:6:VAL:HG12 | 1:A:9:ARG:HB2 | 1.75 | 0.69 |
| 1:A:56:VAL:HG11 | 1:A:202:TYR:CE2 | 2.27 | 0.69 |
| 1:C:454:LYS:O | 1:C:458:GLY:HA3 | 1.92 | 0.69 |
| 2:D:21:GLU:HG3 | 2:D:22:SER:N | 2.08 | 0.69 |
| 1:B:7:SER:H | 1:B:322:LEU:HD11 | 1.57 | 0.69 |
| 1:B:58:SER:HB3 | 1:B:226:HIS:O | 1.92 | 0.69 |
| 1:A:311:ALA:CB | 1:A:334:GLY:H | 2.05 | 0.69 |
| 1:A:343:ALA:O | 1:A:344:GLN:HB3 | 1.93 | 0.69 |
| 1:A:477:LEU:HD23 | 1:A:477:LEU:O | 1.93 | 0.69 |
| 1:A:191:GLU:HG3 | 1:A:290:LYS:HB2 | 1.75 | 0.69 |
| 1:B:38:LYS:HA | 1:B:300:LEU:CD1 | 2.22 | 0.68 |
| 1:B:99:ARG:HH21 | 1:B:103:ASN:CB | 2.06 | 0.68 |
| 1:B:214:HIS:H | 2:E:7:HIS:CE1 | 2.11 | 0.68 |
| 1:C:148:HIS:O | 1:C:152:ILE:HG23 | 1.93 | 0.68 |
| 2:D:67:ILE:CA | 2:D:70:ILE:HG22 | 2.20 | 0.68 |
| 1:B:12:VAL:HG12 | 1:B:33:VAL:HA | 1.76 | 0.68 |
| 1:A:154:ASN:OD1 | 1:A:156:THR:HG22 | 1.94 | 0.68 |
| 1:C:135:LEU:O | 1:C:171:PRO:HD3 | 1.93 | 0.68 |
| 1:B:43:ILE:HD12 | 1:B:43:ILE:H | 1.58 | 0.68 |
| 1:A:360:THR:HG23 | 1:A:377:GLU:HB2 | 1.76 | 0.68 |
| 1:C:283:ARG:HB2 | 1:C:283:ARG:CZ | 2.23 | 0.68 |
| 2:D:29:LEU:O | 2:D:32:VAL:HG12 | 1.93 | 0.68 |
| 2:D:55:SER:HA | 2:D:60:LYS:CE | 2.20 | 0.68 |
| 1:B:37:ASP:C | 1:B:300:LEU:HD11 | 2.13 | 0.68 |
| 1:B:343:ALA:CB | 1:B:389:ILE:HG22 | 2.24 | 0.68 |
| 1:B:471:LEU:O | 1:B:475:LEU:HG | 1.94 | 0.68 |
| 1:C:12:VAL:CG1 | 1:C:33:VAL:HG13 | 2.17 | 0.68 |
| 2:D:2:VAL:HG13 | 2:D:2:VAL:O | 1.93 | 0.68 |
| 1:B:57:ARG:NH1 | 1:B:225:TRP:CD1 | 2.62 | 0.68 |
| 1:C:12:VAL:HG13 | 1:C:12:VAL:O | 1.93 | 0.68 |
| 1:B:187:GLY:O | 1:B:188:LEU:HD23 | 1.94 | 0.68 |
| 1:A:18:GLY:O | 1:A:19:THR:OG1 | 2.11 | 0.68 |
| 1:A:300:LEU:N | 1:A:300:LEU:CD1 | 2.55 | 0.68 |
| 1:A:387:ILE:O | 1:A:388:VAL:HG13 | 1.93 | 0.68 |
| 1:B:221:ILE:CD1 | 2:E:4:LEU:HA | 2.19 | 0.68 |
| 1:B:343:ALA:HB1 | 1:B:389:ILE:HG22 | 1.76 | 0.68 |
| 1:A:59:TYR:CE2 | 1:A:221:ILE:HB | 2.27 | 0.68 |
| 2:E:24:GLU:O | 2:E:27:LYS:HG2 | 1.94 | 0.68 |
| 1:C:441:LEU:O | 1:C:444:GLY:N | 2.25 | 0.68 |
| 1:B:313:THR:H | 1:B:330:VAL:HG13 | 1.58 | 0.68 |
| 1:B:32:THR:HA | 1:B:42:ASP:CB | 2.24 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:100:GLY:CA | 1:B:108:PHE:CE1 | 2.76 | 0.67 |
| 1:B:225:TRP:CE3 | 1:B:226:HIS:N | 2.62 | 0.67 |
| 1:A:138:ARG:HH21 | 1:A:140:MET:CE | 2.07 | 0.67 |
| 1:A:158:HIS:HB3 | 1:A:166:LYS:CE | 2.13 | 0.67 |
| 1:C:141:LEU:O | 1:C:164:ARG:HA | 1.94 | 0.67 |
| 1:B:93:LYS:HB3 | 1:B:245:PHE:CD2 | 2.29 | 0.67 |
| 1:A:261:GLN:NE2 | 1:C:263:GLY:HA3 | 2.09 | 0.67 |
| 1:C:240:GLU:OE2 | 1:C:241:ALA:N | 2.26 | 0.67 |
| 1:B:56:VAL:HG11 | 1:B:202:TYR:CD2 | 2.30 | 0.67 |
| 1:A:302:GLY:HA3 | 1:A:305:TYR:HD2 | 1.58 | 0.67 |
| 1:A:454:LYS:HB2 | 1:A:454:LYS:NZ | 2.10 | 0.67 |
| 1:A:73:ARG:CZ | 1:A:77:GLN:HB3 | 2.23 | 0.67 |
| 1:A:345:MET:O | 1:A:354:PRO:HA | 1.94 | 0.67 |
| 1:C:65:ILE:H | 1:C:257:VAL:CG1 | 2.07 | 0.67 |
| 1:C:97:VAL:HG21 | 1:C:113:LEU:CD2 | 2.25 | 0.67 |
| 1:B:91:VAL:HG11 | 1:B:243:VAL:HG21 | 1.74 | 0.67 |
| 1:C:161:ASP:HB3 | 1:C:164:ARG:O | 1.95 | 0.67 |
| 1:C:345:MET:CB | 1:C:355:VAL:O | 2.41 | 0.67 |
| 1:B:58:SER:OG | 1:B:124:LYS:HD2 | 1.95 | 0.67 |
| 1:B:277:MET:HG3 | 1:B:279:GLY:N | 2.09 | 0.67 |
| 1:B:284:LEU:HD12 | 1:B:285:SER:O | 1.95 | 0.67 |
| 1:A:27:HIS:HD2 | 1:A:285:SER:HA | 1.59 | 0.67 |
| 1:C:1:ILE:HD12 | 1:C:147:GLN:OE1 | 1.95 | 0.67 |
| 1:C:37:ASP:O | 1:C:300:LEU:HB2 | 1.94 | 0.67 |
| 1:B:75:PRO:HB3 | 1:B:110:LYS:HB2 | 1.77 | 0.67 |
| 2:F:9:THR:HG22 | 2:F:10:ARG:HH22 | 1.59 | 0.67 |
| 1:A:143:VAL:HG12 | 1:A:144:HIS:H | 1.59 | 0.67 |
| 1:C:375:MET:N | 1:C:375:MET:SD | 2.67 | 0.67 |
| 1:B:181:GLY:C | 1:B:183:PHE:N | 2.48 | 0.67 |
| 1:A:426:ASP:C | 1:A:428:ALA:H | 1.97 | 0.67 |
| 1:C:426:ASP:CB | 1:C:446:HIS:HB2 | 2.25 | 0.67 |
| 1:B:187:GLY:H | 1:B:293:LEU:HD12 | 1.59 | 0.67 |
| 1:C:144:HIS:O | 1:C:145:GLY:C | 2.34 | 0.66 |
| 1:C:245:PHE:HA | 1:C:254:THR:O | 1.94 | 0.66 |
| 1:B:54:ALA:HB3 | 1:B:129:SER:HB3 | 1.77 | 0.66 |
| 1:A:56:VAL:HG23 | 1:B:78:GLY:CA | 2.25 | 0.66 |
| 1:B:180:LEU:HD12 | 1:B:180:LEU:N | 1.99 | 0.66 |
| 1:B:189:ASP:HB2 | 1:B:292:ARG:HB3 | 1.77 | 0.66 |
| 1:B:225:TRP:CE3 | 1:B:226:HIS:HA | 2.30 | 0.66 |
| 1:A:73:ARG:HH21 | 1:A:77:GLN:HB3 | 1.60 | 0.66 |
| 1:B:186:LEU:HD23 | 1:B:298:LEU:HD11 | 1.76 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:459:GLY:HA2 | 2:D:9:THR:HG23 | 1.76 | 0.66 |
| 1:C:1:ILE:HD12 | 1:C:1:ILE:N | 2.10 | 0.66 |
| 1:C:138:ARG:HB3 | 1:C:138:ARG:CZ | 2.23 | 0.66 |
| 1:B:56:VAL:HG22 | 1:B:57:ARG:HG3 | 1.78 | 0.66 |
| 1:C:392:GLY:O | 1:C:395:LYS:HE3 | 1.95 | 0.66 |
| 1:B:180:LEU:HD11 | 1:B:186:LEU:HD11 | 1.76 | 0.66 |
| 1:B:283:ARG:CZ | 1:B:283:ARG:HB3 | 2.24 | 0.66 |
| 1:A:169:ILE:CD1 | 1:A:190:CYS:HB2 | 2.25 | 0.66 |
| 1:A:178:ALA:HB1 | 1:A:180:LEU:HD21 | 1.76 | 0.66 |
| 1:A:226:HIS:CG | 1:A:234:PRO:HB3 | 2.31 | 0.66 |
| 1:C:70:SER:OG | 1:C:253:GLN:NE2 | 2.28 | 0.66 |
| 1:C:295:MET:HE1 | 1:C:298:LEU:HB3 | 1.76 | 0.66 |
| 1:C:89:GLN:HA | 1:C:239:LYS:HZ3 | 1.61 | 0.66 |
| 1:B:445:ILE:HG23 | 1:B:446:HIS:N | 2.10 | 0.66 |
| 1:A:1:ILE:HG22 | 1:A:2:ARG:N | 2.11 | 0.66 |
| 1:A:493:GLY:O | 1:A:496:ILE:HB | 1.96 | 0.66 |
| 1:C:295:MET:HE1 | 1:C:298:LEU:HD12 | 1.77 | 0.66 |
| 1:B:20:TRP:CE3 | 1:B:292:ARG:NH2 | 2.64 | 0.66 |
| 1:A:359:ILE:CD1 | 1:A:377:GLU:HG2 | 2.20 | 0.66 |
| 1:B:38:LYS:CA | 1:B:300:LEU:HD11 | 2.25 | 0.66 |
| 1:B:65:ILE:HD12 | 1:B:65:ILE:O | 1.96 | 0.66 |
| 1:A:333:ALA:O | 1:A:370:GLU:HA | 1.95 | 0.65 |
| 1:A:472:LEU:HD23 | 1:A:492:GLY:HA2 | 1.78 | 0.65 |
| 1:C:47:THR:HG23 | 1:C:283:ARG:HD3 | 1.77 | 0.65 |
| 1:A:348:ASP:HB2 | 1:A:350:GLN:CG | 2.26 | 0.65 |
| 1:C:26:GLU:CB | 1:C:288:HIS:HA | 2.26 | 0.65 |
| 1:B:56:VAL:HG11 | 1:B:202:TYR:HD2 | 1.60 | 0.65 |
| 1:B:158:HIS:CB | 1:B:164:ARG:HD3 | 2.26 | 0.65 |
| 1:B:187:GLY:N | 1:B:293:LEU:HD12 | 2.12 | 0.65 |
| 1:B:393:GLU:HG3 | 1:B:394:LYS:N | 2.11 | 0.65 |
| 1:A:266:HIS:O | 2:D:20:LEU:HD11 | 1.96 | 0.65 |
| 1:B:281:LYS:NZ | 1:B:281:LYS:HB3 | 2.11 | 0.65 |
| 1:B:74:CYS:HB3 | 1:B:75:PRO:HD2 | 1.77 | 0.65 |
| 1:B:137:TYR:CD2 | 1:B:289:LEU:HD13 | 2.32 | 0.65 |
| 1:B:479:THR:HG21 | 1:B:485:SER:OG | 1.96 | 0.65 |
| 1:A:203:TYR:HE2 | 1:A:277:MET:HE1 | 1.62 | 0.65 |
| 1:B:159:GLU:HA | 1:B:164:ARG:O | 1.97 | 0.65 |
| 2:F:4:LEU:HD23 | 2:F:5:PRO:CD | 2.26 | 0.65 |
| 1:A:43:ILE:CG2 | 1:A:141:LEU:HD21 | 2.25 | 0.65 |
| 1:A:97:VAL:HG11 | 1:A:113:LEU:HD13 | 1.79 | 0.65 |
| 1:B:306:SER:O | 1:B:339:CYS:HB2 | 1.95 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:47:ALA:O | 2:F:51:TRP:HB2 | 1.96 | 0.65 |
| 2:F:56:SER:HB3 | 2:F:59:GLN:CG | 2.27 | 0.65 |
| 1:B:141:LEU:HD12 | 1:B:165:ALA:O | 1.97 | 0.65 |
| 1:B:180:LEU:HD11 | 1:B:186:LEU:CD1 | 2.26 | 0.65 |
| 2:F:3:THR:C | 2:F:5:PRO:HD2 | 2.17 | 0.65 |
| 1:C:84:LYS:O | 1:C:86:SER:N | 2.30 | 0.65 |
| 1:A:58:SER:OG | 1:A:126:THR:HG22 | 1.97 | 0.65 |
| 1:A:265:VAL:CG2 | 2:D:4:LEU:HD13 | 2.23 | 0.65 |
| 1:A:305:TYR:HB3 | 1:A:340:LYS:HG3 | 1.78 | 0.65 |
| 1:A:365:ILE:HG22 | 1:A:368:SER:HB2 | 1.79 | 0.65 |
| 1:C:260:SER:OG | 1:C:261:GLN:N | 2.27 | 0.65 |
| 1:C:427:THR:HG22 | 1:C:427:THR:O | 1.97 | 0.65 |
| 1:B:491:LEU:HA | 1:B:494:VAL:HG23 | 1.79 | 0.65 |
| 1:A:156:THR:O | 1:A:158:HIS:N | 2.29 | 0.64 |
| 1:A:251:LYS:HE2 | 1:A:252:ARG:HE | 1.61 | 0.64 |
| 2:D:30:ILE:HG13 | 2:D:31:ARG:N | 2.12 | 0.64 |
| 1:A:27:HIS:NE2 | 1:A:48:THR:HG22 | 2.13 | 0.64 |
| 1:C:73:ARG:HG2 | 1:C:79:GLU:N | 2.12 | 0.64 |
| 1:C:185:SER:O | 1:C:297:LYS:HB2 | 1.96 | 0.64 |
| 1:B:74:CYS:CB | 1:B:75:PRO:HD2 | 2.26 | 0.64 |
| 1:B:338:PRO:HD3 | 1:B:367:GLU:HG2 | 1.77 | 0.64 |
| 2:E:70:ILE:C | 2:E:72:PRO:HD2 | 2.16 | 0.64 |
| 2:F:67:ILE:C | 2:F:69:LEU:H | 2.00 | 0.64 |
| 1:A:63:ALA:HB1 | 1:A:119:PHE:HE1 | 1.61 | 0.64 |
| 1:B:474:TRP:HZ2 | 2:E:58:SER:HB2 | 1.61 | 0.64 |
| 1:C:334:GLY:CA | 1:C:370:GLU:HA | 2.28 | 0.64 |
| 1:A:96:LEU:HD12 | 1:A:96:LEU:H | 1.62 | 0.64 |
| 1:C:39:PRO:CG | 1:C:300:LEU:HA | 2.27 | 0.64 |
| 1:B:56:VAL:O | 1:B:227:ALA:HB1 | 1.96 | 0.64 |
| 1:B:186:LEU:CD2 | 1:B:293:LEU:HD11 | 2.28 | 0.64 |
| 1:A:225:TRP:NE1 | 1:A:237:ASN:ND2 | 2.44 | 0.64 |
| 1:C:298:LEU:C | 1:C:298:LEU:HD13 | 2.18 | 0.64 |
| 1:B:345:MET:HG2 | 1:B:378:LEU:CD2 | 2.26 | 0.64 |
| 2:F:51:TRP:HA | 2:F:60:LYS:HD2 | 1.80 | 0.64 |
| 1:A:86:SER:OG | 1:B:235:HIS:HB2 | 1.97 | 0.64 |
| 1:C:240:GLU:HA | 1:C:243:VAL:HB | 1.80 | 0.64 |
| 1:C:357:ARG:HG2 | 1:C:358:LEU:N | 2.12 | 0.64 |
| 1:B:154:ASN:HB2 | 1:B:158:HIS:HE1 | 1.60 | 0.64 |
| 1:B:258:LEU:HD23 | 1:B:259:GLY:H | 1.62 | 0.64 |
| 1:B:472:LEU:HD23 | 1:B:475:LEU:HD12 | 1.79 | 0.64 |
| 2:E:65:VAL:HG22 | 2:E:69:LEU:CD1 | 2.27 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:27:HIS:HE1 | 1:C:48:THR:HG22 | 1.58 | 0.64 |
| 1:A:83:ASP:OD1 | 1:A:83:ASP:N | 2.30 | 0.64 |
| 1:B:309:THR:HA | 1:B:391:VAL:CG2 | 2.27 | 0.64 |
| 1:A:38:LYS:HE2 | 1:A:298:LEU:O | 1.97 | 0.63 |
| 1:A:312:PHE:CD1 | 1:A:389:ILE:HB | 2.32 | 0.63 |
| 1:C:36:GLN:O | 1:C:38:LYS:HG3 | 1.97 | 0.63 |
| 1:C:63:ALA:HB2 | 1:C:242:LEU:HD12 | 1.79 | 0.63 |
| 1:C:70:SER:CB | 1:C:115:THR:HA | 2.28 | 0.63 |
| 1:C:167:VAL:HG13 | 1:C:168:GLU:N | 2.13 | 0.63 |
| 1:B:429:TRP:HE1 | 1:B:446:HIS:HD2 | 1.45 | 0.63 |
| 1:A:45:LEU:HD12 | 1:A:138:ARG:O | 1.97 | 0.63 |
| 2:D:23:ARG:CA | 2:D:27:LYS:HE3 | 2.27 | 0.63 |
| 2:D:71:ALA:HB3 | 2:D:72:PRO:HD3 | 1.79 | 0.63 |
| 1:B:135:LEU:C | 1:B:135:LEU:HD12 | 2.19 | 0.63 |
| 1:B:349:MET:N | 1:B:349:MET:SD | 2.72 | 0.63 |
| 1:A:456:LEU:HD13 | 1:A:457:PHE:CD2 | 2.33 | 0.63 |
| 1:C:90:TYR:HD1 | 1:C:90:TYR:H | 1.46 | 0.63 |
| 2:D:1:ALA:H1 | 2:F:27:LYS:HD3 | 1.63 | 0.63 |
| 1:A:215:LYS:HB2 | 1:A:215:LYS:NZ | 2.13 | 0.63 |
| 1:A:248:ALA:HB1 | 1:A:252:ARG:NH2 | 2.13 | 0.63 |
| 1:B:360:THR:O | 1:B:361:ALA:HB3 | 1.98 | 0.63 |
| 2:F:27:LYS:O | 2:F:29:LEU:N | 2.30 | 0.63 |
| 1:A:162:GLU:HG3 | 1:A:181:GLY:O | 1.98 | 0.63 |
| 1:C:439:ASN:C | 1:C:441:LEU:N | 2.47 | 0.63 |
| 2:D:60:LYS:HD3 | 2:D:60:LYS:N | 2.12 | 0.63 |
| 1:B:19:THR:CB | 1:B:295:MET:H | 2.12 | 0.63 |
| 1:B:20:TRP:HE3 | 1:B:292:ARG:HH21 | 1.47 | 0.63 |
| 1:B:41:VAL:CG2 | 1:B:143:VAL:HG22 | 2.18 | 0.63 |
| 1:C:90:TYR:N | 1:C:90:TYR:CD1 | 2.67 | 0.63 |
| 1:C:445:ILE:HA | 1:C:448:ILE:HD12 | 1.81 | 0.63 |
| 1:B:344:GLN:OE1 | 1:B:352:LEU:HG | 1.98 | 0.63 |
| 1:A:157:GLY:C | 1:A:159:GLU:N | 2.49 | 0.63 |
| 1:B:225:TRP:CE3 | 1:B:225:TRP:C | 2.71 | 0.63 |
| 1:A:115:THR:HG21 | 1:A:253:GLN:O | 1.99 | 0.63 |
| 1:A:330:VAL:HG22 | 1:A:374:MET:HG3 | 1.81 | 0.63 |
| 1:B:110:LYS:O | 1:B:111:GLY:O | 2.17 | 0.63 |
| 1:B:162:GLU:HA | 1:B:162:GLU:OE1 | 1.99 | 0.63 |
| 1:B:489:LEU:O | 1:B:489:LEU:HD23 | 1.98 | 0.63 |
| 2:F:56:SER:O | 2:F:60:LYS:HG2 | 1.98 | 0.63 |
| 1:A:9:ARG:HA | 1:A:30:CYS:O | 1.99 | 0.63 |
| 1:C:180:LEU:HD23 | 1:C:184:GLY:O | 1.99 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:127:GLY:HA3 | 1:B:218:PHE:CZ | 2.34 | 0.63 |
| 1:B:216:GLU:OE1 | 1:B:216:GLU:HA | 1.98 | 0.63 |
| 2:F:19:TRP:CG | 2:F:20:LEU:N | 2.64 | 0.63 |
| 1:C:40:THR:O | 1:C:143:VAL:HG13 | 1.98 | 0.62 |
| 1:C:305:TYR:HB3 | 1:C:339:CYS:HA | 1.81 | 0.62 |
| 2:D:56:SER:HB3 | 2:D:59:GLN:CG | 2.04 | 0.62 |
| 2:D:60:LYS:HD3 | 2:D:60:LYS:H | 1.64 | 0.62 |
| 2:D:69:LEU:O | 2:D:69:LEU:HD23 | 1.99 | 0.62 |
| 2:D:69:LEU:HD22 | 2:F:70:ILE:HD12 | 1.81 | 0.62 |
| 1:B:71:ASP:OD2 | 1:B:80:ALA:HB1 | 1.99 | 0.62 |
| 1:C:2:ARG:HH12 | 1:C:155:ASP:CG | 2.02 | 0.62 |
| 1:C:63:ALA:HB2 | 1:C:242:LEU:CD1 | 2.29 | 0.62 |
| 1:B:32:THR:CB | 1:B:42:ASP:HB3 | 2.29 | 0.62 |
| 1:A:101:TRP:HZ2 | 1:C:316:LYS:HB2 | 1.63 | 0.62 |
| 1:A:423:VAL:C | 1:A:425:GLY:H | 2.01 | 0.62 |
| 1:B:420:ARG:HB3 | 1:B:420:ARG:NH1 | 2.14 | 0.62 |
| 1:A:497:PHE:C | 1:A:499:SER:H | 2.03 | 0.62 |
| 1:B:169:ILE:HD12 | 1:B:169:ILE:N | 2.15 | 0.62 |
| 1:B:302:GLY:O | 1:B:304:SER:N | 2.29 | 0.62 |
| 1:B:479:THR:HG21 | 1:B:485:SER:HB2 | 1.81 | 0.62 |
| 1:A:321:THR:OG1 | 1:A:325:THR:OG1 | 2.17 | 0.62 |
| 1:A:355:VAL:O | 1:A:355:VAL:HG12 | 1.99 | 0.62 |
| 1:C:34:MET:CE | 1:C:359:ILE:HD12 | 2.30 | 0.62 |
| 1:C:93:LYS:O | 1:C:114:VAL:HA | 2.00 | 0.62 |
| 1:C:213:VAL:HG11 | 1:C:217:TRP:CE3 | 2.34 | 0.62 |
| 2:D:21:GLU:O | 2:D:23:ARG:N | 2.33 | 0.62 |
| 1:B:36:GLN:O | 1:B:300:LEU:HD21 | 1.98 | 0.62 |
| 1:B:101:TRP:CD1 | 1:B:108:PHE:CE2 | 2.88 | 0.62 |
| 1:B:417:GLY:O | 1:B:421:MET:HB2 | 2.00 | 0.62 |
| 1:A:294:LYS:HB3 | 1:A:296:ASP:OD1 | 1.99 | 0.62 |
| 1:C:330:VAL:HG23 | 1:C:374:MET:CE | 2.28 | 0.62 |
| 1:A:290:LYS:HE3 | 1:A:292:ARG:HH12 | 1.64 | 0.62 |
| 1:A:392:GLY:C | 1:A:394:LYS:N | 2.46 | 0.62 |
| 1:A:475:LEU:CD1 | 2:F:53:LEU:HB2 | 2.29 | 0.62 |
| 1:B:415:VAL:HG12 | 1:B:419:LYS:HE3 | 1.80 | 0.62 |
| 1:B:487:MET:HA | 1:B:490:ALA:HB3 | 1.80 | 0.62 |
| 1:A:150:GLY:O | 1:A:152:ILE:N | 2.32 | 0.62 |
| 1:B:227:ALA:C | 1:B:229:ALA:H | 2.02 | 0.62 |
| 2:E:54:GLY:O | 2:E:56:SER:N | 2.33 | 0.62 |
| 1:A:72:SER:HB2 | 1:A:99:ARG:HH11 | 1.65 | 0.62 |
| 1:C:56:VAL:HG12 | 1:C:127:GLY:O | 1.99 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:70:SER:CB | 1:C:253:GLN:HE22 | 2.12 | 0.62 |
| 1:B:139:ILE:HD13 | 1:B:167:VAL:HG23 | 1.80 | 0.62 |
| 1:C:1:ILE:HG21 | 1:C:4:ILE:HG23 | 1.82 | 0.62 |
| 1:C:21:VAL:HA | 1:C:433:SER:HB2 | 1.80 | 0.62 |
| 1:C:211:TRP:HE1 | 1:C:269:LEU:CD1 | 1.97 | 0.62 |
| 1:B:426:ASP:C | 1:B:428:ALA:N | 2.53 | 0.62 |
| 1:A:2:ARG:HB2 | 1:A:142:SER:HB2 | 1.79 | 0.61 |
| 1:B:1:ILE:HD12 | 1:B:2:ARG:H | 1.64 | 0.61 |
| 2:E:42:PHE:O | 2:E:46:ALA:CB | 2.48 | 0.61 |
| 1:A:3:CYS:O | 1:A:9:ARG:HD3 | 2.00 | 0.61 |
| 1:A:291:CYS:C | 1:A:292:ARG:HD2 | 2.20 | 0.61 |
| 1:A:356:GLY:O | 1:A:357:ARG:CB | 2.48 | 0.61 |
| 2:D:12:LEU:H | 2:D:12:LEU:CD1 | 2.12 | 0.61 |
| 1:B:137:TYR:HB2 | 1:B:169:ILE:CD1 | 2.31 | 0.61 |
| 1:B:201:LEU:HD12 | 1:B:212:LEU:HB3 | 1.82 | 0.61 |
| 1:C:179:THR:C | 1:C:180:LEU:HD22 | 2.20 | 0.61 |
| 2:D:12:LEU:HD12 | 2:D:12:LEU:N | 2.15 | 0.61 |
| 1:B:93:LYS:HB3 | 1:B:245:PHE:CE2 | 2.34 | 0.61 |
| 1:B:238:ASN:O | 1:B:239:LYS:CB | 2.49 | 0.61 |
| 2:F:50:ALA:HB2 | 2:F:67:ILE:HD12 | 1.83 | 0.61 |
| 1:A:115:THR:HG22 | 1:A:253:GLN:HE22 | 1.64 | 0.61 |
| 1:C:273:LEU:HB2 | 2:F:12:LEU:HD11 | 1.82 | 0.61 |
| 1:B:73:ARG:HD2 | 1:B:77:GLN:HG3 | 1.83 | 0.61 |
| 1:B:82:LEU:O | 1:B:84:LYS:N | 2.32 | 0.61 |
| 1:B:130:ILE:HG13 | 1:B:130:ILE:O | 2.00 | 0.61 |
| 1:B:261:GLN:OE1 | 1:B:261:GLN:HA | 1.98 | 0.61 |
| 1:B:409:LYS:NZ | 1:B:413:ALA:HB2 | 2.15 | 0.61 |
| 1:A:49:THR:HG23 | 1:A:136:GLU:HG3 | 1.80 | 0.61 |
| 1:A:348:ASP:HB2 | 1:A:350:GLN:HG2 | 1.82 | 0.61 |
| 1:C:178:ALA:O | 1:C:185:SER:CB | 2.48 | 0.61 |
| 1:B:127:GLY:HA2 | 1:B:204:LEU:HD12 | 1.82 | 0.61 |
| 1:A:1:ILE:N | 1:A:144:HIS:NE2 | 2.48 | 0.61 |
| 1:A:34:MET:SD | 1:A:34:MET:N | 2.74 | 0.61 |
| 1:A:199:SER:O | 1:A:200:ASP:HB2 | 2.00 | 0.61 |
| 1:C:308:CYS:HB3 | 1:C:332:TYR:HE2 | 1.66 | 0.61 |
| 1:B:45:LEU:HA | 1:B:139:ILE:CG2 | 2.30 | 0.61 |
| 1:B:137:TYR:HB2 | 1:B:169:ILE:HD11 | 1.83 | 0.61 |
| 1:B:185:SER:O | 1:B:186:LEU:HG | 2.01 | 0.61 |
| 1:B:190:CYS:C | 1:B:192:PRO:HD3 | 2.20 | 0.61 |
| 1:A:331:GLN:HG2 | 1:A:372:SER:O | 2.01 | 0.61 |
| 1:A:423:VAL:O | 1:A:424:LEU:HB2 | 2.00 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:164:ARG:HG2 | 1:C:164:ARG:NH1 | 2.15 | 0.61 |
| 1:B:60:CYS:HB3 | 1:B:224:PRO:CG | 2.14 | 0.61 |
| 1:B:265:VAL:O | 1:B:269:LEU:HB2 | 2.00 | 0.61 |
| 2:F:7:HIS:C | 2:F:9:THR:H | 2.03 | 0.61 |
| 1:A:341:VAL:HG21 | 1:A:374:MET:HE3 | 1.83 | 0.61 |
| 1:C:113:LEU:HD11 | 1:C:253:GLN:NE2 | 2.16 | 0.61 |
| 1:C:277:MET:HA | 1:C:282:GLY:HA2 | 1.83 | 0.61 |
| 1:C:338:PRO:HA | 1:C:365:ILE:O | 2.00 | 0.61 |
| 1:C:409:LYS:HA | 1:C:409:LYS:NZ | 2.15 | 0.61 |
| 1:C:428:ALA:O | 1:C:430:ASP:N | 2.33 | 0.61 |
| 2:D:9:THR:HG22 | 2:D:10:ARG:HG2 | 1.82 | 0.61 |
| 1:B:415:VAL:HA | 1:B:418:ALA:CB | 2.30 | 0.61 |
| 1:A:324:GLY:CA | 1:A:402:ARG:HH22 | 2.13 | 0.61 |
| 1:B:95:THR:O | 1:B:112:SER:HA | 2.01 | 0.61 |
| 1:C:90:TYR:CZ | 1:C:118:LYS:HG3 | 2.35 | 0.61 |
| 1:B:225:TRP:CE3 | 1:B:226:HIS:CA | 2.83 | 0.61 |
| 1:B:341:VAL:HG23 | 1:B:363:PRO:HB2 | 1.83 | 0.61 |
| 1:A:135:LEU:HD23 | 1:A:135:LEU:H | 1.66 | 0.60 |
| 1:C:471:LEU:HD23 | 2:F:62:ILE:HD11 | 1.82 | 0.60 |
| 1:A:48:THR:HG23 | 1:A:284:LEU:HG | 1.83 | 0.60 |
| 1:A:235:HIS:HD2 | 1:B:86:SER:HA | 1.65 | 0.60 |
| 1:A:470:THR:C | 1:A:472:LEU:H | 2.05 | 0.60 |
| 1:C:47:THR:HB | 1:C:138:ARG:HB2 | 1.81 | 0.60 |
| 1:C:131:GLN:O | 1:C:133:GLU:O | 2.19 | 0.60 |
| 1:C:286:SER:HB3 | 2:F:16:SER:HB2 | 1.83 | 0.60 |
| 1:C:330:VAL:HG23 | 1:C:374:MET:HE3 | 1.82 | 0.60 |
| 1:B:45:LEU:HA | 1:B:139:ILE:HG22 | 1.83 | 0.60 |
| 1:B:137:TYR:HE2 | 1:B:289:LEU:HD13 | 1.66 | 0.60 |
| 1:B:366:THR:O | 1:B:368:SER:N | 2.34 | 0.60 |
| 1:A:143:VAL:HG11 | 1:A:183:PHE:CD2 | 2.36 | 0.60 |
| 1:A:228:GLY:HA3 | 1:B:73:ARG:HH12 | 1.66 | 0.60 |
| 1:A:338:PRO:HA | 1:A:365:ILE:O | 2.01 | 0.60 |
| 1:A:376:LEU:HD12 | 1:A:376:LEU:O | 2.02 | 0.60 |
| 1:B:341:VAL:CG2 | 1:B:363:PRO:HB2 | 2.32 | 0.60 |
| 1:B:181:GLY:O | 1:B:183:PHE:N | 2.32 | 0.60 |
| 1:B:382:PHE:N | 1:B:382:PHE:CD1 | 2.69 | 0.60 |
| 1:A:382:PHE:CD2 | 1:A:406:THR:HA | 2.37 | 0.60 |
| 1:C:329:GLU:CG | 1:C:375:MET:HB3 | 2.31 | 0.60 |
| 1:C:461:SER:O | 1:C:464:SER:OG | 2.15 | 0.60 |
| 2:D:47:ALA:HA | 2:D:64:LEU:HD23 | 1.84 | 0.60 |
| 1:B:75:PRO:HB3 | 1:B:110:LYS:CB | 2.32 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:216:GLU:O | 1:B:218:PHE:N | 2.33 | 0.60 |
| 1:A:1:ILE:HG12 | 1:A:147:GLN:CB | 2.32 | 0.60 |
| 1:A:2:ARG:NH1 | 1:A:140:MET:HG3 | 2.16 | 0.60 |
| 1:A:238:ASN:O | 1:A:240:GLU:N | 2.35 | 0.60 |
| 1:A:244:GLU:O | 1:A:255:VAL:HA | 2.01 | 0.60 |
| 1:C:20:TRP:CD1 | 1:C:20:TRP:O | 2.54 | 0.60 |
| 1:C:175:ARG:HG2 | 1:C:189:ASP:OD1 | 2.01 | 0.60 |
| 2:D:72:PRO:O | 2:D:73:ALA:HB3 | 2.01 | 0.60 |
| 1:B:4:ILE:HD11 | 1:B:144:HIS:HE1 | 1.67 | 0.60 |
| 1:B:22:ASP:HB2 | 1:B:433:SER:HA | 1.82 | 0.60 |
| 1:B:196:LEU:HD21 | 1:B:287:GLY:HA2 | 1.84 | 0.60 |
| 1:B:277:MET:HG3 | 1:B:279:GLY:H | 1.66 | 0.60 |
| 2:F:54:GLY:O | 2:F:59:GLN:NE2 | 2.35 | 0.60 |
| 1:A:150:GLY:CA | 1:A:152:ILE:HD13 | 2.32 | 0.60 |
| 1:A:238:ASN:C | 1:A:240:GLU:H | 2.04 | 0.60 |
| 1:C:154:ASN:HB2 | 3:C:601:NAG:C8 | 2.30 | 0.60 |
| 1:C:210:HIS:HD2 | 1:C:277:MET:H | 1.47 | 0.60 |
| 2:D:29:LEU:HD23 | 2:D:29:LEU:C | 2.22 | 0.60 |
| 1:B:2:ARG:HH12 | 1:B:140:MET:HB3 | 1.66 | 0.60 |
| 1:B:107:LEU:H | 1:B:107:LEU:CD1 | 2.13 | 0.60 |
| 2:E:11:LYS:C | 2:E:12:LEU:HD12 | 2.21 | 0.60 |
| 2:F:29:LEU:O | 2:F:31:ARG:N | 2.35 | 0.60 |
| 1:A:1:ILE:HD13 | 1:A:144:HIS:CA | 2.29 | 0.60 |
| 1:A:21:VAL:O | 1:A:21:VAL:HG13 | 2.01 | 0.60 |
| 1:A:409:LYS:HB3 | 1:A:409:LYS:HZ2 | 1.65 | 0.60 |
| 1:C:375:MET:HE3 | 1:C:375:MET:N | 2.16 | 0.60 |
| 1:C:443:LYS:O | 1:C:443:LYS:HG2 | 2.02 | 0.60 |
| 1:B:272:ALA:HB2 | 2:E:18:THR:CG2 | 2.27 | 0.60 |
| 1:A:411:PHE:O | 1:A:415:VAL:HG22 | 2.02 | 0.60 |
| 1:C:15:MET:SD | 1:C:36:GLN:CB | 2.90 | 0.60 |
| 1:C:255:VAL:O | 1:C:255:VAL:HG12 | 2.02 | 0.60 |
| 1:C:302:GLY:CA | 1:C:305:TYR:CD2 | 2.85 | 0.60 |
| 1:C:396:ILE:HD12 | 1:C:397:THR:H | 1.65 | 0.60 |
| 1:B:446:HIS:CG | 1:B:446:HIS:O | 2.55 | 0.60 |
| 1:B:491:LEU:HD12 | 1:B:494:VAL:HG21 | 1.84 | 0.60 |
| 1:A:65:ILE:HG23 | 1:A:66:SER:H | 1.66 | 0.59 |
| 1:A:457:PHE:O | 1:A:460:MET:HB2 | 2.02 | 0.59 |
| 1:C:462:TRP:CD1 | 1:C:463:PHE:N | 2.70 | 0.59 |
| 1:B:191:GLU:O | 1:B:193:ARG:N | 2.28 | 0.59 |
| 1:A:349:MET:O | 1:A:349:MET:SD | 2.60 | 0.59 |
| 1:C:1:ILE:O | 1:C:2:ARG:HB3 | 2.03 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:61:TYR:HE1 | 1:C:123:LYS:HE2 | 1.66 | 0.59 |
| 1:C:70:SER:HA | 1:C:82:LEU:HD11 | 1.84 | 0.59 |
| 1:C:407:ILE:HG22 | 1:C:407:ILE:O | 2.02 | 0.59 |
| 1:C:426:ASP:C | 1:C:428:ALA:H | 2.05 | 0.59 |
| 1:B:23:VAL:HG21 | 1:B:31:VAL:HG21 | 1.82 | 0.59 |
| 1:A:261:GLN:OE1 | 2:D:2:VAL:HG21 | 2.02 | 0.59 |
| 1:C:1:ILE:N | 1:C:1:ILE:CD1 | 2.65 | 0.59 |
| 1:C:373:LYS:NZ | 1:C:373:LYS:HB3 | 2.16 | 0.59 |
| 2:D:66:MET:HA | 2:D:66:MET:CE | 2.32 | 0.59 |
| 1:B:23:VAL:CG2 | 1:B:31:VAL:HG21 | 2.33 | 0.59 |
| 1:A:418:ALA:HA | 1:A:421:MET:HB2 | 1.84 | 0.59 |
| 1:B:160:THR:O | 1:B:160:THR:HG22 | 2.03 | 0.59 |
| 1:B:171:PRO:CA | 1:B:192:PRO:HB2 | 2.30 | 0.59 |
| 1:B:364:VAL:N | 1:B:374:MET:CE | 2.65 | 0.59 |
| 1:A:43:ILE:HD12 | 1:A:43:ILE:O | 2.02 | 0.59 |
| 1:A:90:TYR:N | 1:A:239:LYS:NZ | 2.49 | 0.59 |
| 1:A:342:PRO:O | 1:A:390:GLY:N | 2.33 | 0.59 |
| 1:B:286:SER:HB2 | 2:E:14:THR:HG21 | 1.85 | 0.59 |
| 1:B:345:MET:CG | 1:B:378:LEU:HD23 | 2.31 | 0.59 |
| 1:A:156:THR:O | 1:A:157:GLY:C | 2.37 | 0.59 |
| 1:A:261:GLN:HE21 | 1:A:261:GLN:N | 2.01 | 0.59 |
| 1:A:419:LYS:O | 1:A:423:VAL:HG12 | 2.02 | 0.59 |
| 1:C:72:SER:HB3 | 1:C:113:LEU:HD13 | 1.85 | 0.59 |
| 2:D:41:GLY:C | 2:D:43:ALA:N | 2.55 | 0.59 |
| 1:B:49:THR:HG22 | 1:B:283:ARG:CG | 2.32 | 0.59 |
| 1:B:66:SER:HG | 1:B:118:LYS:HB3 | 1.68 | 0.59 |
| 2:F:4:LEU:N | 2:F:5:PRO:HD2 | 2.17 | 0.59 |
| 1:C:307:LEU:N | 1:C:307:LEU:HD12 | 2.17 | 0.59 |
| 1:B:1:ILE:CD1 | 1:B:142:SER:OG | 2.49 | 0.59 |
| 1:B:109:GLY:O | 1:B:110:LYS:HB2 | 2.02 | 0.59 |
| 2:E:12:LEU:HD12 | 2:E:12:LEU:N | 2.18 | 0.59 |
| 1:A:131:GLN:C | 1:A:133:GLU:H | 2.06 | 0.59 |
| 1:A:307:LEU:N | 1:A:307:LEU:CD2 | 2.64 | 0.59 |
| 1:C:125:MET:HB3 | 1:C:206:MET:HB3 | 1.85 | 0.59 |
| 1:B:185:SER:C | 1:B:186:LEU:HG | 2.21 | 0.59 |
| 1:B:258:LEU:HD23 | 1:B:259:GLY:N | 2.17 | 0.59 |
| 2:F:50:ALA:HB1 | 2:F:63:TYR:HB3 | 1.84 | 0.59 |
| 1:B:46:VAL:HG13 | 1:B:47:THR:H | 1.68 | 0.59 |
| 1:B:418:ALA:HA | 1:B:421:MET:HE3 | 1.84 | 0.59 |
| 1:B:303:VAL:O | 1:B:303:VAL:HG12 | 2.02 | 0.59 |
| 1:B:415:VAL:HA | 1:B:418:ALA:HB3 | 1.85 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:382:PHE:CE2 | 1:A:406:THR:HA | 2.38 | 0.58 |
| 1:C:268:ALA:HB1 | 2:F:5:PRO:O | 2.03 | 0.58 |
| 2:D:1:ALA:O | 2:D:2:VAL:C | 2.42 | 0.58 |
| 2:D:27:LYS:HA | 2:D:30:ILE:HG12 | 1.85 | 0.58 |
| 1:B:190:CYS:O | 1:B:192:PRO:HD3 | 2.03 | 0.58 |
| 1:B:459:GLY:H | 1:B:460:MET:HE3 | 1.67 | 0.58 |
| 1:C:22:ASP:HA | 1:C:292:ARG:HG2 | 1.85 | 0.58 |
| 1:C:496:ILE:O | 1:C:500:THR:OG1 | 2.19 | 0.58 |
| 2:E:33:GLU:C | 2:E:35:TRP:H | 2.05 | 0.58 |
| 2:F:56:SER:HB3 | 2:F:59:GLN:CB | 2.33 | 0.58 |
| 1:A:220:ASP:OD2 | 2:F:38:ARG:HD2 | 2.03 | 0.58 |
| 1:C:65:ILE:H | 1:C:257:VAL:HG11 | 1.67 | 0.58 |
| 1:C:180:LEU:CB | 1:C:183:PHE:HB2 | 2.33 | 0.58 |
| 1:C:416:ARG:O | 1:C:420:ARG:HG3 | 2.03 | 0.58 |
| 1:B:12:VAL:CG1 | 1:B:12:VAL:O | 2.52 | 0.58 |
| 2:F:61:VAL:C | 2:F:63:TYR:H | 2.06 | 0.58 |
| 1:A:39:PRO:HG3 | 1:A:300:LEU:HA | 1.85 | 0.58 |
| 1:C:334:GLY:HA2 | 1:C:370:GLU:HA | 1.85 | 0.58 |
| 1:B:137:TYR:HD2 | 1:B:289:LEU:CD2 | 2.12 | 0.58 |
| 1:B:151:MET:HG2 | 1:B:152:ILE:HG12 | 1.85 | 0.58 |
| 2:E:21:GLU:O | 2:E:24:GLU:CB | 2.52 | 0.58 |
| 1:A:96:LEU:HD12 | 1:A:96:LEU:N | 2.17 | 0.58 |
| 1:C:65:ILE:CD1 | 1:C:257:VAL:HG12 | 2.31 | 0.58 |
| 1:B:38:LYS:N | 1:B:300:LEU:HD11 | 2.19 | 0.58 |
| 1:B:170:THR:O | 1:B:192:PRO:HG2 | 2.03 | 0.58 |
| 1:B:322:LEU:O | 1:B:323:HIS:CD2 | 2.56 | 0.58 |
| 1:C:214:HIS:NE2 | 1:C:216:GLU:HG3 | 2.19 | 0.58 |
| 1:C:262:GLU:OE1 | 1:C:262:GLU:N | 2.36 | 0.58 |
| 2:D:26:THR:O | 2:D:29:LEU:HB3 | 2.02 | 0.58 |
| 2:D:27:LYS:HB3 | 2:F:2:VAL:HG21 | 1.84 | 0.58 |
| 1:A:63:ALA:HB1 | 1:A:119:PHE:CE1 | 2.38 | 0.58 |
| 1:A:305:TYR:HE1 | 1:A:338:PRO:CG | 2.16 | 0.58 |
| 1:A:313:THR:HG23 | 1:A:313:THR:O | 2.04 | 0.58 |
| 1:C:355:VAL:HG12 | 1:C:356:GLY:N | 2.18 | 0.58 |
| 1:B:73:ARG:HH11 | 1:B:77:GLN:HG3 | 1.67 | 0.58 |
| 1:B:272:ALA:CA | 2:E:18:THR:HG22 | 2.34 | 0.58 |
| 1:B:314:PHE:HA | 1:B:330:VAL:HG22 | 1.86 | 0.58 |
| 1:B:360:THR:HG21 | 1:B:363:PRO:HB3 | 1.86 | 0.58 |
| 2:E:26:THR:O | 2:E:30:ILE:HG13 | 2.04 | 0.58 |
| 1:A:107:LEU:N | 1:A:107:LEU:HD23 | 2.17 | 0.58 |
| 1:A:225:TRP:C | 1:A:225:TRP:CD1 | 2.76 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:389:ILE:HD11 | 1:C:396:ILE:O | 2.04 | 0.58 |
| 1:C:423:VAL:HG23 | 1:C:502:VAL:HG11 | 1.86 | 0.58 |
| 1:B:1:ILE:CG2 | 1:B:147:GLN:HB2 | 2.23 | 0.58 |
| 1:B:31:VAL:HG13 | 1:B:43:ILE:CD1 | 2.34 | 0.58 |
| 1:B:38:LYS:CG | 1:B:39:PRO:HD2 | 2.32 | 0.58 |
| 1:B:268:ALA:HB2 | 2:E:4:LEU:HD11 | 1.85 | 0.58 |
| 1:B:364:VAL:N | 1:B:374:MET:HE1 | 2.18 | 0.58 |
| 1:A:383:GLY:O | 1:A:401:HIS:ND1 | 2.36 | 0.58 |
| 1:C:39:PRO:CG | 1:C:183:PHE:HE2 | 2.15 | 0.58 |
| 1:C:154:ASN:CA | 3:C:601:NAG:H82 | 2.34 | 0.58 |
| 1:C:257:VAL:O | 1:C:258:LEU:CB | 2.52 | 0.58 |
| 1:C:307:LEU:HD12 | 1:C:307:LEU:H | 1.68 | 0.58 |
| 2:D:10:ARG:HH21 | 2:D:10:ARG:CG | 2.17 | 0.58 |
| 1:B:202:TYR:CE1 | 1:B:215:LYS:HB2 | 2.38 | 0.58 |
| 1:C:211:TRP:HB3 | 1:C:274:GLU:HA | 1.85 | 0.58 |
| 1:C:301:LYS:NZ | 1:C:301:LYS:HB3 | 2.18 | 0.58 |
| 1:B:38:LYS:HG2 | 1:B:39:PRO:N | 2.18 | 0.58 |
| 1:B:375:MET:O | 1:B:376:LEU:HG | 2.04 | 0.57 |
| 1:C:395:LYS:O | 1:C:395:LYS:HD3 | 2.04 | 0.57 |
| 1:C:445:ILE:HA | 1:C:448:ILE:CD1 | 2.34 | 0.57 |
| 2:D:46:ALA:O | 2:D:49:ILE:HG12 | 2.03 | 0.57 |
| 2:E:14:THR:HG23 | 2:E:16:SER:O | 2.04 | 0.57 |
| 2:E:70:ILE:HG13 | 2:E:75:SER:C | 2.25 | 0.57 |
| 1:A:331:GLN:HA | 1:A:373:LYS:HA | 1.86 | 0.57 |
| 1:C:213:VAL:HG12 | 1:C:214:HIS:N | 2.18 | 0.57 |
| 1:B:100:GLY:O | 1:B:105:CYS:HB2 | 2.04 | 0.57 |
| 2:F:27:LYS:CG | 2:F:28:HIS:H | 2.16 | 0.57 |
| 1:A:246:LYS:O | 1:A:253:GLN:HA | 2.03 | 0.57 |
| 1:C:101:TRP:N | 1:C:101:TRP:CD1 | 2.70 | 0.57 |
| 1:C:164:ARG:O | 1:C:164:ARG:HG3 | 2.04 | 0.57 |
| 1:C:171:PRO:HB2 | 1:C:193:ARG:HH11 | 1.69 | 0.57 |
| 1:C:340:LYS:HG2 | 1:C:341:VAL:N | 2.18 | 0.57 |
| 1:C:373:LYS:HB3 | 1:C:373:LYS:HZ3 | 1.68 | 0.57 |
| 2:E:51:TRP:HA | 2:E:60:LYS:HE3 | 1.86 | 0.57 |
| 2:E:65:VAL:HG22 | 2:E:69:LEU:HG | 1.86 | 0.57 |
| 1:A:10:ASP:O | 1:A:31:VAL:HG13 | 2.05 | 0.57 |
| 1:C:65:ILE:CD1 | 1:C:243:VAL:HG22 | 2.20 | 0.57 |
| 1:C:469:GLY:O | 1:C:472:LEU:HB2 | 2.04 | 0.57 |
| 1:B:4:ILE:N | 1:B:151:MET:HE3 | 2.09 | 0.57 |
| 1:B:137:TYR:CE2 | 1:B:289:LEU:HB2 | 2.38 | 0.57 |
| 1:B:351:THR:O | 1:B:353:THR:N | 2.35 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:24:VAL:HG11 | 1:A:424:LEU:HD21 | 1.85 | 0.57 |
| 1:A:327:THR:HG21 | 1:C:108:PHE:HE2 | 1.70 | 0.57 |
| 1:A:479:THR:CG2 | 1:A:480:LYS:H | 2.03 | 0.57 |
| 2:D:25:TYR:HD1 | 2:D:25:TYR:C | 2.07 | 0.57 |
| 1:B:73:ARG:HB3 | 1:B:77:GLN:NE2 | 2.19 | 0.57 |
| 1:B:101:TRP:CD1 | 1:B:108:PHE:CD2 | 2.92 | 0.57 |
| 1:B:309:THR:O | 1:B:310:ALA:HB2 | 2.04 | 0.57 |
| 1:A:314:PHE:CD1 | 1:A:314:PHE:N | 2.72 | 0.57 |
| 1:C:95:THR:O | 1:C:96:LEU:HD23 | 2.04 | 0.57 |
| 1:C:462:TRP:CE3 | 1:C:499:SER:HB2 | 2.39 | 0.57 |
| 1:B:23:VAL:HG21 | 1:B:31:VAL:CG1 | 2.32 | 0.57 |
| 1:B:205:THR:HG23 | 1:B:210:HIS:HD2 | 1.70 | 0.57 |
| 1:B:332:TYR:CD1 | 1:B:333:ALA:N | 2.73 | 0.57 |
| 1:A:216:GLU:HB3 | 2:F:38:ARG:HD3 | 1.86 | 0.57 |
| 1:C:26:GLU:HG2 | 1:C:28:GLY:H | 1.68 | 0.57 |
| 1:B:6:VAL:C | 1:B:8:ASN:N | 2.57 | 0.57 |
| 1:B:55:GLU:CD | 1:B:55:GLU:N | 2.58 | 0.57 |
| 1:B:241:ALA:O | 1:B:242:LEU:HG | 2.05 | 0.57 |
| 2:E:28:HIS:H | 2:E:28:HIS:CD2 | 2.21 | 0.57 |
| 1:C:240:GLU:H | 1:C:240:GLU:CD | 2.07 | 0.57 |
| 1:B:225:TRP:CB | 1:B:237:ASN:HD22 | 2.18 | 0.57 |
| 1:B:457:PHE:CD2 | 1:B:495:LEU:HD21 | 2.40 | 0.57 |
| 1:B:415:VAL:C | 1:B:417:GLY:H | 2.07 | 0.57 |
| 1:A:6:VAL:CG1 | 1:A:9:ARG:HB2 | 2.35 | 0.56 |
| 2:D:1:ALA:HB1 | 2:F:23:ARG:HD2 | 1.84 | 0.56 |
| 2:D:67:ILE:HD12 | 2:D:70:ILE:CG2 | 2.34 | 0.56 |
| 1:B:39:PRO:HG3 | 1:B:183:PHE:HD1 | 1.68 | 0.56 |
| 1:B:95:THR:HG22 | 1:B:96:LEU:HD23 | 1.87 | 0.56 |
| 1:B:99:ARG:NH2 | 1:B:105:CYS:SG | 2.78 | 0.56 |
| 2:E:62:ILE:O | 2:E:65:VAL:N | 2.37 | 0.56 |
| 1:A:85:GLN:NE2 | 1:A:94:ARG:HH22 | 2.01 | 0.56 |
| 1:A:101:TRP:CZ2 | 1:C:316:LYS:HB2 | 2.39 | 0.56 |
| 1:C:19:THR:HG22 | 1:C:19:THR:O | 2.04 | 0.56 |
| 1:B:11:PHE:HA | 1:B:32:THR:HG22 | 1.86 | 0.56 |
| 1:B:246:LYS:O | 1:B:254:THR:CG2 | 2.53 | 0.56 |
| 1:A:44:GLU:CG | 1:A:46:VAL:HG23 | 2.34 | 0.56 |
| 1:A:55:GLU:HA | 1:A:128:LYS:HA | 1.86 | 0.56 |
| 1:C:33:VAL:O | 1:C:40:THR:HA | 2.05 | 0.56 |
| 1:C:251:LYS:HG3 | 1:C:251:LYS:O | 2.04 | 0.56 |
| 1:C:276:GLU:HG2 | 1:C:276:GLU:O | 2.05 | 0.56 |
| 1:C:315:THR:HG21 | 1:C:373:LYS:CE | 2.31 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:467:LEU:HD13 | 2:F:69:LEU:CD2 | 2.35 | 0.56 |
| 1:B:39:PRO:HG3 | 1:B:183:PHE:CD1 | 2.40 | 0.56 |
| 1:B:62:GLU:HA | 1:B:260:SER:HA | 1.86 | 0.56 |
| 1:B:133:GLU:O | 1:B:134:ASN:CB | 2.53 | 0.56 |
| 1:B:135:LEU:HD12 | 1:B:136:GLU:N | 2.19 | 0.56 |
| 1:B:335:THR:O | 1:B:335:THR:HG22 | 2.05 | 0.56 |
| 1:B:365:ILE:CA | 1:B:374:MET:SD | 2.94 | 0.56 |
| 1:A:2:ARG:HB3 | 1:A:42:ASP:HB3 | 1.87 | 0.56 |
| 1:A:364:VAL:HG12 | 1:A:365:ILE:N | 2.20 | 0.56 |
| 1:C:421:MET:C | 1:C:421:MET:SD | 2.84 | 0.56 |
| 1:A:182:GLY:O | 1:A:301:LYS:HA | 2.05 | 0.56 |
| 1:A:348:ASP:C | 1:A:350:GLN:H | 2.08 | 0.56 |
| 1:C:212:LEU:HD13 | 1:C:284:LEU:HD23 | 1.85 | 0.56 |
| 1:B:63:ALA:HB2 | 1:B:242:LEU:HD22 | 1.88 | 0.56 |
| 1:B:100:GLY:HA3 | 1:B:108:PHE:CZ | 2.39 | 0.56 |
| 1:A:193:ARG:NH1 | 1:A:193:ARG:HB2 | 2.20 | 0.56 |
| 1:A:366:THR:O | 1:A:367:GLU:HG3 | 2.05 | 0.56 |
| 1:C:148:HIS:CB | 1:C:151:MET:HB3 | 2.36 | 0.56 |
| 2:D:41:GLY:O | 2:D:43:ALA:N | 2.39 | 0.56 |
| 1:B:21:VAL:CG1 | 1:B:293:LEU:CB | 2.75 | 0.56 |
| 1:B:53:MET:HB3 | 1:B:130:ILE:HG22 | 1.88 | 0.56 |
| 1:B:214:HIS:CE1 | 1:B:216:GLU:HB2 | 2.40 | 0.56 |
| 2:E:4:LEU:C | 2:E:4:LEU:CD2 | 2.73 | 0.56 |
| 1:A:329:GLU:HB2 | 1:C:101:TRP:HZ3 | 1.69 | 0.56 |
| 1:C:11:PHE:CD1 | 1:C:32:THR:OG1 | 2.58 | 0.56 |
| 1:C:315:THR:OG1 | 1:C:373:LYS:HE3 | 2.06 | 0.56 |
| 2:D:25:TYR:C | 2:D:25:TYR:CD1 | 2.78 | 0.56 |
| 1:A:56:VAL:HG22 | 1:A:57:ARG:HG3 | 1.88 | 0.56 |
| 1:A:238:ASN:C | 1:A:240:GLU:N | 2.59 | 0.56 |
| 1:A:51:SER:HB2 | 1:A:134:ASN:HB3 | 1.88 | 0.56 |
| 1:A:209:LYS:HB2 | 1:A:211:TRP:CH2 | 2.41 | 0.56 |
| 1:A:261:GLN:HA | 1:A:261:GLN:NE2 | 2.19 | 0.56 |
| 1:C:469:GLY:HA2 | 1:C:472:LEU:HD12 | 1.88 | 0.56 |
| 1:B:24:VAL:HG11 | 1:B:424:LEU:HD21 | 1.86 | 0.56 |
| 1:B:27:HIS:HB3 | 1:B:287:GLY:H | 1.70 | 0.56 |
| 1:B:247:ASP:HA | 1:B:253:GLN:HA | 1.87 | 0.56 |
| 1:B:364:VAL:H | 1:B:374:MET:HE3 | 1.69 | 0.56 |
| 2:E:56:SER:C | 2:E:58:SER:H | 2.09 | 0.56 |
| 1:A:65:ILE:HG23 | 1:A:66:SER:N | 2.20 | 0.56 |
| 1:A:148:HIS:HD2 | 1:A:151:MET:HE1 | 1.71 | 0.56 |
| 1:A:466:ILE:O | 1:A:470:THR:N | 2.39 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:9:ARG:HA | 1:C:30:CYS:O | 2.06 | 0.56 |
| 1:C:222:PRO:O | 1:C:223:LEU:HD23 | 2.05 | 0.56 |
| 1:C:302:GLY:HA2 | 1:C:305:TYR:CE2 | 2.41 | 0.56 |
| 1:C:358:LEU:HG | 1:C:360:THR:O | 2.06 | 0.56 |
| 2:D:19:TRP:O | 2:D:21:GLU:N | 2.40 | 0.56 |
| 1:A:150:GLY:O | 1:A:152:ILE:HD13 | 2.06 | 0.55 |
| 1:C:315:THR:CG2 | 1:C:331:GLN:HG2 | 2.36 | 0.55 |
| 1:B:44:GLU:O | 1:B:46:VAL:N | 2.39 | 0.55 |
| 2:F:27:LYS:CG | 2:F:28:HIS:N | 2.69 | 0.55 |
| 1:A:82:LEU:O | 1:A:85:GLN:HG3 | 2.05 | 0.55 |
| 1:C:9:ARG:NH1 | 1:C:32:THR:HG21 | 2.16 | 0.55 |
| 1:C:58:SER:HB2 | 1:C:226:HIS:HB3 | 1.88 | 0.55 |
| 1:C:207:ASN:O | 1:C:208:ASN:HB2 | 2.06 | 0.55 |
| 1:B:72:SER:OG | 1:B:99:ARG:NH1 | 2.40 | 0.55 |
| 1:B:149:SER:C | 1:B:151:MET:H | 2.08 | 0.55 |
| 1:B:244:GLU:HB3 | 1:B:256:VAL:HG23 | 1.88 | 0.55 |
| 1:B:429:TRP:NE1 | 1:B:446:HIS:HD2 | 2.04 | 0.55 |
| 2:E:22:SER:O | 2:E:23:ARG:HB2 | 2.06 | 0.55 |
| 1:C:41:VAL:CG2 | 1:C:143:VAL:HG22 | 2.33 | 0.55 |
| 2:D:3:THR:O | 2:D:4:LEU:C | 2.45 | 0.55 |
| 1:B:152:ILE:HG22 | 1:B:153:VAL:N | 2.21 | 0.55 |
| 1:A:65:ILE:CD1 | 1:A:257:VAL:HG22 | 2.34 | 0.55 |
| 1:C:32:THR:HG22 | 1:C:42:ASP:OD2 | 2.06 | 0.55 |
| 1:C:336:ASP:C | 1:C:336:ASP:OD1 | 2.45 | 0.55 |
| 1:B:99:ARG:NH2 | 1:B:103:ASN:HD22 | 2.03 | 0.55 |
| 1:B:345:MET:HB3 | 1:B:387:ILE:HA | 1.88 | 0.55 |
| 1:A:91:VAL:HG22 | 1:A:239:LYS:HE3 | 1.89 | 0.55 |
| 1:A:163:ASN:O | 1:A:164:ARG:HD2 | 2.06 | 0.55 |
| 1:A:360:THR:HG23 | 1:A:377:GLU:H | 1.70 | 0.55 |
| 1:A:370:GLU:O | 1:A:371:ASN:HB2 | 2.06 | 0.55 |
| 1:C:217:TRP:CE2 | 2:F:5:PRO:HB2 | 2.42 | 0.55 |
| 1:B:148:HIS:C | 1:B:150:GLY:N | 2.60 | 0.55 |
| 2:E:19:TRP:CD1 | 2:E:20:LEU:HG | 2.41 | 0.55 |
| 1:A:225:TRP:CD1 | 1:A:226:HIS:N | 2.75 | 0.55 |
| 1:A:246:LYS:HE2 | 2:F:17:GLN:HB3 | 1.88 | 0.55 |
| 2:D:32:VAL:O | 2:D:32:VAL:HG22 | 2.06 | 0.55 |
| 1:B:38:LYS:HE3 | 1:B:39:PRO:O | 2.07 | 0.55 |
| 1:B:385:SER:C | 1:B:386:TYR:CD2 | 2.80 | 0.55 |
| 1:B:484:ILE:O | 1:B:484:ILE:HG22 | 2.07 | 0.55 |
| 1:A:49:THR:CG2 | 1:A:136:GLU:HG3 | 2.37 | 0.55 |
| 1:C:114:VAL:O | 1:C:114:VAL:CG1 | 2.55 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:179:THR:O | 1:C:180:LEU:HD13 | 2.07 | 0.55 |
| 1:C:261:GLN:O | 1:C:265:VAL:HG22 | 2.07 | 0.55 |
| 1:C:456:LEU:HB3 | 1:C:457:PHE:CD1 | 2.42 | 0.55 |
| 1:B:11:PHE:N | 1:B:11:PHE:CD1 | 2.75 | 0.55 |
| 1:B:261:GLN:NE2 | 2:E:1:ALA:H3 | 2.05 | 0.55 |
| 1:B:472:LEU:HD12 | 1:B:492:GLY:HA2 | 1.88 | 0.55 |
| 2:E:53:LEU:C | 2:E:55:SER:H | 2.10 | 0.55 |
| 1:A:237:ASN:O | 1:A:238:ASN:HB2 | 2.06 | 0.55 |
| 1:B:338:PRO:HG3 | 1:B:367:GLU:HG2 | 1.89 | 0.55 |
| 1:B:389:ILE:HG13 | 1:B:389:ILE:O | 2.07 | 0.55 |
| 1:B:472:LEU:HA | 1:B:475:LEU:HG | 1.89 | 0.55 |
| 1:A:19:THR:O | 1:A:294:LYS:HA | 2.06 | 0.55 |
| 1:A:31:VAL:O | 1:A:43:ILE:HD12 | 2.07 | 0.55 |
| 1:A:132:PRO:O | 1:A:135:LEU:HD21 | 2.07 | 0.55 |
| 1:C:40:THR:HG21 | 1:C:360:THR:HA | 1.87 | 0.55 |
| 1:B:12:VAL:HG12 | 1:B:33:VAL:HG12 | 1.86 | 0.55 |
| 1:B:37:ASP:O | 1:B:300:LEU:HD11 | 2.07 | 0.55 |
| 1:B:38:LYS:HG3 | 1:B:298:LEU:HB2 | 1.87 | 0.55 |
| 1:B:186:LEU:HD21 | 1:B:298:LEU:HD21 | 1.88 | 0.55 |
| 1:B:382:PHE:HD1 | 1:B:382:PHE:H | 1.53 | 0.55 |
| 1:B:420:ARG:HB3 | 1:B:420:ARG:HH11 | 1.72 | 0.55 |
| 2:F:7:HIS:C | 2:F:9:THR:N | 2.59 | 0.55 |
| 1:A:89:GLN:O | 1:A:89:GLN:HG2 | 2.06 | 0.55 |
| 1:A:197:ASP:O | 1:A:199:SER:O | 2.24 | 0.55 |
| 1:A:203:TYR:HE2 | 1:A:277:MET:HE2 | 1.71 | 0.55 |
| 1:A:263:GLY:O | 1:A:267:THR:CG2 | 2.42 | 0.55 |
| 1:A:324:GLY:HA3 | 1:A:402:ARG:HH22 | 1.71 | 0.55 |
| 1:C:20:TRP:O | 1:C:20:TRP:HD1 | 1.90 | 0.55 |
| 1:C:315:THR:HG23 | 1:C:331:GLN:HG2 | 1.89 | 0.55 |
| 1:B:71:ASP:HB2 | 1:B:82:LEU:CD1 | 2.21 | 0.55 |
| 1:B:415:VAL:C | 1:B:417:GLY:N | 2.60 | 0.55 |
| 1:A:224:PRO:HA | 1:A:237:ASN:O | 2.06 | 0.54 |
| 1:A:290:LYS:HB3 | 1:A:290:LYS:NZ | 2.21 | 0.54 |
| 1:C:329:GLU:HG3 | 1:C:375:MET:CB | 2.34 | 0.54 |
| 1:C:445:ILE:HD13 | 1:C:448:ILE:CD1 | 2.37 | 0.54 |
| 1:B:4:ILE:HD11 | 1:B:144:HIS:CE1 | 2.42 | 0.54 |
| 1:B:107:LEU:N | 1:B:107:LEU:CD1 | 2.67 | 0.54 |
| 1:B:135:LEU:CD1 | 1:B:136:GLU:N | 2.70 | 0.54 |
| 1:B:197:ASP:C | 1:B:199:SER:N | 2.60 | 0.54 |
| 1:B:322:LEU:O | 1:B:323:HIS:CG | 2.60 | 0.54 |
| 1:B:364:VAL:H | 1:B:374:MET:CE | 2.20 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:71:ALA:O | 2:F:75:SER:HB3 | 2.07 | 0.54 |
| 1:A:241:ALA:O | 1:A:242:LEU:HD12 | 2.06 | 0.54 |
| 1:C:1:ILE:HD13 | 1:C:152:ILE:HG22 | 1.88 | 0.54 |
| 1:C:47:THR:HG22 | 1:C:49:THR:HG23 | 1.89 | 0.54 |
| 2:D:47:ALA:O | 2:D:50:ALA:HB3 | 2.06 | 0.54 |
| 1:B:276:GLU:O | 1:B:283:ARG:O | 2.25 | 0.54 |
| 1:C:201:LEU:CD2 | 1:C:212:LEU:HD23 | 2.37 | 0.54 |
| 1:B:21:VAL:O | 1:B:21:VAL:CG2 | 2.56 | 0.54 |
| 1:B:365:ILE:N | 1:B:374:MET:SD | 2.80 | 0.54 |
| 1:A:311:ALA:O | 1:A:332:TYR:HA | 2.08 | 0.54 |
| 1:A:464:SER:O | 1:A:465:GLN:C | 2.45 | 0.54 |
| 1:C:113:LEU:HD21 | 1:C:253:GLN:HE21 | 1.71 | 0.54 |
| 1:C:302:GLY:CA | 1:C:305:TYR:CE2 | 2.90 | 0.54 |
| 1:B:81:TYR:O | 1:B:82:LEU:CB | 2.54 | 0.54 |
| 1:A:49:THR:HB | 1:A:283:ARG:NH2 | 2.22 | 0.54 |
| 1:A:72:SER:CB | 1:A:99:ARG:HH11 | 2.21 | 0.54 |
| 1:A:113:LEU:HD21 | 1:A:253:GLN:HE21 | 1.72 | 0.54 |
| 1:A:416:ARG:C | 1:A:418:ALA:H | 2.11 | 0.54 |
| 1:C:74:CYS:CB | 1:C:75:PRO:HD2 | 2.37 | 0.54 |
| 1:C:322:LEU:HD12 | 1:C:322:LEU:N | 2.23 | 0.54 |
| 2:D:19:TRP:C | 2:D:21:GLU:H | 2.11 | 0.54 |
| 2:D:70:ILE:O | 2:D:70:ILE:HD13 | 2.07 | 0.54 |
| 1:B:7:SER:HA | 1:B:322:LEU:HD13 | 1.89 | 0.54 |
| 1:B:371:ASN:O | 1:B:371:ASN:OD1 | 2.26 | 0.54 |
| 1:A:265:VAL:C | 1:A:267:THR:H | 2.11 | 0.54 |
| 1:A:332:TYR:CD2 | 1:A:335:THR:HB | 2.34 | 0.54 |
| 1:A:443:LYS:HB3 | 1:A:443:LYS:HZ3 | 1.69 | 0.54 |
| 2:D:51:TRP:HA | 2:D:60:LYS:NZ | 2.23 | 0.54 |
| 1:B:7:SER:HA | 1:B:322:LEU:CD1 | 2.38 | 0.54 |
| 1:B:236:TRP:HB2 | 1:B:239:LYS:CE | 2.28 | 0.54 |
| 1:B:330:VAL:CG1 | 1:B:331:GLN:N | 2.71 | 0.54 |
| 1:B:338:PRO:HG3 | 1:B:367:GLU:CG | 2.37 | 0.54 |
| 1:B:358:LEU:O | 1:B:359:ILE:C | 2.44 | 0.54 |
| 1:A:37:ASP:N | 1:A:37:ASP:OD1 | 2.40 | 0.54 |
| 1:A:74:CYS:SG | 1:A:75:PRO:HD2 | 2.47 | 0.54 |
| 1:A:204:LEU:CD2 | 1:A:204:LEU:N | 2.66 | 0.54 |
| 1:A:233:THR:O | 1:A:234:PRO:C | 2.45 | 0.54 |
| 1:A:259:GLY:O | 1:A:261:GLN:NE2 | 2.41 | 0.54 |
| 1:A:332:TYR:O | 1:A:372:SER:OG | 2.24 | 0.54 |
| 1:C:28:GLY:HA3 | 2:F:15:ARG:CG | 2.33 | 0.54 |
| 1:B:169:ILE:CD1 | 1:B:169:ILE:H | 2.20 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:260:SER:O | 1:B:261:GLN:CB | 2.54 | 0.54 |
| 1:A:38:LYS:HE3 | 1:A:38:LYS:CA | 2.33 | 0.54 |
| 1:A:224:PRO:HD2 | 1:A:242:LEU:HD22 | 1.89 | 0.54 |
| 1:A:315:THR:O | 1:A:316:LYS:HG2 | 2.08 | 0.54 |
| 1:A:363:PRO:HB2 | 1:A:374:MET:HE3 | 1.88 | 0.54 |
| 1:B:5:GLY:C | 1:B:7:SER:H | 2.11 | 0.54 |
| 1:B:151:MET:CG | 1:B:152:ILE:HG12 | 2.37 | 0.54 |
| 1:B:204:LEU:HG | 1:B:205:THR:H | 1.73 | 0.54 |
| 1:B:310:ALA:HB1 | 1:B:333:ALA:HB2 | 1.90 | 0.54 |
| 1:B:357:ARG:CG | 1:B:358:LEU:N | 2.71 | 0.54 |
| 1:B:447:GLN:C | 1:B:449:PHE:H | 2.11 | 0.54 |
| 1:B:472:LEU:HD23 | 1:B:475:LEU:CD1 | 2.37 | 0.54 |
| 1:A:125:MET:HG2 | 1:A:125:MET:O | 2.08 | 0.54 |
| 1:C:127:GLY:O | 1:C:128:LYS:C | 2.45 | 0.54 |
| 1:C:131:GLN:O | 1:C:133:GLU:N | 2.41 | 0.54 |
| 1:C:170:THR:O | 1:C:192:PRO:HG2 | 2.08 | 0.54 |
| 1:C:357:ARG:CG | 1:C:358:LEU:N | 2.69 | 0.54 |
| 1:C:423:VAL:O | 1:C:423:VAL:HG12 | 2.08 | 0.54 |
| 1:B:223:LEU:HD12 | 1:B:223:LEU:N | 2.23 | 0.54 |
| 1:C:314:PHE:H | 1:C:314:PHE:HD1 | 1.56 | 0.54 |
| 1:C:399:HIS:CE1 | 1:B:191:GLU:OE1 | 2.61 | 0.54 |
| 1:B:396:ILE:O | 1:B:396:ILE:CG1 | 2.55 | 0.53 |
| 1:A:466:ILE:HG13 | 1:A:467:LEU:H | 1.73 | 0.53 |
| 1:C:127:GLY:HA3 | 1:C:218:PHE:CE2 | 2.43 | 0.53 |
| 1:C:349:MET:HE1 | 1:C:352:LEU:HD22 | 1.89 | 0.53 |
| 1:B:57:ARG:CZ | 1:B:225:TRP:HE1 | 2.19 | 0.53 |
| 1:B:73:ARG:CA | 1:B:77:GLN:HE21 | 2.21 | 0.53 |
| 1:B:313:THR:CA | 1:B:396:ILE:HD12 | 2.36 | 0.53 |
| 1:A:396:ILE:HD12 | 1:A:396:ILE:N | 2.22 | 0.53 |
| 1:A:472:LEU:HA | 1:A:475:LEU:HD23 | 1.90 | 0.53 |
| 1:C:1:ILE:HG21 | 1:C:4:ILE:HG13 | 1.89 | 0.53 |
| 1:C:1:ILE:O | 1:C:2:ARG:CB | 2.56 | 0.53 |
| 1:C:72:SER:HA | 1:C:112:SER:O | 2.08 | 0.53 |
| 1:C:262:GLU:O | 1:C:263:GLY:C | 2.47 | 0.53 |
| 1:A:273:LEU:HG | 2:D:12:LEU:HB2 | 1.90 | 0.53 |
| 1:A:398:HIS:ND1 | 1:A:399:HIS:O | 2.42 | 0.53 |
| 1:C:32:THR:HA | 1:C:41:VAL:O | 2.07 | 0.53 |
| 1:B:351:THR:O | 1:B:351:THR:HG22 | 2.09 | 0.53 |
| 2:D:9:THR:CG2 | 2:D:10:ARG:N | 2.67 | 0.53 |
| 1:B:223:LEU:HB3 | 1:B:242:LEU:HD11 | 1.91 | 0.53 |
| 2:E:40:PRO:HG2 | 2:E:41:GLY:N | 2.23 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:108:PHE:HB2 | 1:C:320:GLU:O | 2.08 | 0.53 |
| 1:A:273:LEU:CG | 2:D:12:LEU:HD22 | 2.39 | 0.53 |
| 1:A:156:THR:C | 1:A:158:HIS:N | 2.61 | 0.53 |
| 1:A:341:VAL:HG21 | 1:A:374:MET:CE | 2.39 | 0.53 |
| 1:A:426:ASP:OD1 | 1:A:446:HIS:HB3 | 2.09 | 0.53 |
| 1:C:320:GLU:OE2 | 1:C:324:GLY:HA2 | 2.09 | 0.53 |
| 1:B:56:VAL:HG13 | 1:B:57:ARG:H | 1.73 | 0.53 |
| 1:B:217:TRP:CD1 | 2:E:7:HIS:HB2 | 2.44 | 0.53 |
| 1:B:268:ALA:CA | 2:E:4:LEU:HD21 | 2.37 | 0.53 |
| 1:B:268:ALA:CB | 2:E:4:LEU:HD21 | 2.39 | 0.53 |
| 1:B:283:ARG:HG2 | 1:B:283:ARG:HH11 | 1.72 | 0.53 |
| 1:B:330:VAL:HG12 | 1:B:331:GLN:N | 2.23 | 0.53 |
| 1:A:2:ARG:CB | 1:A:142:SER:HB3 | 2.36 | 0.53 |
| 1:A:359:ILE:HG12 | 1:A:377:GLU:HB3 | 1.91 | 0.53 |
| 1:C:113:LEU:HD11 | 1:C:253:GLN:HE22 | 1.73 | 0.53 |
| 1:B:20:TRP:O | 1:B:22:ASP:N | 2.41 | 0.53 |
| 1:B:326:VAL:HG12 | 1:B:380:PRO:HD3 | 1.91 | 0.53 |
| 2:E:63:TYR:O | 2:E:67:ILE:HG22 | 2.08 | 0.53 |
| 1:A:74:CYS:O | 1:A:76:THR:N | 2.42 | 0.53 |
| 1:A:101:TRP:HB3 | 1:C:152:ILE:HD11 | 1.91 | 0.53 |
| 1:C:34:MET:HE3 | 1:C:359:ILE:HD12 | 1.90 | 0.53 |
| 2:E:71:ALA:N | 2:E:72:PRO:CD | 2.66 | 0.53 |
| 2:F:48:ALA:HA | 2:F:51:TRP:HB3 | 1.90 | 0.53 |
| 1:A:130:ILE:HG21 | 1:A:198:PHE:CD2 | 2.41 | 0.53 |
| 1:A:347:VAL:CG2 | 1:A:355:VAL:HB | 2.37 | 0.53 |
| 1:C:355:VAL:CG1 | 1:C:356:GLY:N | 2.72 | 0.53 |
| 1:B:99:ARG:NH2 | 1:B:103:ASN:HB3 | 2.21 | 0.53 |
| 1:B:113:LEU:HD13 | 1:B:113:LEU:C | 2.29 | 0.53 |
| 1:B:332:TYR:O | 1:B:333:ALA:C | 2.48 | 0.53 |
| 2:F:62:ILE:HG23 | 2:F:62:ILE:O | 2.08 | 0.53 |
| 1:A:70:SER:HA | 1:A:115:THR:HA | 1.91 | 0.52 |
| 1:A:378:LEU:HD23 | 1:A:379:ASP:N | 2.24 | 0.52 |
| 2:D:64:LEU:O | 2:D:68:LEU:HB2 | 2.08 | 0.52 |
| 1:B:2:ARG:HG2 | 1:B:3:CYS:H | 1.74 | 0.52 |
| 1:B:74:CYS:C | 1:B:76:THR:H | 2.11 | 0.52 |
| 1:B:75:PRO:HG2 | 1:B:107:LEU:HB2 | 1.90 | 0.52 |
| 1:B:169:ILE:HD12 | 1:B:169:ILE:H | 1.71 | 0.52 |
| 1:B:180:LEU:H | 1:B:180:LEU:CD1 | 1.98 | 0.52 |
| 1:B:338:PRO:CD | 1:B:367:GLU:HG2 | 2.39 | 0.52 |
| 1:A:23:VAL:HG22 | 1:A:24:VAL:N | 2.24 | 0.52 |
| 1:A:140:MET:SD | 1:A:158:HIS:CE1 | 3.03 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:352:LEU:H | 1:A:352:LEU:CD1 | 2.16 | 0.52 |
| 1:C:115:THR:CG2 | 1:C:253:GLN:HB3 | 2.37 | 0.52 |
| 2:D:9:THR:HG21 | 2:D:10:ARG:NH2 | 2.24 | 0.52 |
| 1:B:4:ILE:HG13 | 1:B:9:ARG:HH21 | 1.73 | 0.52 |
| 1:B:442:GLY:C | 1:B:444:GLY:N | 2.62 | 0.52 |
| 2:F:32:VAL:HG13 | 2:F:72:PRO:HG2 | 1.90 | 0.52 |
| 1:C:113:LEU:HD12 | 1:C:114:VAL:N | 2.24 | 0.52 |
| 1:C:300:LEU:CD2 | 1:C:301:LYS:O | 2.57 | 0.52 |
| 1:C:399:HIS:CE1 | 1:C:400:TRP:O | 2.62 | 0.52 |
| 2:D:53:LEU:CD1 | 2:F:62:ILE:HG21 | 2.37 | 0.52 |
| 1:B:40:THR:CG2 | 1:B:144:HIS:CD2 | 2.86 | 0.52 |
| 1:B:62:GLU:HB3 | 1:B:122:SER:HB2 | 1.91 | 0.52 |
| 1:A:150:GLY:HA2 | 1:A:375:MET:HE1 | 1.92 | 0.52 |
| 1:C:56:VAL:HG13 | 1:C:57:ARG:N | 2.24 | 0.52 |
| 1:C:155:ASP:OD1 | 1:C:158:HIS:CE1 | 2.63 | 0.52 |
| 1:C:225:TRP:HB2 | 1:C:237:ASN:HD22 | 1.73 | 0.52 |
| 1:C:226:HIS:CD2 | 1:C:234:PRO:HB2 | 2.44 | 0.52 |
| 2:D:30:ILE:HG13 | 2:D:31:ARG:H | 1.72 | 0.52 |
| 1:B:364:VAL:C | 1:B:374:MET:SD | 2.88 | 0.52 |
| 1:A:34:MET:HB3 | 1:A:40:THR:CG2 | 2.39 | 0.52 |
| 1:C:69:ALA:O | 1:C:116:CYS:N | 2.39 | 0.52 |
| 1:C:188:LEU:N | 1:C:188:LEU:HD23 | 2.24 | 0.52 |
| 1:C:494:VAL:HG13 | 1:C:495:LEU:HD23 | 1.92 | 0.52 |
| 1:B:22:ASP:H | 1:B:433:SER:HB3 | 1.75 | 0.52 |
| 1:B:374:MET:HB3 | 1:B:376:LEU:HD11 | 1.90 | 0.52 |
| 1:B:388:VAL:CG2 | 1:B:388:VAL:O | 2.57 | 0.52 |
| 1:A:74:CYS:C | 1:A:76:THR:H | 2.13 | 0.52 |
| 1:A:366:THR:O | 1:A:367:GLU:CG | 2.58 | 0.52 |
| 1:C:201:LEU:HD21 | 1:C:212:LEU:HD23 | 1.90 | 0.52 |
| 1:C:420:ARG:HD2 | 1:C:431:PHE:CE2 | 2.44 | 0.52 |
| 1:B:52:ASN:C | 1:B:53:MET:HG2 | 2.30 | 0.52 |
| 1:A:22:ASP:O | 1:A:23:VAL:HB | 2.10 | 0.52 |
| 1:A:366:THR:C | 1:A:367:GLU:HG3 | 2.30 | 0.52 |
| 1:C:387:ILE:HG22 | 1:C:387:ILE:O | 2.10 | 0.52 |
| 1:C:389:ILE:CD1 | 1:C:396:ILE:O | 2.58 | 0.52 |
| 1:C:420:ARG:O | 1:C:428:ALA:HB1 | 2.09 | 0.52 |
| 2:E:4:LEU:HD23 | 2:E:5:PRO:N | 2.24 | 0.52 |
| 1:C:258:LEU:HD21 | 2:F:1:ALA:HA | 1.92 | 0.52 |
| 1:C:273:LEU:HB2 | 2:F:12:LEU:HD13 | 1.92 | 0.52 |
| 1:C:466:ILE:HD13 | 1:C:496:ILE:HG22 | 1.92 | 0.52 |
| 1:B:223:LEU:CB | 1:B:224:PRO:CD | 2.78 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:49:ILE:O | 2:E:53:LEU:CD2 | 2.57 | 0.52 |
| 1:C:107:LEU:HD12 | 1:C:108:PHE:H | 1.74 | 0.52 |
| 1:C:203:TYR:CE2 | 1:C:277:MET:HB2 | 2.44 | 0.52 |
| 1:C:391:VAL:O | 1:C:395:LYS:HB3 | 2.09 | 0.52 |
| 2:D:9:THR:CG2 | 2:D:10:ARG:HH21 | 2.23 | 0.52 |
| 1:B:38:LYS:HD3 | 1:B:298:LEU:HD13 | 1.91 | 0.52 |
| 1:B:142:SER:HA | 1:B:163:ASN:O | 2.10 | 0.52 |
| 1:A:171:PRO:HB3 | 1:A:192:PRO:HB2 | 1.92 | 0.52 |
| 1:A:342:PRO:HG2 | 1:A:389:ILE:CG1 | 2.40 | 0.52 |
| 1:C:244:GLU:HG2 | 2:D:20:LEU:HD23 | 1.91 | 0.52 |
| 1:C:346:ALA:HB2 | 1:C:388:VAL:HG23 | 1.91 | 0.52 |
| 2:D:49:ILE:O | 2:D:52:LEU:HB2 | 2.10 | 0.52 |
| 1:B:41:VAL:HG23 | 1:B:143:VAL:HG13 | 1.92 | 0.52 |
| 1:B:60:CYS:H | 1:B:224:PRO:CD | 2.18 | 0.52 |
| 1:A:97:VAL:CG1 | 1:A:113:LEU:HD22 | 2.40 | 0.51 |
| 1:A:141:LEU:O | 1:A:164:ARG:HA | 2.09 | 0.51 |
| 1:A:320:GLU:O | 1:C:108:PHE:HB2 | 2.09 | 0.51 |
| 1:C:93:LYS:HD2 | 1:C:245:PHE:CE1 | 2.45 | 0.51 |
| 1:C:308:CYS:HB3 | 1:C:332:TYR:CE2 | 2.45 | 0.51 |
| 1:C:460:MET:HE1 | 1:C:464:SER:HB2 | 1.92 | 0.51 |
| 1:B:191:GLU:HG3 | 1:B:290:LYS:HE3 | 1.91 | 0.51 |
| 1:A:114:VAL:HG22 | 1:A:115:THR:N | 2.24 | 0.51 |
| 1:A:387:ILE:C | 1:A:388:VAL:HG22 | 2.31 | 0.51 |
| 1:C:45:LEU:HD22 | 1:C:289:LEU:HB3 | 1.92 | 0.51 |
| 1:C:65:ILE:H | 1:C:257:VAL:HG12 | 1.75 | 0.51 |
| 2:D:54:GLY:HA2 | 2:F:59:GLN:OE1 | 2.10 | 0.51 |
| 1:B:43:ILE:HD12 | 1:B:43:ILE:N | 2.26 | 0.51 |
| 1:B:421:MET:O | 1:B:425:GLY:N | 2.43 | 0.51 |
| 2:E:56:SER:HB3 | 2:E:59:GLN:HB3 | 1.88 | 0.51 |
| 1:A:4:ILE:HG22 | 1:A:4:ILE:O | 2.10 | 0.51 |
| 1:A:317:ILE:HG23 | 1:A:317:ILE:O | 2.10 | 0.51 |
| 1:A:348:ASP:HB2 | 1:A:350:GLN:HG3 | 1.92 | 0.51 |
| 1:A:467:LEU:C | 1:A:469:GLY:H | 2.12 | 0.51 |
| 2:D:38:ARG:O | 2:D:40:PRO:HD3 | 2.09 | 0.51 |
| 1:B:283:ARG:CG | 1:B:283:ARG:HH11 | 2.24 | 0.51 |
| 1:C:133:GLU:O | 1:C:134:ASN:CB | 2.52 | 0.51 |
| 1:C:138:ARG:HB3 | 1:C:138:ARG:NH2 | 2.25 | 0.51 |
| 1:C:477:LEU:HD23 | 1:C:489:LEU:HD23 | 1.91 | 0.51 |
| 2:D:19:TRP:C | 2:D:21:GLU:N | 2.64 | 0.51 |
| 1:B:28:GLY:O | 1:B:29:GLY:O | 2.29 | 0.51 |
| 1:B:175:ARG:CZ | 1:B:175:ARG:CB | 2.85 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:175:ARG:O | 1:B:176:ALA:O | 2.29 | 0.51 |
| 1:B:202:TYR:N | 1:B:202:TYR:CD1 | 2.79 | 0.51 |
| 1:B:330:VAL:HG21 | 1:B:389:ILE:HD11 | 1.91 | 0.51 |
| 1:C:340:LYS:NZ | 1:C:340:LYS:CB | 2.73 | 0.51 |
| 1:C:453:PHE:CZ | 1:C:495:LEU:HD22 | 2.46 | 0.51 |
| 1:B:313:THR:O | 1:B:330:VAL:HG13 | 2.11 | 0.51 |
| 1:B:314:PHE:CE2 | 1:B:398:HIS:HB2 | 2.45 | 0.51 |
| 1:B:320:GLU:OE2 | 1:B:324:GLY:HA2 | 2.11 | 0.51 |
| 1:A:412:GLU:OE2 | 1:A:416:ARG:HB2 | 2.11 | 0.51 |
| 1:A:470:THR:C | 1:A:472:LEU:N | 2.64 | 0.51 |
| 1:C:225:TRP:O | 1:C:236:TRP:HA | 2.11 | 0.51 |
| 2:D:72:PRO:C | 2:D:74:TYR:H | 2.14 | 0.51 |
| 1:B:283:ARG:HB3 | 1:B:283:ARG:NH1 | 2.26 | 0.51 |
| 1:A:273:LEU:HB2 | 2:D:12:LEU:HD22 | 1.93 | 0.51 |
| 1:C:201:LEU:HD12 | 1:C:213:VAL:O | 2.09 | 0.51 |
| 1:B:202:TYR:CE1 | 1:B:215:LYS:HG3 | 2.45 | 0.51 |
| 1:B:357:ARG:HB3 | 1:B:379:ASP:HB3 | 1.91 | 0.51 |
| 2:E:19:TRP:CG | 2:E:20:LEU:HG | 2.46 | 0.51 |
| 1:C:66:SER:HB3 | 1:C:118:LYS:HB3 | 1.93 | 0.51 |
| 1:C:400:TRP:CZ3 | 1:C:401:HIS:O | 2.64 | 0.51 |
| 1:C:409:LYS:HA | 1:C:409:LYS:HZ3 | 1.74 | 0.51 |
| 1:C:423:VAL:HG13 | 2:F:13:GLN:HB3 | 1.93 | 0.51 |
| 1:C:439:ASN:O | 1:C:441:LEU:N | 2.44 | 0.51 |
| 2:D:18:THR:OG1 | 2:D:19:TRP:N | 2.44 | 0.51 |
| 1:B:41:VAL:CG2 | 1:B:143:VAL:HG13 | 2.41 | 0.51 |
| 2:F:38:ARG:HB3 | 2:F:38:ARG:HH11 | 1.76 | 0.51 |
| 1:A:256:VAL:HG13 | 1:C:209:LYS:NZ | 2.26 | 0.51 |
| 1:C:467:LEU:CD1 | 2:F:69:LEU:HD21 | 2.39 | 0.51 |
| 1:C:471:LEU:HD23 | 2:F:62:ILE:CD1 | 2.41 | 0.51 |
| 2:D:69:LEU:CD2 | 2:F:70:ILE:HD12 | 2.39 | 0.51 |
| 1:C:60:CYS:O | 1:C:223:LEU:HD13 | 2.11 | 0.51 |
| 1:C:93:LYS:O | 1:C:114:VAL:HG23 | 2.10 | 0.51 |
| 1:C:468:ILE:O | 1:C:472:LEU:HG | 2.11 | 0.51 |
| 1:B:13:GLU:O | 1:B:14:GLY:O | 2.28 | 0.51 |
| 1:B:445:ILE:CG2 | 1:B:446:HIS:H | 2.21 | 0.51 |
| 1:A:65:ILE:HB | 1:A:257:VAL:HG22 | 1.92 | 0.50 |
| 1:A:306:SER:O | 1:A:339:CYS:HB2 | 2.11 | 0.50 |
| 1:C:27:HIS:NE2 | 1:C:48:THR:HG22 | 2.26 | 0.50 |
| 2:D:9:THR:HG22 | 2:D:10:ARG:CG | 2.41 | 0.50 |
| 2:E:42:PHE:O | 2:E:46:ALA:HB2 | 2.11 | 0.50 |
| 1:A:131:GLN:O | 1:A:133:GLU:O | 2.30 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:22:ASP:OD1 | 1:C:433:SER:HA | 2.11 | 0.50 |
| 1:C:203:TYR:HE2 | 1:C:277:MET:HB2 | 1.77 | 0.50 |
| 1:C:320:GLU:HA | 1:C:325:THR:O | 2.11 | 0.50 |
| 1:B:156:THR:O | 1:B:159:GLU:HG2 | 2.11 | 0.50 |
| 1:B:272:ALA:HA | 2:E:18:THR:HA | 1.94 | 0.50 |
| 1:B:483:SER:C | 1:B:485:SER:H | 2.15 | 0.50 |
| 2:E:50:ALA:O | 2:E:60:LYS:HG2 | 2.11 | 0.50 |
| 2:E:65:VAL:HG22 | 2:E:69:LEU:HD11 | 1.92 | 0.50 |
| 1:A:135:LEU:N | 1:A:135:LEU:CD2 | 2.74 | 0.50 |
| 1:A:199:SER:O | 1:A:200:ASP:CB | 2.59 | 0.50 |
| 1:A:232:GLY:O | 1:A:233:THR:C | 2.50 | 0.50 |
| 1:A:453:PHE:HA | 1:A:456:LEU:HD11 | 1.91 | 0.50 |
| 1:C:91:VAL:HG13 | 1:C:91:VAL:O | 2.11 | 0.50 |
| 1:C:133:GLU:HB2 | 1:C:193:ARG:NH1 | 2.23 | 0.50 |
| 1:C:312:PHE:CZ | 1:C:341:VAL:HG11 | 2.46 | 0.50 |
| 1:C:396:ILE:HD12 | 1:C:397:THR:N | 2.26 | 0.50 |
| 1:C:457:PHE:CD1 | 1:C:457:PHE:N | 2.79 | 0.50 |
| 1:B:11:PHE:HD1 | 1:B:11:PHE:H | 1.59 | 0.50 |
| 1:B:169:ILE:HG21 | 1:B:190:CYS:HB2 | 1.94 | 0.50 |
| 1:B:234:PRO:O | 1:B:236:TRP:CD1 | 2.64 | 0.50 |
| 1:B:444:GLY:O | 1:B:447:GLN:CB | 2.58 | 0.50 |
| 1:A:300:LEU:CD1 | 1:A:300:LEU:H | 2.23 | 0.50 |
| 1:A:322:LEU:HG | 1:A:323:HIS:N | 2.22 | 0.50 |
| 1:A:366:THR:C | 1:A:368:SER:N | 2.63 | 0.50 |
| 1:C:84:LYS:O | 1:C:87:ASP:N | 2.44 | 0.50 |
| 1:C:236:TRP:O | 1:C:239:LYS:HG3 | 2.12 | 0.50 |
| 1:B:38:LYS:C | 1:B:39:PRO:O | 2.48 | 0.50 |
| 1:A:62:GLU:OE2 | 1:A:260:SER:HB2 | 2.12 | 0.50 |
| 1:C:265:VAL:O | 1:C:266:HIS:C | 2.49 | 0.50 |
| 1:C:273:LEU:CD2 | 1:C:286:SER:HB2 | 2.36 | 0.50 |
| 1:B:21:VAL:HG13 | 1:B:293:LEU:CA | 2.41 | 0.50 |
| 1:B:61:TYR:O | 1:B:61:TYR:CD1 | 2.65 | 0.50 |
| 2:E:49:ILE:O | 2:E:53:LEU:HD22 | 2.11 | 0.50 |
| 2:F:61:VAL:O | 2:F:63:TYR:N | 2.44 | 0.50 |
| 1:A:423:VAL:HG22 | 1:A:424:LEU:H | 1.77 | 0.50 |
| 1:A:425:GLY:O | 1:A:426:ASP:HB3 | 2.11 | 0.50 |
| 1:C:90:TYR:HA | 1:C:117:ALA:O | 2.11 | 0.50 |
| 1:B:31:VAL:O | 1:B:31:VAL:HG13 | 2.11 | 0.50 |
| 1:B:323:HIS:HD2 | 1:B:416:ARG:HH12 | 1.58 | 0.50 |
| 1:A:47:THR:OG1 | 1:A:138:ARG:HB2 | 2.11 | 0.50 |
| 1:A:191:GLU:HG3 | 1:A:290:LYS:CB | 2.41 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:271:GLY:O | 2:D:11:LYS:HA | 2.12 | 0.50 |
| 1:C:375:MET:N | 1:C:375:MET:CE | 2.74 | 0.50 |
| 1:B:474:TRP:C | 1:B:476:GLY:N | 2.65 | 0.50 |
| 1:B:487:MET:HA | 1:B:490:ALA:CB | 2.42 | 0.50 |
| 1:A:423:VAL:O | 1:A:425:GLY:N | 2.42 | 0.50 |
| 1:C:213:VAL:HG11 | 1:C:217:TRP:CZ3 | 2.46 | 0.50 |
| 1:C:434:VAL:HG13 | 1:C:434:VAL:O | 2.11 | 0.50 |
| 1:B:57:ARG:HA | 1:B:227:ALA:HB1 | 1.88 | 0.50 |
| 1:B:415:VAL:CG1 | 1:B:419:LYS:HE3 | 2.42 | 0.50 |
| 1:A:65:ILE:HG22 | 1:A:66:SER:N | 2.27 | 0.50 |
| 1:A:101:TRP:HZ2 | 1:C:316:LYS:CB | 2.24 | 0.50 |
| 1:A:418:ALA:O | 1:A:421:MET:HB2 | 2.12 | 0.50 |
| 1:C:201:LEU:HD12 | 1:C:214:HIS:HA | 1.93 | 0.50 |
| 1:C:382:PHE:CD1 | 1:C:382:PHE:C | 2.86 | 0.50 |
| 2:D:18:THR:HG23 | 2:D:21:GLU:CB | 2.28 | 0.50 |
| 1:B:7:SER:CA | 1:B:322:LEU:HD13 | 2.42 | 0.50 |
| 1:B:91:VAL:O | 1:B:91:VAL:CG1 | 2.59 | 0.50 |
| 1:B:113:LEU:HD13 | 1:B:113:LEU:O | 2.12 | 0.50 |
| 2:E:50:ALA:CB | 2:E:64:LEU:HA | 2.42 | 0.50 |
| 2:F:19:TRP:CD1 | 2:F:20:LEU:N | 2.80 | 0.50 |
| 2:F:54:GLY:HA2 | 2:F:63:TYR:CD2 | 2.47 | 0.50 |
| 1:A:74:CYS:HA | 1:A:99:ARG:HD3 | 1.92 | 0.49 |
| 1:A:214:HIS:ND1 | 2:D:10:ARG:HG3 | 2.26 | 0.49 |
| 1:A:263:GLY:HA3 | 1:C:260:SER:O | 2.12 | 0.49 |
| 1:A:265:VAL:C | 1:A:267:THR:N | 2.64 | 0.49 |
| 1:C:424:LEU:HB2 | 1:C:428:ALA:HB2 | 1.94 | 0.49 |
| 1:B:312:PHE:CZ | 1:B:341:VAL:HG12 | 2.46 | 0.49 |
| 2:F:73:ALA:O | 2:F:75:SER:N | 2.43 | 0.49 |
| 1:A:99:ARG:HB2 | 1:A:99:ARG:NH2 | 2.27 | 0.49 |
| 1:A:172:ASN:C | 1:A:172:ASN:OD1 | 2.51 | 0.49 |
| 1:A:221:ILE:HG22 | 1:A:223:LEU:HB2 | 1.94 | 0.49 |
| 1:A:463:PHE:HD1 | 1:A:466:ILE:HD11 | 1.77 | 0.49 |
| 1:C:131:GLN:O | 1:C:132:PRO:C | 2.50 | 0.49 |
| 1:C:133:GLU:HG2 | 1:C:134:ASN:N | 2.26 | 0.49 |
| 1:C:345:MET:CE | 1:C:378:LEU:HB3 | 2.42 | 0.49 |
| 1:B:139:ILE:CD1 | 1:B:167:VAL:HG23 | 2.41 | 0.49 |
| 1:B:222:PRO:C | 1:B:223:LEU:CD1 | 2.80 | 0.49 |
| 1:B:429:TRP:CE3 | 1:B:442:GLY:HA3 | 2.47 | 0.49 |
| 1:A:1:ILE:HG23 | 1:A:152:ILE:CG2 | 2.41 | 0.49 |
| 1:A:119:PHE:O | 1:A:120:ALA:HB2 | 2.11 | 0.49 |
| 1:A:496:ILE:O | 1:A:499:SER:HB2 | 2.12 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:247:ASP:OD2 | 1:C:250:ALA:O | 2.29 | 0.49 |
| 1:C:295:MET:HE3 | 1:C:298:LEU:HB3 | 1.91 | 0.49 |
| 1:B:20:TRP:HE3 | 1:B:292:ARG:NH2 | 2.08 | 0.49 |
| 1:B:81:TYR:O | 1:B:82:LEU:HB3 | 2.13 | 0.49 |
| 2:F:58:SER:O | 2:F:61:VAL:HG23 | 2.12 | 0.49 |
| 1:A:99:ARG:HB2 | 1:A:99:ARG:HH21 | 1.76 | 0.49 |
| 1:A:236:TRP:HB2 | 1:A:239:LYS:HG2 | 1.94 | 0.49 |
| 1:A:276:GLU:OE1 | 1:A:283:ARG:HG2 | 2.13 | 0.49 |
| 1:A:296:ASP:O | 1:A:298:LEU:N | 2.45 | 0.49 |
| 1:A:345:MET:CE | 1:A:378:LEU:HD21 | 2.42 | 0.49 |
| 1:C:34:MET:HB3 | 1:C:40:THR:HB | 1.93 | 0.49 |
| 1:C:191:GLU:HG3 | 1:C:191:GLU:O | 2.13 | 0.49 |
| 2:D:3:THR:HB | 2:F:31:ARG:NH1 | 2.27 | 0.49 |
| 2:D:21:GLU:O | 2:D:22:SER:C | 2.51 | 0.49 |
| 1:B:7:SER:N | 1:B:322:LEU:HD11 | 2.26 | 0.49 |
| 1:B:20:TRP:HE3 | 1:B:292:ARG:HE | 1.58 | 0.49 |
| 1:B:74:CYS:C | 1:B:76:THR:N | 2.66 | 0.49 |
| 1:B:157:GLY:HA3 | 3:B:601:NAG:O6 | 2.12 | 0.49 |
| 1:B:225:TRP:O | 1:B:236:TRP:CE3 | 2.65 | 0.49 |
| 1:B:272:ALA:CB | 2:E:18:THR:CG2 | 2.82 | 0.49 |
| 1:A:262:GLU:HG2 | 1:C:259:GLY:HA3 | 1.94 | 0.49 |
| 1:A:392:GLY:O | 1:A:395:LYS:HB3 | 2.11 | 0.49 |
| 1:A:443:LYS:HB3 | 1:A:443:LYS:HZ2 | 1.73 | 0.49 |
| 1:A:456:LEU:HD13 | 1:A:457:PHE:HD2 | 1.77 | 0.49 |
| 1:C:36:GLN:C | 1:C:38:LYS:H | 2.15 | 0.49 |
| 1:C:214:HIS:HB2 | 2:F:7:HIS:NE2 | 2.26 | 0.49 |
| 1:C:430:ASP:OD1 | 1:C:443:LYS:HD2 | 2.13 | 0.49 |
| 1:B:148:HIS:HB2 | 1:B:373:LYS:HG3 | 1.94 | 0.49 |
| 1:B:444:GLY:O | 1:B:447:GLN:HB3 | 2.11 | 0.49 |
| 2:E:59:GLN:C | 2:E:61:VAL:N | 2.64 | 0.49 |
| 1:A:43:ILE:CG2 | 1:A:141:LEU:CD2 | 2.89 | 0.49 |
| 1:A:332:TYR:OH | 1:A:389:ILE:CD1 | 2.60 | 0.49 |
| 1:C:61:TYR:CE1 | 1:C:123:LYS:HE2 | 2.45 | 0.49 |
| 1:C:138:ARG:HH21 | 1:C:138:ARG:HG3 | 1.78 | 0.49 |
| 1:C:298:LEU:HD13 | 1:C:298:LEU:O | 2.13 | 0.49 |
| 2:D:63:TYR:O | 2:D:66:MET:HB2 | 2.13 | 0.49 |
| 1:B:203:TYR:OH | 1:B:275:ALA:HB1 | 2.13 | 0.49 |
| 2:E:38:ARG:C | 2:E:40:PRO:HD3 | 2.33 | 0.49 |
| 1:C:182:GLY:O | 1:C:299:ARG:NH1 | 2.45 | 0.49 |
| 1:B:65:ILE:HG13 | 1:B:257:VAL:HB | 1.93 | 0.49 |
| 2:F:48:ALA:HA | 2:F:51:TRP:CB | 2.42 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:246:LYS:CE | 2:F:17:GLN:HB3 | 2.42 | 0.49 |
| 1:A:358:LEU:O | 1:A:377:GLU:HB3 | 2.13 | 0.49 |
| 1:C:39:PRO:HG3 | 1:C:300:LEU:HA | 1.94 | 0.49 |
| 1:C:42:ASP:O | 1:C:141:LEU:HA | 2.13 | 0.49 |
| 1:C:325:THR:HB | 1:C:377:GLU:HG3 | 1.94 | 0.49 |
| 1:B:1:ILE:HG12 | 1:B:147:GLN:HG3 | 1.94 | 0.49 |
| 1:B:175:ARG:HB2 | 1:B:175:ARG:NH1 | 2.27 | 0.49 |
| 2:E:51:TRP:CD1 | 2:E:60:LYS:NZ | 2.72 | 0.49 |
| 1:A:49:THR:HB | 1:A:283:ARG:HH22 | 1.78 | 0.49 |
| 1:A:225:TRP:HD1 | 1:A:226:HIS:N | 2.10 | 0.49 |
| 1:A:385:SER:O | 1:A:400:TRP:N | 2.43 | 0.49 |
| 1:C:97:VAL:CG2 | 1:C:113:LEU:HD23 | 2.42 | 0.49 |
| 1:C:263:GLY:O | 1:C:265:VAL:N | 2.46 | 0.49 |
| 1:C:288:HIS:CE1 | 1:C:424:LEU:HD22 | 2.48 | 0.49 |
| 1:C:460:MET:C | 2:D:75:SER:O | 2.51 | 0.49 |
| 1:B:143:VAL:HG23 | 1:B:163:ASN:O | 2.13 | 0.49 |
| 1:A:133:GLU:O | 1:A:134:ASN:HB2 | 2.13 | 0.49 |
| 1:A:272:ALA:HB2 | 2:D:7:HIS:ND1 | 2.26 | 0.49 |
| 1:C:70:SER:HA | 1:C:82:LEU:CD1 | 2.42 | 0.49 |
| 1:C:207:ASN:O | 1:C:208:ASN:CB | 2.60 | 0.49 |
| 1:C:306:SER:O | 1:C:308:CYS:N | 2.46 | 0.49 |
| 1:C:475:LEU:HB3 | 1:C:488:CYS:SG | 2.53 | 0.49 |
| 1:B:152:ILE:HG22 | 1:B:153:VAL:H | 1.76 | 0.49 |
| 1:B:225:TRP:H | 1:B:236:TRP:HE3 | 1.60 | 0.49 |
| 1:B:261:GLN:OE1 | 1:B:264:ALA:HB3 | 2.13 | 0.49 |
| 1:B:263:GLY:O | 1:B:266:HIS:HB2 | 2.13 | 0.49 |
| 1:B:300:LEU:HB3 | 1:B:362:ASN:ND2 | 2.28 | 0.49 |
| 2:E:58:SER:HA | 2:E:61:VAL:HG21 | 1.94 | 0.49 |
| 2:F:4:LEU:N | 2:F:5:PRO:CD | 2.75 | 0.49 |
| 1:A:15:MET:SD | 1:A:295:MET:HG3 | 2.53 | 0.48 |
| 1:A:233:THR:O | 1:A:235:HIS:N | 2.46 | 0.48 |
| 1:A:244:GLU:OE2 | 1:A:244:GLU:HA | 2.12 | 0.48 |
| 1:A:314:PHE:HE2 | 1:A:318:PRO:CD | 2.21 | 0.48 |
| 1:A:454:LYS:HB2 | 1:A:454:LYS:HZ2 | 1.77 | 0.48 |
| 2:D:54:GLY:O | 2:D:55:SER:HB2 | 2.11 | 0.48 |
| 1:B:25:LEU:HD13 | 1:B:139:ILE:CG2 | 2.27 | 0.48 |
| 1:B:97:VAL:HG13 | 1:B:251:LYS:CA | 2.38 | 0.48 |
| 1:B:457:PHE:CE2 | 1:B:495:LEU:HD11 | 2.48 | 0.48 |
| 1:A:7:SER:O | 1:A:8:ASN:CB | 2.61 | 0.48 |
| 1:A:399:HIS:ND1 | 1:A:400:TRP:N | 2.61 | 0.48 |
| 1:C:384:ASP:O | 1:C:385:SER:CB | 2.56 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:5:GLY:HA2 | 1:B:322:LEU:CD1 | 2.43 | 0.48 |
| 1:B:30:CYS:SG | 1:B:43:ILE:O | 2.71 | 0.48 |
| 1:B:357:ARG:HD3 | 1:B:359:ILE:CD1 | 2.43 | 0.48 |
| 2:E:65:VAL:HG22 | 2:E:69:LEU:CG | 2.43 | 0.48 |
| 2:F:54:GLY:HA2 | 2:F:63:TYR:CE2 | 2.47 | 0.48 |
| 1:A:61:TYR:HE2 | 1:A:262:GLU:HB2 | 1.77 | 0.48 |
| 1:A:255:VAL:HG12 | 1:A:256:VAL:N | 2.29 | 0.48 |
| 1:A:261:GLN:O | 1:A:264:ALA:HB3 | 2.13 | 0.48 |
| 1:A:290:LYS:HB3 | 1:A:290:LYS:HZ2 | 1.78 | 0.48 |
| 1:A:409:LYS:HB3 | 1:A:409:LYS:HZ3 | 1.77 | 0.48 |
| 1:C:31:VAL:HG12 | 1:C:32:THR:N | 2.26 | 0.48 |
| 1:C:149:SER:OG | 1:C:373:LYS:NZ | 2.39 | 0.48 |
| 1:C:312:PHE:HB3 | 1:C:330:VAL:CG1 | 2.43 | 0.48 |
| 1:C:418:ALA:O | 1:C:422:ALA:HB3 | 2.13 | 0.48 |
| 1:C:420:ARG:HG2 | 1:C:431:PHE:CE2 | 2.48 | 0.48 |
| 1:B:59:TYR:CE2 | 1:B:221:ILE:O | 2.66 | 0.48 |
| 1:B:97:VAL:O | 1:B:99:ARG:N | 2.46 | 0.48 |
| 1:B:338:PRO:CG | 1:B:367:GLU:HG2 | 2.43 | 0.48 |
| 2:E:31:ARG:CZ | 2:E:31:ARG:HB2 | 2.43 | 0.48 |
| 2:F:67:ILE:C | 2:F:69:LEU:N | 2.67 | 0.48 |
| 1:A:47:THR:OG1 | 1:A:138:ARG:CD | 2.54 | 0.48 |
| 1:A:228:GLY:CA | 1:B:73:ARG:HH12 | 2.26 | 0.48 |
| 1:C:24:VAL:HG22 | 1:C:290:LYS:HG3 | 1.96 | 0.48 |
| 1:C:25:LEU:HD12 | 1:C:25:LEU:H | 1.78 | 0.48 |
| 1:B:32:THR:OG1 | 1:B:42:ASP:HB3 | 2.14 | 0.48 |
| 1:B:97:VAL:CG1 | 1:B:251:LYS:HA | 2.37 | 0.48 |
| 1:B:409:LYS:HZ3 | 1:B:413:ALA:HB2 | 1.78 | 0.48 |
| 1:A:12:VAL:C | 1:A:14:GLY:N | 2.67 | 0.48 |
| 1:A:54:ALA:HB3 | 1:B:76:THR:O | 2.14 | 0.48 |
| 1:A:72:SER:C | 1:A:73:ARG:HG2 | 2.34 | 0.48 |
| 1:A:232:GLY:O | 1:A:234:PRO:N | 2.45 | 0.48 |
| 1:A:265:VAL:O | 1:A:267:THR:N | 2.47 | 0.48 |
| 1:A:429:TRP:HB2 | 1:A:443:LYS:HE2 | 1.95 | 0.48 |
| 1:C:55:GLU:CA | 1:C:128:LYS:HA | 2.31 | 0.48 |
| 1:C:180:LEU:HD22 | 1:C:180:LEU:N | 2.28 | 0.48 |
| 1:C:214:HIS:HD2 | 1:C:216:GLU:HB2 | 1.78 | 0.48 |
| 1:C:399:HIS:ND1 | 1:C:400:TRP:N | 2.61 | 0.48 |
| 1:C:471:LEU:HD13 | 1:C:471:LEU:O | 2.14 | 0.48 |
| 2:D:33:GLU:C | 2:D:35:TRP:N | 2.65 | 0.48 |
| 1:B:61:TYR:CE1 | 1:B:262:GLU:HG2 | 2.48 | 0.48 |
| 1:B:302:GLY:C | 1:B:304:SER:H | 2.15 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:35:ALA:O | 1:A:37:ASP:N | 2.46 | 0.48 |
| 1:A:38:LYS:HG3 | 1:A:298:LEU:HB2 | 1.94 | 0.48 |
| 1:A:73:ARG:NH2 | 1:A:77:GLN:CB | 2.56 | 0.48 |
| 1:A:101:TRP:N | 1:A:106:GLY:HA2 | 2.27 | 0.48 |
| 1:A:215:LYS:O | 1:A:216:GLU:C | 2.51 | 0.48 |
| 1:C:39:PRO:CD | 1:C:298:LEU:HD11 | 2.33 | 0.48 |
| 1:C:61:TYR:CE1 | 1:C:123:LYS:HB2 | 2.49 | 0.48 |
| 1:C:343:ALA:HA | 1:C:388:VAL:O | 2.13 | 0.48 |
| 1:C:357:ARG:CG | 1:C:358:LEU:H | 2.26 | 0.48 |
| 1:B:90:TYR:CD1 | 1:B:90:TYR:N | 2.82 | 0.48 |
| 1:B:148:HIS:C | 1:B:150:GLY:H | 2.16 | 0.48 |
| 1:B:196:LEU:HB2 | 1:B:198:PHE:CZ | 2.48 | 0.48 |
| 1:B:244:GLU:O | 1:B:255:VAL:HA | 2.13 | 0.48 |
| 1:B:255:VAL:HG23 | 1:B:255:VAL:O | 2.14 | 0.48 |
| 1:B:272:ALA:HB3 | 2:E:12:LEU:HD13 | 1.94 | 0.48 |
| 1:A:12:VAL:HG23 | 1:A:33:VAL:HG22 | 1.96 | 0.48 |
| 1:A:58:SER:HA | 1:A:126:THR:HA | 1.95 | 0.48 |
| 1:A:215:LYS:HB2 | 1:A:215:LYS:HZ2 | 1.78 | 0.48 |
| 1:A:235:HIS:CD2 | 1:B:86:SER:HA | 2.47 | 0.48 |
| 1:C:55:GLU:HA | 1:C:128:LYS:CA | 2.31 | 0.48 |
| 2:D:60:LYS:H | 2:D:60:LYS:CD | 2.24 | 0.48 |
| 1:B:382:PHE:CB | 1:B:404:GLY:O | 2.57 | 0.48 |
| 2:E:50:ALA:HB2 | 2:E:64:LEU:HA | 1.96 | 0.48 |
| 1:A:60:CYS:O | 1:A:223:LEU:HG | 2.13 | 0.48 |
| 1:A:97:VAL:HG23 | 1:A:98:ASP:N | 2.28 | 0.48 |
| 1:A:312:PHE:CZ | 1:A:388:VAL:O | 2.67 | 0.48 |
| 1:C:61:TYR:HB2 | 1:C:261:GLN:HB2 | 1.96 | 0.48 |
| 1:C:139:ILE:HB | 1:C:167:VAL:HG12 | 1.93 | 0.48 |
| 1:C:154:ASN:HA | 3:C:601:NAG:H82 | 1.94 | 0.48 |
| 1:C:223:LEU:HB3 | 1:C:224:PRO:CD | 2.43 | 0.48 |
| 1:C:302:GLY:HA2 | 1:C:305:TYR:CD2 | 2.49 | 0.48 |
| 1:C:305:TYR:CZ | 1:C:338:PRO:HB2 | 2.49 | 0.48 |
| 1:B:240:GLU:C | 1:B:242:LEU:H | 2.17 | 0.48 |
| 1:B:247:ASP:HB3 | 1:B:253:GLN:HG3 | 1.94 | 0.48 |
| 1:B:336:ASP:O | 1:B:368:SER:O | 2.31 | 0.48 |
| 1:B:465:GLN:HG3 | 1:B:499:SER:HB3 | 1.95 | 0.48 |
| 1:A:113:LEU:HD23 | 1:A:113:LEU:C | 2.34 | 0.48 |
| 1:A:423:VAL:HG22 | 1:A:424:LEU:N | 2.29 | 0.48 |
| 1:A:425:GLY:O | 1:A:426:ASP:CB | 2.62 | 0.48 |
| 1:A:462:TRP:NE1 | 1:A:499:SER:HB3 | 2.29 | 0.48 |
| 1:C:434:VAL:HG23 | 1:C:439:ASN:OD1 | 2.14 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:191:GLU:C | 1:B:193:ARG:H | 2.14 | 0.48 |
| 2:F:46:ALA:HA | 2:F:49:ILE:HB | 1.96 | 0.48 |
| 1:A:87:ASP:C | 1:A:89:GLN:H | 2.17 | 0.48 |
| 1:A:96:LEU:HA | 1:A:112:SER:HA | 1.96 | 0.48 |
| 1:A:240:GLU:HA | 1:A:243:VAL:CG2 | 2.38 | 0.48 |
| 1:C:213:VAL:CG1 | 1:C:214:HIS:N | 2.76 | 0.48 |
| 1:C:273:LEU:H | 2:F:12:LEU:CD2 | 2.22 | 0.48 |
| 2:D:11:LYS:O | 2:D:13:GLN:N | 2.46 | 0.48 |
| 1:B:302:GLY:HA2 | 1:B:364:VAL:HG11 | 1.94 | 0.48 |
| 2:F:24:GLU:O | 2:F:27:LYS:HG2 | 2.14 | 0.48 |
| 1:A:99:ARG:NH2 | 1:A:99:ARG:CB | 2.76 | 0.47 |
| 1:C:40:THR:HG23 | 1:C:144:HIS:HB2 | 1.96 | 0.47 |
| 1:C:441:LEU:O | 1:C:443:LYS:N | 2.47 | 0.47 |
| 1:C:465:GLN:OE1 | 1:C:499:SER:HB3 | 2.14 | 0.47 |
| 1:B:114:VAL:O | 1:B:114:VAL:HG13 | 2.14 | 0.47 |
| 1:B:226:HIS:O | 1:B:227:ALA:HB2 | 2.14 | 0.47 |
| 1:B:300:LEU:HD12 | 1:B:300:LEU:N | 2.29 | 0.47 |
| 1:B:313:THR:H | 1:B:330:VAL:CG1 | 2.25 | 0.47 |
| 2:E:21:GLU:O | 2:E:24:GLU:HB3 | 2.13 | 0.47 |
| 2:E:72:PRO:HG2 | 2:E:73:ALA:H | 1.79 | 0.47 |
| 1:A:10:ASP:HB2 | 1:A:431:PHE:HZ | 1.78 | 0.47 |
| 1:A:17:GLY:C | 1:A:19:THR:H | 2.17 | 0.47 |
| 1:C:31:VAL:HG12 | 1:C:32:THR:O | 2.14 | 0.47 |
| 2:D:9:THR:CG2 | 2:D:10:ARG:NH2 | 2.77 | 0.47 |
| 1:B:479:THR:HG23 | 1:B:481:ASN:O | 2.14 | 0.47 |
| 2:F:44:LEU:O | 2:F:47:ALA:HB3 | 2.14 | 0.47 |
| 2:F:56:SER:OG | 2:F:57:THR:N | 2.44 | 0.47 |
| 1:A:43:ILE:HA | 1:A:140:MET:O | 2.14 | 0.47 |
| 1:A:50:VAL:CG1 | 1:A:130:ILE:HD12 | 2.10 | 0.47 |
| 1:A:171:PRO:HB2 | 1:A:193:ARG:HH12 | 1.79 | 0.47 |
| 1:A:311:ALA:CB | 1:A:334:GLY:N | 2.77 | 0.47 |
| 1:A:434:VAL:O | 1:A:434:VAL:HG23 | 2.14 | 0.47 |
| 1:C:277:MET:HG3 | 1:C:282:GLY:HA2 | 1.96 | 0.47 |
| 1:C:471:LEU:CD2 | 2:F:62:ILE:HG12 | 2.43 | 0.47 |
| 1:C:497:PHE:HA | 1:C:500:THR:OG1 | 2.14 | 0.47 |
| 1:B:73:ARG:HB3 | 1:B:77:GLN:CG | 2.44 | 0.47 |
| 1:B:338:PRO:HG3 | 1:B:367:GLU:CB | 2.44 | 0.47 |
| 1:B:345:MET:HA | 1:B:386:TYR:O | 2.15 | 0.47 |
| 1:B:456:LEU:HD12 | 1:B:457:PHE:HE1 | 1.78 | 0.47 |
| 2:F:3:THR:HG22 | 2:F:5:PRO:HG2 | 1.95 | 0.47 |
| 1:A:196:LEU:HG | 1:A:287:GLY:HA2 | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:476:GLY:CA | 1:A:489:LEU:HG | 2.41 | 0.47 |
| 1:C:202:TYR:CZ | 1:C:215:LYS:HG3 | 2.48 | 0.47 |
| 2:D:10:ARG:HG2 | 2:D:10:ARG:NH2 | 2.22 | 0.47 |
| 1:B:36:GLN:OE1 | 1:B:36:GLN:CA | 2.62 | 0.47 |
| 1:B:61:TYR:O | 1:B:62:GLU:HB2 | 2.13 | 0.47 |
| 1:B:65:ILE:HD12 | 1:B:65:ILE:C | 2.34 | 0.47 |
| 1:B:377:GLU:C | 1:B:378:LEU:HD12 | 2.35 | 0.47 |
| 1:B:419:LYS:C | 1:B:421:MET:H | 2.18 | 0.47 |
| 1:A:65:ILE:HD13 | 1:A:255:VAL:HG11 | 1.96 | 0.47 |
| 1:A:416:ARG:C | 1:A:418:ALA:N | 2.64 | 0.47 |
| 1:C:97:VAL:HG23 | 1:C:113:LEU:HB3 | 1.96 | 0.47 |
| 1:C:205:THR:HG23 | 1:C:210:HIS:ND1 | 2.30 | 0.47 |
| 2:D:62:ILE:O | 2:D:66:MET:HG2 | 2.14 | 0.47 |
| 1:B:73:ARG:HB3 | 1:B:77:GLN:HG2 | 1.95 | 0.47 |
| 1:B:137:TYR:HE2 | 1:B:289:LEU:HB2 | 1.79 | 0.47 |
| 1:A:34:MET:HB3 | 1:A:40:THR:OG1 | 2.14 | 0.47 |
| 1:A:37:ASP:O | 1:A:300:LEU:HD21 | 2.15 | 0.47 |
| 1:C:125:MET:SD | 1:C:206:MET:CE | 3.02 | 0.47 |
| 1:C:209:LYS:O | 1:C:211:TRP:CZ3 | 2.68 | 0.47 |
| 1:C:209:LYS:HB2 | 1:C:211:TRP:HZ3 | 1.79 | 0.47 |
| 1:B:61:TYR:CZ | 1:B:123:LYS:CB | 2.97 | 0.47 |
| 2:E:65:VAL:HG13 | 2:E:66:MET:N | 2.29 | 0.47 |
| 2:F:20:LEU:C | 2:F:20:LEU:HD12 | 2.35 | 0.47 |
| 1:A:151:MET:O | 1:A:151:MET:CG | 2.61 | 0.47 |
| 1:A:152:ILE:CG1 | 1:A:153:VAL:N | 2.58 | 0.47 |
| 1:A:204:LEU:HD21 | 1:A:213:VAL:HG13 | 1.97 | 0.47 |
| 1:A:312:PHE:CD2 | 1:A:396:ILE:HB | 2.32 | 0.47 |
| 1:A:423:VAL:C | 1:A:425:GLY:N | 2.66 | 0.47 |
| 1:C:13:GLU:CG | 1:C:34:MET:HG3 | 2.33 | 0.47 |
| 1:C:119:PHE:C | 1:C:119:PHE:CD1 | 2.88 | 0.47 |
| 1:C:148:HIS:C | 1:C:375:MET:HE2 | 2.35 | 0.47 |
| 1:C:171:PRO:CA | 1:C:192:PRO:HB2 | 2.43 | 0.47 |
| 1:C:277:MET:HG3 | 1:C:282:GLY:CA | 2.44 | 0.47 |
| 1:C:300:LEU:CD2 | 1:C:301:LYS:N | 2.69 | 0.47 |
| 1:C:399:HIS:CD2 | 1:B:191:GLU:HA | 2.50 | 0.47 |
| 2:D:13:GLN:O | 2:D:14:THR:HG23 | 2.15 | 0.47 |
| 2:D:18:THR:O | 2:D:21:GLU:HB3 | 2.13 | 0.47 |
| 1:B:20:TRP:CZ3 | 1:B:292:ARG:NH2 | 2.83 | 0.47 |
| 1:B:172:ASN:C | 1:B:174:PRO:HD3 | 2.34 | 0.47 |
| 1:B:175:ARG:CA | 1:B:188:LEU:O | 2.52 | 0.47 |
| 1:B:370:GLU:HG3 | 1:B:371:ASN:N | 2.30 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:21:GLU:O | 2:F:22:SER:C | 2.52 | 0.47 |
| 2:F:27:LYS:O | 2:F:28:HIS:C | 2.53 | 0.47 |
| 1:A:31:VAL:O | 1:A:43:ILE:CD1 | 2.63 | 0.47 |
| 1:C:75:PRO:O | 1:C:77:GLN:N | 2.48 | 0.47 |
| 1:C:429:TRP:CD1 | 1:C:442:GLY:HA3 | 2.49 | 0.47 |
| 1:C:468:ILE:HD13 | 2:D:42:PHE:CZ | 2.50 | 0.47 |
| 1:B:21:VAL:O | 1:B:292:ARG:HA | 2.14 | 0.47 |
| 1:B:99:ARG:NH2 | 1:B:103:ASN:ND2 | 2.63 | 0.47 |
| 1:A:399:HIS:ND1 | 1:A:399:HIS:C | 2.68 | 0.47 |
| 1:C:209:LYS:CB | 1:C:211:TRP:HZ3 | 2.28 | 0.47 |
| 1:C:247:ASP:CG | 1:C:252:ARG:O | 2.53 | 0.47 |
| 1:C:326:VAL:CG2 | 1:C:380:PRO:HG2 | 2.41 | 0.47 |
| 1:C:389:ILE:CD1 | 1:C:396:ILE:HG23 | 2.33 | 0.47 |
| 1:C:420:ARG:HG2 | 1:C:431:PHE:HE2 | 1.80 | 0.47 |
| 1:C:436:GLY:O | 1:C:439:ASN:OD1 | 2.32 | 0.47 |
| 1:C:473:MET:O | 1:C:477:LEU:HG | 2.15 | 0.47 |
| 1:B:38:LYS:O | 1:B:39:PRO:O | 2.33 | 0.47 |
| 1:B:281:LYS:HB3 | 1:B:281:LYS:HZ3 | 1.77 | 0.47 |
| 1:B:457:PHE:HA | 1:B:460:MET:HE1 | 1.96 | 0.47 |
| 1:B:491:LEU:HD12 | 1:B:494:VAL:CG2 | 2.44 | 0.47 |
| 1:A:93:LYS:HB3 | 1:A:245:PHE:CD2 | 2.50 | 0.47 |
| 1:A:264:ALA:HB1 | 2:D:4:LEU:HD12 | 1.97 | 0.47 |
| 1:A:305:TYR:HB2 | 1:A:340:LYS:CG | 2.33 | 0.47 |
| 1:A:313:THR:CG2 | 1:A:331:GLN:O | 2.63 | 0.47 |
| 1:C:331:GLN:OE1 | 1:C:371:ASN:CB | 2.50 | 0.47 |
| 1:C:349:MET:CE | 1:C:352:LEU:HD22 | 2.45 | 0.47 |
| 1:B:222:PRO:O | 1:B:223:LEU:CG | 2.60 | 0.47 |
| 1:B:309:THR:O | 1:B:310:ALA:CB | 2.62 | 0.47 |
| 1:B:310:ALA:HB3 | 1:B:332:TYR:CE1 | 2.50 | 0.47 |
| 1:A:203:TYR:CE2 | 1:A:277:MET:HE1 | 2.46 | 0.46 |
| 1:A:366:THR:C | 1:A:368:SER:H | 2.18 | 0.46 |
| 1:A:454:LYS:HG2 | 1:A:455:SER:N | 2.30 | 0.46 |
| 1:C:1:ILE:HG21 | 1:C:4:ILE:CG2 | 2.44 | 0.46 |
| 1:C:307:LEU:HD23 | 1:C:342:PRO:HG3 | 1.96 | 0.46 |
| 1:C:347:VAL:O | 1:C:348:ASP:CB | 2.61 | 0.46 |
| 2:D:33:GLU:C | 2:D:35:TRP:H | 2.18 | 0.46 |
| 1:B:41:VAL:HG13 | 1:B:142:SER:O | 2.15 | 0.46 |
| 1:B:147:GLN:O | 1:B:375:MET:HB3 | 2.16 | 0.46 |
| 1:B:148:HIS:CG | 1:B:148:HIS:O | 2.68 | 0.46 |
| 1:B:357:ARG:HH11 | 1:B:357:ARG:CB | 2.22 | 0.46 |
| 1:B:479:THR:CG2 | 1:B:485:SER:OG | 2.64 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:234:PRO:O | 1:A:236:TRP:N | 2.48 | 0.46 |
| 1:C:312:PHE:CD2 | 1:C:331:GLN:O | 2.68 | 0.46 |
| 1:C:340:LYS:HB3 | 1:C:340:LYS:HZ3 | 1.80 | 0.46 |
| 1:C:347:VAL:O | 1:C:347:VAL:HG22 | 2.15 | 0.46 |
| 1:C:437:ALA:C | 1:C:439:ASN:N | 2.69 | 0.46 |
| 2:F:48:ALA:C | 2:F:50:ALA:N | 2.68 | 0.46 |
| 1:A:89:GLN:CA | 1:A:239:LYS:HZ3 | 2.29 | 0.46 |
| 1:A:427:THR:HG22 | 1:A:427:THR:O | 2.15 | 0.46 |
| 1:C:20:TRP:HB2 | 1:C:292:ARG:HD2 | 1.97 | 0.46 |
| 1:C:292:ARG:HG3 | 1:C:292:ARG:NH1 | 2.30 | 0.46 |
| 1:C:300:LEU:HD23 | 1:C:301:LYS:O | 2.16 | 0.46 |
| 1:C:311:ALA:HB2 | 1:C:394:LYS:HE2 | 1.98 | 0.46 |
| 1:C:460:MET:HE1 | 1:C:468:ILE:HD12 | 1.96 | 0.46 |
| 1:B:61:TYR:CZ | 1:B:123:LYS:HB2 | 2.50 | 0.46 |
| 1:B:225:TRP:CD2 | 1:B:226:HIS:N | 2.84 | 0.46 |
| 1:B:360:THR:HG23 | 1:B:376:LEU:HD22 | 1.96 | 0.46 |
| 1:B:426:ASP:O | 1:B:428:ALA:N | 2.48 | 0.46 |
| 2:F:61:VAL:C | 2:F:63:TYR:N | 2.67 | 0.46 |
| 1:C:307:LEU:H | 1:C:307:LEU:CD1 | 2.28 | 0.46 |
| 1:C:397:THR:OG1 | 1:B:175:ARG:HD3 | 2.15 | 0.46 |
| 1:C:463:PHE:CE1 | 1:C:467:LEU:HD11 | 2.50 | 0.46 |
| 1:C:490:ALA:O | 1:C:494:VAL:HG12 | 2.15 | 0.46 |
| 2:E:59:GLN:O | 2:E:60:LYS:C | 2.53 | 0.46 |
| 2:E:67:ILE:O | 2:E:70:ILE:HG23 | 2.15 | 0.46 |
| 1:A:157:GLY:O | 1:A:159:GLU:N | 2.48 | 0.46 |
| 1:A:312:PHE:CD2 | 1:A:389:ILE:HB | 2.50 | 0.46 |
| 1:A:355:VAL:O | 1:A:355:VAL:CG1 | 2.64 | 0.46 |
| 1:C:200:ASP:HA | 1:C:215:LYS:HB2 | 1.96 | 0.46 |
| 1:C:373:LYS:HZ3 | 1:C:373:LYS:CB | 2.26 | 0.46 |
| 1:B:223:LEU:HA | 1:B:241:ALA:HB3 | 1.96 | 0.46 |
| 1:B:386:TYR:O | 1:B:388:VAL:N | 2.49 | 0.46 |
| 1:B:442:GLY:O | 1:B:444:GLY:N | 2.49 | 0.46 |
| 1:A:24:VAL:HG23 | 1:A:430:ASP:O | 2.15 | 0.46 |
| 1:A:202:TYR:HE1 | 1:A:215:LYS:HB2 | 1.81 | 0.46 |
| 1:A:362:ASN:N | 1:A:363:PRO:CD | 2.78 | 0.46 |
| 1:C:22:ASP:CA | 1:C:292:ARG:HG2 | 2.46 | 0.46 |
| 1:C:292:ARG:HG3 | 1:C:292:ARG:HH11 | 1.79 | 0.46 |
| 1:C:386:TYR:O | 1:C:387:ILE:HG13 | 2.15 | 0.46 |
| 1:C:423:VAL:HG21 | 1:C:502:VAL:HG11 | 1.94 | 0.46 |
| 1:B:128:LYS:O | 1:B:202:TYR:HB3 | 2.15 | 0.46 |
| 1:B:360:THR:O | 1:B:361:ALA:CB | 2.64 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:364:VAL:O | 1:B:374:MET:HE3 | 2.15 | 0.46 |
| 1:A:12:VAL:CG2 | 1:A:33:VAL:HG22 | 2.45 | 0.46 |
| 1:A:69:ALA:O | 1:A:70:SER:HB2 | 2.15 | 0.46 |
| 1:A:96:LEU:H | 1:A:96:LEU:CD1 | 2.18 | 0.46 |
| 1:C:35:ALA:HB3 | 1:C:38:LYS:HD2 | 1.97 | 0.46 |
| 1:C:39:PRO:HG3 | 1:C:300:LEU:HG | 1.97 | 0.46 |
| 1:C:374:MET:C | 1:C:374:MET:SD | 2.93 | 0.46 |
| 1:B:9:ARG:HG3 | 1:B:11:PHE:CE1 | 2.51 | 0.46 |
| 1:B:494:VAL:HG12 | 1:B:498:LEU:HD11 | 1.96 | 0.46 |
| 2:E:33:GLU:C | 2:E:35:TRP:N | 2.69 | 0.46 |
| 1:A:101:TRP:CZ2 | 1:C:316:LYS:HG3 | 2.51 | 0.46 |
| 1:C:19:THR:HG23 | 1:C:295:MET:O | 2.16 | 0.46 |
| 1:C:25:LEU:HD12 | 1:C:289:LEU:O | 2.16 | 0.46 |
| 1:B:26:GLU:OE2 | 1:B:420:ARG:HG2 | 2.16 | 0.46 |
| 1:A:61:TYR:CE2 | 1:A:262:GLU:HB2 | 2.50 | 0.46 |
| 1:A:149:SER:O | 1:A:151:MET:N | 2.49 | 0.46 |
| 1:A:150:GLY:CA | 1:A:152:ILE:HG23 | 2.44 | 0.46 |
| 1:A:193:ARG:HB2 | 1:A:193:ARG:HH11 | 1.80 | 0.46 |
| 1:A:378:LEU:HD11 | 1:A:387:ILE:HG22 | 1.98 | 0.46 |
| 1:C:40:THR:CG2 | 1:C:360:THR:HA | 2.46 | 0.46 |
| 1:C:139:ILE:O | 1:C:167:VAL:HG12 | 2.15 | 0.46 |
| 1:C:148:HIS:HB3 | 1:C:151:MET:HB3 | 1.96 | 0.46 |
| 2:D:40:PRO:C | 2:D:42:PHE:N | 2.69 | 0.46 |
| 1:B:7:SER:N | 1:B:322:LEU:CD1 | 2.79 | 0.46 |
| 1:B:36:GLN:OE1 | 1:B:36:GLN:HA | 2.16 | 0.46 |
| 1:B:474:TRP:C | 1:B:476:GLY:H | 2.18 | 0.46 |
| 2:E:31:ARG:HG3 | 2:E:32:VAL:H | 1.81 | 0.46 |
| 1:A:179:THR:C | 1:A:180:LEU:HD23 | 2.36 | 0.46 |
| 1:A:223:LEU:HD13 | 2:D:4:LEU:HD21 | 1.98 | 0.46 |
| 1:A:261:GLN:CA | 1:A:261:GLN:NE2 | 2.63 | 0.46 |
| 1:A:264:ALA:CB | 2:D:4:LEU:HD12 | 2.46 | 0.46 |
| 1:A:292:ARG:HD2 | 1:A:292:ARG:N | 2.31 | 0.46 |
| 1:A:321:THR:O | 1:A:322:LEU:O | 2.33 | 0.46 |
| 1:A:396:ILE:HD12 | 1:A:396:ILE:H | 1.81 | 0.46 |
| 1:C:68:MET:HA | 1:C:116:CYS:O | 2.16 | 0.46 |
| 1:C:133:GLU:CB | 1:C:193:ARG:HH12 | 2.26 | 0.46 |
| 1:C:147:GLN:NE2 | 1:C:163:ASN:HB2 | 2.31 | 0.46 |
| 1:C:366:THR:O | 1:C:366:THR:HG22 | 2.16 | 0.46 |
| 1:B:99:ARG:NH2 | 1:B:103:ASN:CB | 2.75 | 0.46 |
| 1:B:149:SER:C | 1:B:151:MET:N | 2.67 | 0.46 |
| 1:B:364:VAL:O | 1:B:364:VAL:HG23 | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:302:GLY:HA3 | 1:A:305:TYR:HE2 | 1.75 | 0.45 |
| 1:A:362:ASN:O | 1:A:364:VAL:HG23 | 2.15 | 0.45 |
| 1:C:4:ILE:HG12 | 1:C:152:ILE:HD12 | 1.98 | 0.45 |
| 1:C:89:GLN:HA | 1:C:239:LYS:HZ2 | 1.80 | 0.45 |
| 1:C:180:LEU:HB3 | 1:C:183:PHE:HB2 | 1.97 | 0.45 |
| 1:C:462:TRP:CG | 1:C:463:PHE:N | 2.84 | 0.45 |
| 1:B:1:ILE:HG21 | 1:B:147:GLN:CG | 2.46 | 0.45 |
| 1:B:202:TYR:N | 1:B:202:TYR:HD1 | 2.14 | 0.45 |
| 1:B:221:ILE:HA | 1:B:222:PRO:HD3 | 1.75 | 0.45 |
| 1:A:52:ASN:C | 1:A:53:MET:HG3 | 2.35 | 0.45 |
| 1:A:202:TYR:OH | 1:A:215:LYS:HD3 | 2.15 | 0.45 |
| 1:A:364:VAL:CG1 | 1:A:365:ILE:N | 2.77 | 0.45 |
| 1:B:93:LYS:HD2 | 1:B:94:ARG:N | 2.30 | 0.45 |
| 1:A:396:ILE:H | 1:A:396:ILE:CD1 | 2.30 | 0.45 |
| 1:A:464:SER:HB3 | 2:F:75:SER:HB2 | 1.99 | 0.45 |
| 1:C:220:ASP:HB3 | 2:D:34:ASN:OD1 | 2.17 | 0.45 |
| 2:E:23:ARG:HB2 | 2:E:23:ARG:HH11 | 1.81 | 0.45 |
| 1:A:62:GLU:HG2 | 1:A:260:SER:HA | 1.99 | 0.45 |
| 1:A:204:LEU:HD11 | 1:A:269:LEU:HD21 | 1.97 | 0.45 |
| 1:A:223:LEU:HD12 | 1:A:242:LEU:CD1 | 2.47 | 0.45 |
| 1:A:321:THR:C | 1:A:322:LEU:O | 2.51 | 0.45 |
| 1:A:358:LEU:O | 1:A:359:ILE:CG1 | 2.56 | 0.45 |
| 1:A:378:LEU:CD1 | 1:A:387:ILE:HG22 | 2.46 | 0.45 |
| 1:C:1:ILE:CG2 | 1:C:4:ILE:HG13 | 2.47 | 0.45 |
| 1:C:138:ARG:HH21 | 1:C:138:ARG:CG | 2.29 | 0.45 |
| 1:B:175:ARG:O | 1:B:176:ALA:C | 2.55 | 0.45 |
| 1:B:264:ALA:HA | 1:B:267:THR:HG22 | 1.98 | 0.45 |
| 1:B:360:THR:HG1 | 1:B:376:LEU:HB3 | 1.79 | 0.45 |
| 1:A:49:THR:OG1 | 1:A:281:LYS:HB3 | 2.16 | 0.45 |
| 1:A:163:ASN:C | 1:A:164:ARG:HD2 | 2.37 | 0.45 |
| 1:A:359:ILE:C | 1:A:361:ALA:H | 2.16 | 0.45 |
| 1:A:477:LEU:N | 1:A:489:LEU:HD21 | 2.31 | 0.45 |
| 1:C:186:LEU:HD23 | 1:C:186:LEU:HA | 1.57 | 0.45 |
| 1:B:202:TYR:CE1 | 1:B:215:LYS:CB | 3.00 | 0.45 |
| 1:A:265:VAL:HG23 | 2:D:4:LEU:CD1 | 2.32 | 0.45 |
| 1:A:475:LEU:HD13 | 2:F:53:LEU:HB2 | 1.97 | 0.45 |
| 1:A:480:LYS:O | 1:A:484:ILE:HD11 | 2.17 | 0.45 |
| 1:C:51:SER:HA | 1:C:281:LYS:HB3 | 1.99 | 0.45 |
| 1:C:143:VAL:H | 1:C:163:ASN:HB3 | 1.82 | 0.45 |
| 1:C:333:ALA:O | 1:C:335:THR:HG23 | 2.16 | 0.45 |
| 1:B:41:VAL:CG1 | 1:B:42:ASP:N | 2.80 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:452:ALA:O | 1:B:454:LYS:N | 2.50 | 0.45 |
| 2:E:20:LEU:N | 2:E:20:LEU:HD12 | 2.32 | 0.45 |
| 1:A:93:LYS:HD3 | 1:A:245:PHE:CB | 2.47 | 0.45 |
| 1:A:149:SER:O | 1:A:150:GLY:C | 2.55 | 0.45 |
| 1:A:263:GLY:HA2 | 1:A:266:HIS:HB2 | 1.97 | 0.45 |
| 1:A:273:LEU:HG | 2:D:12:LEU:HD22 | 1.99 | 0.45 |
| 1:A:354:PRO:O | 1:A:355:VAL:HG23 | 2.17 | 0.45 |
| 1:C:36:GLN:C | 1:C:38:LYS:N | 2.70 | 0.45 |
| 1:C:379:ASP:O | 1:C:380:PRO:C | 2.55 | 0.45 |
| 2:D:14:THR:HB | 2:D:15:ARG:H | 1.49 | 0.45 |
| 2:D:64:LEU:C | 2:D:64:LEU:HD13 | 2.37 | 0.45 |
| 1:B:190:CYS:HB3 | 1:B:289:LEU:HD11 | 1.99 | 0.45 |
| 1:B:312:PHE:O | 1:B:313:THR:HG23 | 2.17 | 0.45 |
| 2:E:23:ARG:HA | 2:E:26:THR:HG22 | 1.99 | 0.45 |
| 2:E:28:HIS:CD2 | 2:E:28:HIS:N | 2.84 | 0.45 |
| 2:E:38:ARG:HA | 2:E:38:ARG:HE | 1.81 | 0.45 |
| 1:A:139:ILE:O | 1:A:167:VAL:CG2 | 2.65 | 0.45 |
| 1:A:148:HIS:ND1 | 1:A:373:LYS:HB2 | 2.31 | 0.45 |
| 1:C:59:TYR:O | 1:C:124:LYS:CB | 2.50 | 0.45 |
| 1:C:302:GLY:HA3 | 1:C:305:TYR:CE2 | 2.52 | 0.45 |
| 1:C:324:GLY:HA3 | 1:C:402:ARG:HE | 1.81 | 0.45 |
| 1:C:400:TRP:HZ3 | 1:C:402:ARG:HB2 | 1.81 | 0.45 |
| 2:D:23:ARG:HB3 | 2:D:27:LYS:CE | 2.32 | 0.45 |
| 1:A:20:TRP:HZ3 | 1:A:434:VAL:HA | 1.82 | 0.45 |
| 1:A:357:ARG:O | 1:A:357:ARG:HG2 | 2.17 | 0.45 |
| 1:C:113:LEU:CD2 | 1:C:251:LYS:HD2 | 2.47 | 0.45 |
| 1:C:392:GLY:O | 1:C:395:LYS:CE | 2.65 | 0.45 |
| 1:C:444:GLY:O | 1:C:446:HIS:N | 2.50 | 0.45 |
| 1:B:211:TRP:CD1 | 1:B:211:TRP:N | 2.85 | 0.45 |
| 1:B:340:LYS:HA | 1:B:364:VAL:HG12 | 1.99 | 0.45 |
| 1:B:400:TRP:CG | 1:B:401:HIS:N | 2.85 | 0.45 |
| 1:A:31:VAL:HB | 1:A:43:ILE:CD1 | 2.43 | 0.45 |
| 1:A:223:LEU:HA | 1:A:224:PRO:HD3 | 1.88 | 0.45 |
| 1:A:283:ARG:CZ | 1:A:283:ARG:HB2 | 2.42 | 0.45 |
| 1:A:329:GLU:HG2 | 1:A:375:MET:HG2 | 1.98 | 0.45 |
| 1:A:468:ILE:HG22 | 1:A:468:ILE:O | 2.17 | 0.45 |
| 1:A:497:PHE:C | 1:A:499:SER:N | 2.70 | 0.45 |
| 1:C:6:VAL:HG23 | 1:C:6:VAL:O | 2.17 | 0.45 |
| 1:C:400:TRP:CE3 | 1:C:401:HIS:N | 2.85 | 0.45 |
| 1:C:420:ARG:CG | 1:C:431:PHE:CE2 | 3.00 | 0.45 |
| 2:D:67:ILE:O | 2:D:70:ILE:HG22 | 2.17 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:99:ARG:HG3 | 1:B:99:ARG:HH11 | 1.82 | 0.45 |
| 1:B:151:MET:HG3 | 1:B:152:ILE:N | 2.32 | 0.45 |
| 1:B:180:LEU:O | 1:B:181:GLY:O | 2.35 | 0.45 |
| 1:A:67:ASP:O | 1:A:68:MET:C | 2.56 | 0.44 |
| 1:C:10:ASP:O | 1:C:31:VAL:HA | 2.17 | 0.44 |
| 1:C:60:CYS:HB3 | 1:C:224:PRO:HD2 | 1.98 | 0.44 |
| 1:C:101:TRP:N | 1:C:101:TRP:HD1 | 2.14 | 0.44 |
| 1:C:164:ARG:NH1 | 1:C:164:ARG:CG | 2.74 | 0.44 |
| 1:C:240:GLU:O | 1:C:243:VAL:O | 2.35 | 0.44 |
| 2:D:69:LEU:HD21 | 2:F:74:TYR:CD2 | 2.53 | 0.44 |
| 1:B:21:VAL:CG1 | 1:B:293:LEU:CA | 2.95 | 0.44 |
| 1:B:65:ILE:HG22 | 1:B:117:ALA:HB1 | 1.99 | 0.44 |
| 1:B:151:MET:CG | 1:B:152:ILE:N | 2.79 | 0.44 |
| 1:B:158:HIS:O | 1:B:164:ARG:HB2 | 2.17 | 0.44 |
| 2:E:40:PRO:HG2 | 2:E:41:GLY:H | 1.82 | 0.44 |
| 1:C:100:GLY:HA2 | 1:C:107:LEU:O | 2.18 | 0.44 |
| 2:D:2:VAL:O | 2:D:2:VAL:CG1 | 2.65 | 0.44 |
| 2:D:21:GLU:C | 2:D:23:ARG:N | 2.71 | 0.44 |
| 1:B:345:MET:HE1 | 1:B:385:SER:HB3 | 1.99 | 0.44 |
| 1:B:474:TRP:CZ2 | 2:E:58:SER:HB2 | 2.48 | 0.44 |
| 1:A:73:ARG:N | 1:A:112:SER:O | 2.51 | 0.44 |
| 1:C:53:MET:HB2 | 1:C:129:SER:O | 2.17 | 0.44 |
| 1:C:84:LYS:C | 1:C:86:SER:N | 2.70 | 0.44 |
| 1:C:434:VAL:HG23 | 1:C:439:ASN:CG | 2.38 | 0.44 |
| 1:B:135:LEU:C | 1:B:135:LEU:CD1 | 2.86 | 0.44 |
| 1:B:215:LYS:O | 1:B:216:GLU:C | 2.55 | 0.44 |
| 2:E:65:VAL:CG1 | 2:E:66:MET:N | 2.80 | 0.44 |
| 1:A:154:ASN:CG | 3:A:601:NAG:C8 | 2.81 | 0.44 |
| 1:A:397:THR:O | 1:A:397:THR:CG2 | 2.58 | 0.44 |
| 1:C:84:LYS:C | 1:C:86:SER:H | 2.20 | 0.44 |
| 1:C:217:TRP:HE1 | 2:F:5:PRO:HB2 | 1.79 | 0.44 |
| 1:C:322:LEU:N | 1:C:322:LEU:CD1 | 2.80 | 0.44 |
| 1:C:338:PRO:HB3 | 1:C:366:THR:HA | 1.98 | 0.44 |
| 1:C:392:GLY:O | 1:C:395:LYS:HD2 | 2.17 | 0.44 |
| 2:D:19:TRP:CD2 | 2:D:20:LEU:HG | 2.52 | 0.44 |
| 1:A:178:ALA:HB3 | 1:A:186:LEU:HB3 | 2.00 | 0.44 |
| 1:A:240:GLU:CA | 1:A:243:VAL:HG22 | 2.40 | 0.44 |
| 1:A:290:LYS:HE3 | 1:A:292:ARG:NH1 | 2.32 | 0.44 |
| 1:A:374:MET:SD | 1:A:376:LEU:HD23 | 2.58 | 0.44 |
| 1:A:386:TYR:CB | 1:A:397:THR:HG23 | 2.47 | 0.44 |
| 1:A:445:ILE:O | 1:A:445:ILE:CG2 | 2.64 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:472:LEU:C | 1:A:474:TRP:N | 2.71 | 0.44 |
| 1:C:52:ASN:O | 1:C:134:ASN:CG | 2.56 | 0.44 |
| 1:C:161:ASP:CB | 1:C:164:ARG:O | 2.65 | 0.44 |
| 1:C:169:ILE:HG22 | 1:C:192:PRO:HG3 | 1.99 | 0.44 |
| 1:C:171:PRO:HG2 | 1:C:172:ASN:N | 2.33 | 0.44 |
| 1:C:251:LYS:O | 1:C:251:LYS:CG | 2.65 | 0.44 |
| 1:B:1:ILE:CG1 | 1:B:147:GLN:HG3 | 2.48 | 0.44 |
| 1:B:27:HIS:NE2 | 1:B:46:VAL:O | 2.51 | 0.44 |
| 1:B:85:GLN:OE1 | 1:B:94:ARG:NH1 | 2.47 | 0.44 |
| 1:B:93:LYS:HE2 | 1:B:95:THR:OG1 | 2.17 | 0.44 |
| 1:B:196:LEU:HD21 | 1:B:287:GLY:CA | 2.48 | 0.44 |
| 1:B:344:GLN:OE1 | 1:B:352:LEU:CG | 2.64 | 0.44 |
| 1:B:445:ILE:CG2 | 1:B:446:HIS:N | 2.78 | 0.44 |
| 1:A:312:PHE:HB2 | 1:A:389:ILE:HD12 | 2.00 | 0.44 |
| 1:A:389:ILE:CG2 | 1:A:395:LYS:HA | 2.47 | 0.44 |
| 1:C:315:THR:C | 1:C:316:LYS:HD3 | 2.37 | 0.44 |
| 1:C:461:SER:O | 1:C:462:TRP:C | 2.55 | 0.44 |
| 2:D:51:TRP:HA | 2:D:60:LYS:HZ2 | 1.81 | 0.44 |
| 2:D:67:ILE:CG2 | 2:D:68:LEU:N | 2.80 | 0.44 |
| 1:B:71:ASP:O | 1:B:113:LEU:CB | 2.58 | 0.44 |
| 1:B:249:HIS:HE1 | 1:B:251:LYS:HB2 | 1.83 | 0.44 |
| 1:B:343:ALA:HB2 | 1:B:389:ILE:HG22 | 2.00 | 0.44 |
| 2:E:30:ILE:O | 2:E:34:ASN:HB3 | 2.18 | 0.44 |
| 1:A:26:GLU:HA | 1:A:288:HIS:HA | 2.00 | 0.44 |
| 1:C:49:THR:OG1 | 1:C:136:GLU:OE1 | 2.29 | 0.44 |
| 1:C:60:CYS:HB2 | 1:C:236:TRP:CZ3 | 2.52 | 0.44 |
| 1:C:94:ARG:HH21 | 1:C:94:ARG:HG2 | 1.82 | 0.44 |
| 1:C:97:VAL:HG13 | 1:C:250:ALA:O | 2.18 | 0.44 |
| 1:C:225:TRP:HE3 | 1:C:237:ASN:HD22 | 1.65 | 0.44 |
| 1:C:421:MET:HA | 1:C:428:ALA:CB | 2.48 | 0.44 |
| 1:C:474:TRP:CD1 | 1:C:474:TRP:C | 2.90 | 0.44 |
| 1:C:475:LEU:HD21 | 2:D:52:LEU:HG | 2.00 | 0.44 |
| 2:D:48:ALA:O | 2:D:50:ALA:N | 2.51 | 0.44 |
| 1:B:136:GLU:HG3 | 1:B:137:TYR:N | 2.32 | 0.44 |
| 1:B:204:LEU:HG | 1:B:205:THR:N | 2.32 | 0.44 |
| 1:A:86:SER:HB3 | 1:B:88:THR:HG21 | 1.98 | 0.44 |
| 1:A:89:GLN:C | 1:A:239:LYS:NZ | 2.71 | 0.44 |
| 1:A:169:ILE:O | 1:A:169:ILE:CG1 | 2.62 | 0.44 |
| 1:A:442:GLY:O | 1:A:446:HIS:HB2 | 2.18 | 0.44 |
| 1:C:323:HIS:CD2 | 1:C:416:ARG:HH22 | 2.35 | 0.44 |
| 1:C:345:MET:HE3 | 1:C:378:LEU:HB3 | 1.98 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:420:ARG:CD | 1:C:431:PHE:CE2 | 3.01 | 0.44 |
| 1:C:423:VAL:O | 1:C:424:LEU:HD23 | 2.18 | 0.44 |
| 1:C:437:ALA:O | 1:C:440:SER:N | 2.44 | 0.44 |
| 2:D:26:THR:O | 2:D:29:LEU:N | 2.42 | 0.44 |
| 2:D:40:PRO:O | 2:D:42:PHE:N | 2.50 | 0.44 |
| 1:B:40:THR:HG21 | 1:B:359:ILE:O | 2.18 | 0.44 |
| 1:B:282:GLY:O | 1:B:284:LEU:HD23 | 2.18 | 0.44 |
| 1:B:420:ARG:O | 1:B:424:LEU:HB2 | 2.17 | 0.44 |
| 1:B:428:ALA:C | 1:B:430:ASP:H | 2.21 | 0.44 |
| 1:B:459:GLY:HA2 | 2:E:9:THR:CG2 | 2.47 | 0.44 |
| 1:B:491:LEU:HA | 1:B:494:VAL:CG2 | 2.47 | 0.44 |
| 2:E:30:ILE:O | 2:E:34:ASN:CB | 2.66 | 0.44 |
| 2:E:35:TRP:HE3 | 2:E:36:ILE:HG12 | 1.82 | 0.44 |
| 1:A:56:VAL:HG11 | 1:A:202:TYR:HE2 | 1.79 | 0.44 |
| 1:A:210:HIS:HB2 | 1:A:275:ALA:O | 2.18 | 0.44 |
| 1:A:216:GLU:O | 1:A:217:TRP:C | 2.56 | 0.44 |
| 1:C:84:LYS:HD2 | 1:C:90:TYR:CZ | 2.53 | 0.44 |
| 1:C:161:ASP:N | 1:C:161:ASP:OD1 | 2.51 | 0.44 |
| 1:C:247:ASP:HB2 | 1:C:253:GLN:HA | 1.99 | 0.44 |
| 1:C:283:ARG:CZ | 1:C:283:ARG:CB | 2.93 | 0.44 |
| 1:B:48:THR:HG23 | 1:B:48:THR:O | 2.17 | 0.44 |
| 1:B:54:ALA:O | 1:B:128:LYS:HA | 2.18 | 0.44 |
| 1:A:137:TYR:CE2 | 1:A:289:LEU:HD13 | 2.53 | 0.43 |
| 1:A:386:TYR:C | 1:A:387:ILE:O | 2.54 | 0.43 |
| 1:A:410:ALA:C | 1:A:412:GLU:N | 2.72 | 0.43 |
| 1:C:70:SER:HB3 | 1:C:253:GLN:OE1 | 2.18 | 0.43 |
| 1:C:210:HIS:O | 1:C:275:ALA:O | 2.35 | 0.43 |
| 1:C:382:PHE:O | 1:C:402:ARG:O | 2.35 | 0.43 |
| 1:C:466:ILE:O | 1:C:470:THR:N | 2.32 | 0.43 |
| 1:B:45:LEU:HA | 1:B:139:ILE:HG23 | 1.99 | 0.43 |
| 1:B:331:GLN:OE1 | 1:B:371:ASN:ND2 | 2.51 | 0.43 |
| 1:A:324:GLY:HA3 | 1:A:402:ARG:NH2 | 2.32 | 0.43 |
| 1:C:21:VAL:O | 1:C:22:ASP:C | 2.56 | 0.43 |
| 1:C:300:LEU:CD1 | 1:C:362:ASN:HD22 | 2.32 | 0.43 |
| 1:C:357:ARG:HG2 | 1:C:358:LEU:H | 1.83 | 0.43 |
| 1:C:434:VAL:HG23 | 1:C:439:ASN:ND2 | 2.33 | 0.43 |
| 1:C:503:SER:O | 1:C:504:ALA:HB2 | 2.18 | 0.43 |
| 1:B:17:GLY:O | 1:B:18:GLY:O | 2.36 | 0.43 |
| 1:B:268:ALA:O | 1:B:270:ALA:N | 2.48 | 0.43 |
| 1:B:353:THR:HG23 | 1:B:355:VAL:HG23 | 2.00 | 0.43 |
| 2:E:56:SER:CB | 2:E:59:GLN:HB2 | 2.25 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:24:VAL:HG11 | 1:A:424:LEU:CD2 | 2.49 | 0.43 |
| 1:A:39:PRO:CD | 1:A:300:LEU:HD12 | 2.45 | 0.43 |
| 1:A:101:TRP:HH2 | 1:C:317:ILE:O | 2.00 | 0.43 |
| 1:A:136:GLU:HB2 | 1:A:168:GLU:OE1 | 2.17 | 0.43 |
| 1:A:223:LEU:HD12 | 1:A:242:LEU:HD11 | 2.01 | 0.43 |
| 1:A:345:MET:HE2 | 1:A:380:PRO:HA | 1.99 | 0.43 |
| 1:C:148:HIS:HB2 | 1:C:151:MET:HB3 | 1.99 | 0.43 |
| 1:C:310:ALA:CB | 1:C:332:TYR:CE1 | 3.02 | 0.43 |
| 1:C:382:PHE:C | 1:C:382:PHE:HD1 | 2.21 | 0.43 |
| 2:F:29:LEU:C | 2:F:31:ARG:H | 2.21 | 0.43 |
| 1:C:50:VAL:HG22 | 1:C:135:LEU:CD1 | 2.48 | 0.43 |
| 1:C:324:GLY:HA3 | 1:C:402:ARG:HH21 | 1.83 | 0.43 |
| 1:B:331:GLN:HA | 1:B:372:SER:O | 2.18 | 0.43 |
| 1:B:459:GLY:CA | 2:E:9:THR:HG23 | 2.49 | 0.43 |
| 1:A:32:THR:HA | 1:A:41:VAL:O | 2.17 | 0.43 |
| 1:A:437:ALA:C | 1:A:439:ASN:H | 2.21 | 0.43 |
| 2:D:4:LEU:N | 2:D:5:PRO:HD3 | 2.33 | 0.43 |
| 1:B:204:LEU:HD12 | 1:B:204:LEU:HA | 1.74 | 0.43 |
| 1:A:1:ILE:N | 1:A:144:HIS:CD2 | 2.85 | 0.43 |
| 1:A:314:PHE:HB3 | 1:A:330:VAL:HA | 2.00 | 0.43 |
| 1:A:365:ILE:HG21 | 1:A:368:SER:OG | 2.19 | 0.43 |
| 1:C:27:HIS:CD2 | 1:C:27:HIS:N | 2.87 | 0.43 |
| 1:C:316:LYS:HE2 | 1:C:373:LYS:HE3 | 2.01 | 0.43 |
| 1:C:395:LYS:HD2 | 1:C:395:LYS:H | 1.84 | 0.43 |
| 2:E:36:ILE:O | 2:E:40:PRO:HB3 | 2.18 | 0.43 |
| 1:A:300:LEU:H | 1:A:300:LEU:HD13 | 1.83 | 0.43 |
| 1:C:13:GLU:HG2 | 1:C:34:MET:CG | 2.38 | 0.43 |
| 1:C:20:TRP:CD1 | 1:C:20:TRP:C | 2.91 | 0.43 |
| 1:C:20:TRP:CZ2 | 1:C:434:VAL:CG1 | 3.01 | 0.43 |
| 1:C:202:TYR:CE2 | 1:C:215:LYS:HG3 | 2.54 | 0.43 |
| 1:C:466:ILE:HA | 1:C:496:ILE:HG22 | 2.01 | 0.43 |
| 1:B:186:LEU:CD2 | 1:B:298:LEU:HD11 | 2.47 | 0.43 |
| 1:B:383:GLY:O | 1:B:401:HIS:HA | 2.19 | 0.43 |
| 1:B:407:ILE:HG23 | 1:B:408:GLY:N | 2.33 | 0.43 |
| 2:F:69:LEU:HD12 | 2:F:69:LEU:HA | 1.70 | 0.43 |
| 1:A:259:GLY:HA3 | 1:C:262:GLU:HB3 | 2.00 | 0.43 |
| 1:C:20:TRP:CE3 | 1:C:292:ARG:NE | 2.87 | 0.43 |
| 1:C:169:ILE:HD11 | 1:C:188:LEU:HD12 | 2.00 | 0.43 |
| 1:C:215:LYS:O | 1:C:216:GLU:C | 2.57 | 0.43 |
| 1:B:227:ALA:O | 1:B:229:ALA:N | 2.51 | 0.43 |
| 1:B:231:THR:O | 1:B:232:GLY:C | 2.56 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:452:ALA:O | 1:B:453:PHE:C | 2.57 | 0.43 |
| 1:A:67:ASP:HB2 | 1:A:118:LYS:HB2 | 2.00 | 0.43 |
| 1:A:127:GLY:HA3 | 1:A:218:PHE:CZ | 2.53 | 0.43 |
| 1:A:242:LEU:HD11 | 2:D:2:VAL:HG23 | 1.99 | 0.43 |
| 1:C:71:ASP:OD2 | 1:C:82:LEU:HG | 2.18 | 0.43 |
| 1:C:177:GLU:HA | 1:C:186:LEU:O | 2.19 | 0.43 |
| 1:C:401:HIS:ND1 | 1:C:402:ARG:N | 2.67 | 0.43 |
| 2:D:27:LYS:HD2 | 2:F:2:VAL:CG2 | 2.48 | 0.43 |
| 2:D:63:TYR:HE1 | 2:F:62:ILE:CG2 | 2.32 | 0.43 |
| 1:B:357:ARG:HG3 | 1:B:358:LEU:N | 2.34 | 0.43 |
| 1:B:462:TRP:O | 1:B:463:PHE:C | 2.56 | 0.43 |
| 1:A:139:ILE:O | 1:A:167:VAL:HG23 | 2.19 | 0.43 |
| 1:A:150:GLY:C | 1:A:152:ILE:HD13 | 2.38 | 0.43 |
| 1:A:229:ALA:H | 1:B:73:ARG:HH22 | 1.67 | 0.43 |
| 1:A:253:GLN:HE21 | 1:A:253:GLN:HB3 | 1.47 | 0.43 |
| 1:C:1:ILE:HG21 | 1:C:4:ILE:CG1 | 2.49 | 0.43 |
| 1:C:119:PHE:CD1 | 1:C:120:ALA:N | 2.87 | 0.43 |
| 1:C:240:GLU:CD | 1:C:240:GLU:N | 2.73 | 0.43 |
| 2:D:69:LEU:CD2 | 2:F:74:TYR:CD2 | 3.02 | 0.43 |
| 1:B:2:ARG:NH1 | 1:B:140:MET:HB3 | 2.34 | 0.43 |
| 1:B:40:THR:HG23 | 1:B:40:THR:O | 2.18 | 0.43 |
| 1:B:97:VAL:HG23 | 1:B:113:LEU:HD12 | 2.01 | 0.43 |
| 1:B:449:PHE:O | 1:B:450:GLY:C | 2.58 | 0.43 |
| 1:A:50:VAL:HA | 1:A:134:ASN:O | 2.19 | 0.42 |
| 1:A:90:TYR:N | 1:A:239:LYS:HZ1 | 2.17 | 0.42 |
| 1:A:350:GLN:HE21 | 1:A:350:GLN:HB2 | 1.65 | 0.42 |
| 1:A:424:LEU:HA | 1:A:424:LEU:HD23 | 1.80 | 0.42 |
| 2:D:75:SER:HB2 | 2:F:9:THR:OG1 | 2.19 | 0.42 |
| 1:B:65:ILE:CG2 | 1:B:117:ALA:HB1 | 2.49 | 0.42 |
| 1:B:314:PHE:CZ | 1:B:398:HIS:HB2 | 2.53 | 0.42 |
| 1:B:461:SER:O | 1:B:462:TRP:C | 2.57 | 0.42 |
| 2:F:42:PHE:CZ | 2:F:46:ALA:HB2 | 2.54 | 0.42 |
| 1:A:386:TYR:HB3 | 1:A:397:THR:HG23 | 2.00 | 0.42 |
| 1:C:185:SER:O | 1:C:297:LYS:CB | 2.63 | 0.42 |
| 1:B:128:LYS:O | 1:B:202:TYR:CB | 2.67 | 0.42 |
| 1:B:159:GLU:C | 1:B:161:ASP:H | 2.23 | 0.42 |
| 1:B:472:LEU:CD2 | 1:B:475:LEU:HD12 | 2.48 | 0.42 |
| 1:B:474:TRP:O | 1:B:478:ASN:HB3 | 2.19 | 0.42 |
| 2:E:22:SER:O | 2:E:23:ARG:CB | 2.67 | 0.42 |
| 1:A:23:VAL:HG13 | 1:A:25:LEU:CD2 | 2.45 | 0.42 |
| 1:A:271:GLY:HA2 | 2:D:11:LYS:HG3 | 2.01 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:258:LEU:CD1 | 2:D:20:LEU:HD21 | 2.49 | 0.42 |
| 2:D:9:THR:HG21 | 2:D:10:ARG:HH21 | 1.83 | 0.42 |
| 2:D:64:LEU:O | 2:D:64:LEU:HD22 | 2.18 | 0.42 |
| 1:B:37:ASP:C | 1:B:37:ASP:OD1 | 2.57 | 0.42 |
| 1:B:56:VAL:O | 1:B:227:ALA:CB | 2.66 | 0.42 |
| 1:B:202:TYR:HE1 | 1:B:215:LYS:HB2 | 1.81 | 0.42 |
| 1:B:312:PHE:CZ | 1:B:332:TYR:HE2 | 2.37 | 0.42 |
| 1:B:388:VAL:O | 1:B:388:VAL:HG23 | 2.18 | 0.42 |
| 2:E:19:TRP:CD1 | 2:E:20:LEU:HD11 | 2.54 | 0.42 |
| 1:A:297:LYS:N | 1:A:297:LYS:HD2 | 2.35 | 0.42 |
| 1:C:169:ILE:HD13 | 1:C:190:CYS:SG | 2.59 | 0.42 |
| 1:C:204:LEU:N | 1:C:204:LEU:HD12 | 2.33 | 0.42 |
| 1:C:272:ALA:O | 2:F:19:TRP:HB2 | 2.20 | 0.42 |
| 1:C:376:LEU:N | 1:C:376:LEU:CD1 | 2.82 | 0.42 |
| 1:C:475:LEU:HD11 | 2:D:52:LEU:CB | 2.45 | 0.42 |
| 1:B:82:LEU:O | 1:B:82:LEU:CG | 2.57 | 0.42 |
| 1:B:450:GLY:O | 1:B:454:LYS:HB3 | 2.19 | 0.42 |
| 2:E:21:GLU:O | 2:E:24:GLU:N | 2.52 | 0.42 |
| 1:A:2:ARG:NH2 | 1:A:44:GLU:OE2 | 2.53 | 0.42 |
| 1:A:38:LYS:C | 1:A:39:PRO:O | 2.58 | 0.42 |
| 1:A:286:SER:HB2 | 2:D:16:SER:HB2 | 2.01 | 0.42 |
| 1:C:341:VAL:HG23 | 1:C:365:ILE:HG12 | 2.01 | 0.42 |
| 1:C:392:GLY:O | 1:C:395:LYS:CD | 2.67 | 0.42 |
| 2:D:63:TYR:HE1 | 2:F:62:ILE:HG23 | 1.83 | 0.42 |
| 1:B:38:LYS:CG | 1:B:298:LEU:HB3 | 2.47 | 0.42 |
| 1:B:364:VAL:N | 1:B:374:MET:HE3 | 2.31 | 0.42 |
| 2:E:19:TRP:CD1 | 2:E:20:LEU:CD1 | 3.02 | 0.42 |
| 1:A:20:TRP:CZ3 | 1:A:434:VAL:HG12 | 2.51 | 0.42 |
| 1:A:81:TYR:C | 1:A:81:TYR:CD1 | 2.93 | 0.42 |
| 1:A:252:ARG:HB2 | 1:A:252:ARG:HH11 | 1.80 | 0.42 |
| 1:A:290:LYS:HE2 | 1:A:430:ASP:OD2 | 2.19 | 0.42 |
| 1:A:463:PHE:CD1 | 1:A:463:PHE:O | 2.72 | 0.42 |
| 1:C:47:THR:O | 1:C:138:ARG:HB2 | 2.19 | 0.42 |
| 1:C:74:CYS:HB3 | 1:C:75:PRO:CD | 2.44 | 0.42 |
| 1:C:187:GLY:C | 1:C:188:LEU:HD23 | 2.40 | 0.42 |
| 1:C:276:GLU:OE2 | 1:C:283:ARG:HG2 | 2.20 | 0.42 |
| 1:B:73:ARG:HD2 | 1:B:77:GLN:CG | 2.48 | 0.42 |
| 1:B:76:THR:HB | 1:B:77:GLN:OE1 | 2.20 | 0.42 |
| 1:B:105:CYS:O | 1:B:106:GLY:C | 2.55 | 0.42 |
| 1:B:133:GLU:OE2 | 1:B:193:ARG:NH1 | 2.52 | 0.42 |
| 1:B:142:SER:OG | 1:B:164:ARG:HG2 | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:202:TYR:HD1 | 1:B:202:TYR:H | 1.66 | 0.42 |
| 1:B:360:THR:OG1 | 1:B:377:GLU:N | 2.53 | 0.42 |
| 1:B:395:LYS:O | 1:B:397:THR:HG23 | 2.19 | 0.42 |
| 2:E:20:LEU:O | 2:E:21:GLU:C | 2.58 | 0.42 |
| 1:A:101:TRP:HB2 | 1:A:108:PHE:CZ | 2.54 | 0.42 |
| 1:A:204:LEU:HD21 | 1:A:211:TRP:HB2 | 2.00 | 0.42 |
| 1:A:441:LEU:O | 1:A:444:GLY:N | 2.53 | 0.42 |
| 1:A:470:THR:O | 1:A:472:LEU:N | 2.52 | 0.42 |
| 1:C:281:LYS:HB2 | 1:C:281:LYS:HE3 | 1.79 | 0.42 |
| 1:C:398:HIS:CD2 | 1:B:172:ASN:HA | 2.55 | 0.42 |
| 1:B:191:GLU:C | 1:B:193:ARG:N | 2.73 | 0.42 |
| 1:B:225:TRP:HB3 | 1:B:237:ASN:HD22 | 1.83 | 0.42 |
| 1:B:257:VAL:O | 1:B:257:VAL:HG13 | 2.19 | 0.42 |
| 2:E:4:LEU:HD23 | 2:E:5:PRO:O | 2.18 | 0.42 |
| 1:A:153:VAL:O | 1:A:154:ASN:C | 2.57 | 0.42 |
| 1:A:263:GLY:HA3 | 1:C:261:GLN:NE2 | 2.35 | 0.42 |
| 1:A:396:ILE:N | 1:A:396:ILE:CD1 | 2.83 | 0.42 |
| 1:C:353:THR:HG23 | 1:C:354:PRO:HD2 | 2.02 | 0.42 |
| 2:D:74:TYR:HE2 | 2:F:69:LEU:O | 2.02 | 0.42 |
| 1:B:170:THR:C | 1:B:172:ASN:N | 2.73 | 0.42 |
| 1:A:12:VAL:CG1 | 1:A:432:GLY:HA3 | 2.42 | 0.42 |
| 1:A:20:TRP:HE3 | 1:A:434:VAL:CG1 | 2.23 | 0.42 |
| 1:A:460:MET:C | 1:A:461:SER:O | 2.57 | 0.42 |
| 1:A:496:ILE:O | 1:A:499:SER:CB | 2.68 | 0.42 |
| 1:C:23:VAL:HG21 | 1:C:43:ILE:HD11 | 2.02 | 0.42 |
| 2:D:73:ALA:HB1 | 2:F:73:ALA:CB | 2.50 | 0.42 |
| 1:B:9:ARG:HG3 | 1:B:9:ARG:HH11 | 1.84 | 0.42 |
| 1:B:222:PRO:C | 1:B:223:LEU:CG | 2.88 | 0.42 |
| 1:B:317:ILE:O | 1:B:317:ILE:HG23 | 2.19 | 0.42 |
| 1:A:74:CYS:HA | 1:A:99:ARG:CD | 2.50 | 0.42 |
| 1:A:223:LEU:CD1 | 1:A:242:LEU:HD11 | 2.50 | 0.42 |
| 1:A:225:TRP:HD1 | 1:A:226:HIS:C | 2.23 | 0.42 |
| 1:A:248:ALA:HB2 | 1:A:252:ARG:NH1 | 2.35 | 0.42 |
| 1:A:272:ALA:HB2 | 2:D:7:HIS:CE1 | 2.54 | 0.42 |
| 1:A:412:GLU:C | 1:A:412:GLU:CD | 2.79 | 0.42 |
| 1:B:41:VAL:HG12 | 1:B:42:ASP:N | 2.35 | 0.42 |
| 1:B:158:HIS:CG | 1:B:164:ARG:HD3 | 2.55 | 0.42 |
| 1:B:186:LEU:HB3 | 1:B:293:LEU:CD1 | 2.50 | 0.42 |
| 1:B:221:ILE:HG12 | 1:B:223:LEU:HD11 | 2.00 | 0.42 |
| 2:F:56:SER:HB3 | 2:F:59:GLN:HG3 | 1.99 | 0.42 |
| 1:A:65:ILE:HD12 | 1:A:257:VAL:CG2 | 2.39 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:313:THR:HG22 | 1:A:331:GLN:O | 2.20 | 0.41 |
| 1:A:477:LEU:HD23 | 1:A:477:LEU:C | 2.39 | 0.41 |
| 1:C:107:LEU:HD12 | 1:C:107:LEU:HA | 1.80 | 0.41 |
| 1:C:171:PRO:HG2 | 1:C:172:ASN:H | 1.85 | 0.41 |
| 1:C:351:THR:HG22 | 1:C:388:VAL:HG21 | 2.02 | 0.41 |
| 2:D:17:GLN:H | 2:D:17:GLN:HG3 | 1.45 | 0.41 |
| 1:B:20:TRP:HE3 | 1:B:292:ARG:NE | 2.18 | 0.41 |
| 1:B:82:LEU:HD22 | 1:B:114:VAL:O | 2.19 | 0.41 |
| 1:B:163:ASN:OD1 | 1:B:163:ASN:N | 2.53 | 0.41 |
| 1:B:200:ASP:O | 1:B:201:LEU:HD22 | 2.19 | 0.41 |
| 2:F:26:THR:HG23 | 2:F:27:LYS:N | 2.35 | 0.41 |
| 1:A:1:ILE:HG12 | 1:A:147:GLN:HB2 | 2.00 | 0.41 |
| 1:A:215:LYS:NZ | 1:A:215:LYS:CB | 2.82 | 0.41 |
| 1:A:359:ILE:HD11 | 1:A:377:GLU:CG | 2.31 | 0.41 |
| 1:C:317:ILE:HA | 1:C:318:PRO:HD3 | 1.85 | 0.41 |
| 1:C:389:ILE:HD11 | 1:C:396:ILE:H | 1.84 | 0.41 |
| 1:C:389:ILE:CD1 | 1:C:396:ILE:H | 2.32 | 0.41 |
| 1:B:88:THR:HG23 | 1:B:89:GLN:N | 2.35 | 0.41 |
| 1:B:423:VAL:HG12 | 1:B:424:LEU:HD12 | 2.01 | 0.41 |
| 1:B:460:MET:HB2 | 1:B:464:SER:OG | 2.20 | 0.41 |
| 1:A:40:THR:OG1 | 1:A:359:ILE:O | 2.36 | 0.41 |
| 1:A:159:GLU:CD | 1:A:160:THR:N | 2.74 | 0.41 |
| 1:A:191:GLU:HB3 | 1:A:194:THR:OG1 | 2.20 | 0.41 |
| 1:A:332:TYR:O | 1:A:335:THR:HG22 | 2.20 | 0.41 |
| 1:C:97:VAL:HG23 | 1:C:113:LEU:CB | 2.50 | 0.41 |
| 1:C:273:LEU:HD12 | 1:C:273:LEU:C | 2.40 | 0.41 |
| 2:D:19:TRP:CE2 | 2:D:20:LEU:HG | 2.55 | 0.41 |
| 1:B:45:LEU:CA | 1:B:139:ILE:HG22 | 2.50 | 0.41 |
| 1:B:206:MET:O | 1:B:207:ASN:HB3 | 2.19 | 0.41 |
| 1:B:215:LYS:O | 1:B:218:PHE:HB3 | 2.21 | 0.41 |
| 1:B:454:LYS:HB3 | 1:B:454:LYS:HE3 | 1.91 | 0.41 |
| 2:E:31:ARG:HG3 | 2:E:32:VAL:N | 2.36 | 0.41 |
| 2:F:48:ALA:O | 2:F:49:ILE:C | 2.59 | 0.41 |
| 1:A:72:SER:O | 1:A:73:ARG:HG2 | 2.19 | 0.41 |
| 1:A:196:LEU:CG | 1:A:287:GLY:HA2 | 2.50 | 0.41 |
| 1:A:236:TRP:CB | 1:A:239:LYS:HG2 | 2.50 | 0.41 |
| 1:A:290:LYS:NZ | 1:A:430:ASP:HB3 | 2.36 | 0.41 |
| 1:C:47:THR:CG2 | 1:C:49:THR:HG23 | 2.49 | 0.41 |
| 1:C:180:LEU:HD23 | 1:C:185:SER:HA | 2.01 | 0.41 |
| 1:C:306:SER:O | 1:C:339:CYS:HB2 | 2.19 | 0.41 |
| 1:C:444:GLY:C | 1:C:446:HIS:N | 2.74 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:7:SER:CA | 1:B:322:LEU:CD1 | 2.98 | 0.41 |
| 1:B:293:LEU:HD12 | 1:B:294:LYS:H | 1.84 | 0.41 |
| 1:B:442:GLY:C | 1:B:444:GLY:H | 2.23 | 0.41 |
| 1:B:456:LEU:HD12 | 1:B:457:PHE:CE1 | 2.56 | 0.41 |
| 1:B:481:ASN:HD22 | 1:B:483:SER:HB3 | 1.82 | 0.41 |
| 2:E:31:ARG:NH2 | 2:E:31:ARG:CB | 2.83 | 0.41 |
| 2:F:29:LEU:C | 2:F:31:ARG:N | 2.74 | 0.41 |
| 1:A:139:ILE:HB | 1:A:167:VAL:CG2 | 2.43 | 0.41 |
| 1:A:366:THR:HG22 | 1:A:367:GLU:N | 2.35 | 0.41 |
| 1:C:40:THR:HG22 | 1:C:361:ALA:H | 1.85 | 0.41 |
| 2:D:29:LEU:C | 2:D:29:LEU:CD2 | 2.88 | 0.41 |
| 2:D:69:LEU:HD23 | 2:F:74:TYR:HD2 | 1.85 | 0.41 |
| 1:B:19:THR:HB | 1:B:295:MET:CB | 2.43 | 0.41 |
| 1:A:1:ILE:H1 | 1:A:144:HIS:CD2 | 2.39 | 0.41 |
| 1:A:190:CYS:HB3 | 1:A:290:LYS:O | 2.21 | 0.41 |
| 1:A:204:LEU:CD2 | 1:A:211:TRP:HB2 | 2.50 | 0.41 |
| 1:A:392:GLY:O | 1:A:395:LYS:CB | 2.68 | 0.41 |
| 1:C:42:ASP:N | 1:C:142:SER:O | 2.49 | 0.41 |
| 1:C:312:PHE:CZ | 1:C:341:VAL:HG21 | 2.55 | 0.41 |
| 1:C:420:ARG:CG | 1:C:431:PHE:HE2 | 2.34 | 0.41 |
| 1:B:53:MET:CE | 1:B:130:ILE:HG21 | 2.50 | 0.41 |
| 1:B:93:LYS:C | 1:B:114:VAL:HG23 | 2.41 | 0.41 |
| 1:B:245:PHE:HA | 1:B:255:VAL:HG12 | 2.02 | 0.41 |
| 1:B:290:LYS:O | 1:B:290:LYS:HG2 | 2.20 | 0.41 |
| 1:A:99:ARG:HB3 | 1:A:99:ARG:CZ | 2.51 | 0.41 |
| 1:C:21:VAL:O | 1:C:23:VAL:HG12 | 2.21 | 0.41 |
| 1:C:41:VAL:HG22 | 1:C:42:ASP:N | 2.35 | 0.41 |
| 1:C:52:ASN:O | 1:C:134:ASN:OD1 | 2.39 | 0.41 |
| 1:C:295:MET:CE | 1:C:298:LEU:HD12 | 2.48 | 0.41 |
| 1:C:399:HIS:NE2 | 1:B:193:ARG:HB3 | 2.35 | 0.41 |
| 1:B:6:VAL:HG22 | 1:B:9:ARG:HB3 | 2.02 | 0.41 |
| 1:B:224:PRO:HG3 | 1:B:242:LEU:HD13 | 2.03 | 0.41 |
| 1:B:241:ALA:C | 1:B:242:LEU:HD12 | 2.40 | 0.41 |
| 1:A:72:SER:HB2 | 1:A:99:ARG:NH1 | 2.33 | 0.41 |
| 1:A:445:ILE:O | 1:A:445:ILE:HG22 | 2.20 | 0.41 |
| 1:A:454:LYS:CG | 1:A:455:SER:N | 2.81 | 0.41 |
| 1:C:148:HIS:C | 1:C:375:MET:CE | 2.89 | 0.41 |
| 1:C:471:LEU:HD21 | 2:F:62:ILE:HG12 | 2.01 | 0.41 |
| 1:B:1:ILE:CG2 | 1:B:147:GLN:CG | 2.99 | 0.41 |
| 1:B:50:VAL:CG1 | 1:B:53:MET:HE2 | 2.51 | 0.41 |
| 1:B:213:VAL:HG11 | 1:B:269:LEU:HD21 | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:329:GLU:OE2 | 1:B:375:MET:HB2 | 2.21 | 0.41 |
| 1:B:494:VAL:O | 1:B:497:PHE:HB3 | 2.21 | 0.41 |
| 2:F:3:THR:HG22 | 2:F:5:PRO:CG | 2.51 | 0.41 |
| 2:F:68:LEU:HD23 | 2:F:68:LEU:HA | 1.89 | 0.41 |
| 1:A:1:ILE:CG2 | 1:A:2:ARG:N | 2.80 | 0.41 |
| 1:A:12:VAL:C | 1:A:14:GLY:H | 2.24 | 0.41 |
| 1:A:46:VAL:HG21 | 1:A:140:MET:CG | 2.39 | 0.41 |
| 1:A:68:MET:SD | 1:A:255:VAL:HB | 2.61 | 0.41 |
| 1:A:71:ASP:OD1 | 1:A:72:SER:N | 2.54 | 0.41 |
| 1:A:226:HIS:CE1 | 1:A:230:ASP:HB3 | 2.56 | 0.41 |
| 1:A:365:ILE:CG2 | 1:A:368:SER:HB2 | 2.48 | 0.41 |
| 1:C:97:VAL:HG13 | 1:C:250:ALA:C | 2.41 | 0.41 |
| 1:C:118:LYS:HB3 | 1:C:118:LYS:NZ | 2.36 | 0.41 |
| 1:C:291:CYS:HB3 | 1:C:292:ARG:H | 1.47 | 0.41 |
| 1:C:322:LEU:CD1 | 1:C:322:LEU:H | 2.34 | 0.41 |
| 1:C:437:ALA:C | 1:C:439:ASN:H | 2.24 | 0.41 |
| 1:B:19:THR:OG1 | 1:B:295:MET:HG2 | 2.21 | 0.41 |
| 1:B:23:VAL:O | 1:B:23:VAL:HG13 | 2.21 | 0.41 |
| 1:B:61:TYR:CZ | 1:B:123:LYS:HB3 | 2.56 | 0.41 |
| 1:B:131:GLN:HE21 | 1:B:131:GLN:HB3 | 1.67 | 0.41 |
| 1:B:375:MET:C | 1:B:376:LEU:CG | 2.78 | 0.41 |
| 1:B:432:GLY:O | 1:B:434:VAL:N | 2.54 | 0.41 |
| 2:E:31:ARG:NH2 | 2:E:31:ARG:HB3 | 2.36 | 0.41 |
| 2:E:64:LEU:O | 2:E:67:ILE:HG23 | 2.20 | 0.41 |
| 1:A:38:LYS:HG3 | 1:A:298:LEU:CB | 2.51 | 0.41 |
| 1:A:61:TYR:CE2 | 1:A:123:LYS:NZ | 2.89 | 0.41 |
| 1:A:147:GLN:O | 1:A:375:MET:N | 2.52 | 0.41 |
| 1:A:314:PHE:CD2 | 1:A:318:PRO:HD3 | 2.54 | 0.41 |
| 1:A:466:ILE:HG13 | 1:A:467:LEU:N | 2.36 | 0.41 |
| 1:C:62:GLU:CG | 1:C:122:SER:HB3 | 2.50 | 0.41 |
| 1:C:98:ASP:OD1 | 1:C:110:LYS:CG | 2.60 | 0.41 |
| 1:C:213:VAL:HG12 | 1:C:214:HIS:O | 2.21 | 0.41 |
| 1:C:355:VAL:CG1 | 1:C:356:GLY:H | 2.34 | 0.41 |
| 1:C:420:ARG:HD2 | 1:C:431:PHE:HD2 | 1.75 | 0.41 |
| 2:D:19:TRP:HA | 2:D:19:TRP:CE3 | 2.56 | 0.41 |
| 2:D:23:ARG:O | 2:D:27:LYS:HG2 | 2.21 | 0.41 |
| 2:D:42:PHE:O | 2:D:46:ALA:CB | 2.69 | 0.41 |
| 1:B:217:TRP:CD1 | 2:E:7:HIS:N | 2.89 | 0.41 |
| 1:B:476:GLY:HA3 | 1:B:489:LEU:HD12 | 2.02 | 0.41 |
| 2:F:42:PHE:CE2 | 2:F:46:ALA:HB2 | 2.56 | 0.41 |
| 1:A:484:ILE:C | 1:A:484:ILE:HD12 | 2.41 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:74:CYS:O | 1:C:75:PRO:C | 2.59 | 0.40 |
| 1:C:94:ARG:HG2 | 1:C:94:ARG:NH2 | 2.37 | 0.40 |
| 1:C:257:VAL:O | 1:C:258:LEU:HB3 | 2.21 | 0.40 |
| 1:C:429:TRP:O | 1:C:430:ASP:OD1 | 2.39 | 0.40 |
| 1:B:50:VAL:HB | 1:B:53:MET:CE | 2.51 | 0.40 |
| 1:B:395:LYS:C | 1:B:397:THR:H | 2.24 | 0.40 |
| 1:B:409:LYS:HZ2 | 1:B:413:ALA:HB2 | 1.86 | 0.40 |
| 2:E:35:TRP:CE3 | 2:E:36:ILE:HG12 | 2.56 | 0.40 |
| 2:F:27:LYS:C | 2:F:29:LEU:N | 2.73 | 0.40 |
| 1:A:59:TYR:HD1 | 1:A:59:TYR:HA | 1.74 | 0.40 |
| 1:A:326:VAL:HG23 | 1:A:380:PRO:HG3 | 2.02 | 0.40 |
| 1:A:345:MET:HE2 | 1:A:381:PRO:HD2 | 2.01 | 0.40 |
| 1:A:349:MET:HB2 | 1:A:386:TYR:CD2 | 2.56 | 0.40 |
| 1:A:405:SER:HB2 | 1:A:408:GLY:CA | 2.39 | 0.40 |
| 1:C:143:VAL:O | 1:C:163:ASN:OD1 | 2.38 | 0.40 |
| 2:D:73:ALA:HB1 | 2:F:73:ALA:HB1 | 2.03 | 0.40 |
| 1:B:108:PHE:HD1 | 1:B:109:GLY:N | 2.20 | 0.40 |
| 1:B:151:MET:O | 1:B:152:ILE:C | 2.60 | 0.40 |
| 1:B:153:VAL:HG23 | 1:B:154:ASN:N | 2.36 | 0.40 |
| 1:B:226:HIS:NE2 | 1:B:231:THR:HA | 2.36 | 0.40 |
| 2:F:53:LEU:HD13 | 2:F:53:LEU:HA | 1.98 | 0.40 |
| 1:A:152:ILE:HD11 | 1:C:102:GLY:HA3 | 2.03 | 0.40 |
| 1:C:125:MET:SD | 1:C:206:MET:HE1 | 2.61 | 0.40 |
| 1:C:171:PRO:HB2 | 1:C:193:ARG:CD | 2.43 | 0.40 |
| 1:C:312:PHE:CE2 | 1:C:341:VAL:HG11 | 2.57 | 0.40 |
| 1:B:1:ILE:CG2 | 1:B:147:GLN:HG3 | 2.51 | 0.40 |
| 1:B:24:VAL:HG11 | 1:B:424:LEU:CD2 | 2.52 | 0.40 |
| 1:B:101:TRP:HD1 | 1:B:108:PHE:CE2 | 2.38 | 0.40 |
| 1:B:211:TRP:CG | 1:B:269:LEU:HD11 | 2.57 | 0.40 |
| 1:B:283:ARG:CG | 1:B:283:ARG:NH1 | 2.82 | 0.40 |
| 2:E:42:PHE:O | 2:E:46:ALA:HB3 | 2.19 | 0.40 |
| 1:A:20:TRP:HE1 | 1:A:292:ARG:HG2 | 1.86 | 0.40 |
| 1:A:60:CYS:HB2 | 1:A:236:TRP:CH2 | 2.57 | 0.40 |
| 1:A:61:TYR:CD1 | 1:A:61:TYR:N | 2.90 | 0.40 |
| 1:A:65:ILE:HG13 | 1:A:257:VAL:HG13 | 2.04 | 0.40 |
| 1:A:73:ARG:CG | 1:A:80:ALA:HB2 | 2.51 | 0.40 |
| 1:A:242:LEU:HD11 | 2:D:2:VAL:CG2 | 2.52 | 0.40 |
| 1:A:360:THR:HG21 | 1:A:377:GLU:N | 2.29 | 0.40 |
| 1:C:12:VAL:HG12 | 1:C:32:THR:O | 2.21 | 0.40 |
| 1:B:3:CYS:O | 1:B:9:ARG:CZ | 2.70 | 0.40 |
| 1:B:131:GLN:HG2 | 1:B:133:GLU:O | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:B:209:LYS:O | 1:B:211:TRP:CE2 | 2.73 | 0.40 |
| 1:B:237:ASN:O | 1:B:238:ASN:HB2 | 2.21 | 0.40 |
| 1:B:264:ALA:O | 2:E:4:LEU:CD1 | 2.70 | 0.40 |
| 1:B:373:LYS:O | 1:B:373:LYS:CG | 2.58 | 0.40 |
| 1:B:444:GLY:O | 1:B:447:GLN:HB2 | 2.21 | 0.40 |
| 1:A:9:ARG:NH1 | 1:A:11:PHE:HZ | 2.18 | 0.40 |
| 1:A:34:MET:HG2 | 1:A:34:MET:O | 2.21 | 0.40 |
| 1:A:436:GLY:O | 1:A:440:SER:HB3 | 2.21 | 0.40 |
| 1:C:33:VAL:N | 1:C:41:VAL:O | 2.52 | 0.40 |
| 1:C:153:VAL:O | 1:C:154:ASN:C | 2.60 | 0.40 |
| 1:C:497:PHE:CD2 | 1:C:497:PHE:C | 2.95 | 0.40 |
| 1:B:101:TRP:CD1 | 1:B:101:TRP:N | 2.89 | 0.40 |
| 1:B:312:PHE:CE1 | 1:B:332:TYR:CD2 | 3.09 | 0.40 |
| 1:B:386:TYR:CD2 | 1:B:386:TYR:N | 2.89 | 0.40 |
| 2:E:40:PRO:CG | 2:E:41:GLY:N | 2.84 | 0.40 |
| 2:E:60:LYS:HE2 | 2:E:60:LYS:HB3 | 1.70 | 0.40 |
| 2:F:63:TYR:O | 2:F:67:ILE:HG13 | 2.21 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-----------|-------------|----|
| 1 | A | 502/504 (100%) | 332 (66%) | 123 (24%) | 47 (9%) | 0 | 8 |
| 1 | B | 502/504 (100%) | 331 (66%) | 104 (21%) | 67 (13%) | 0 | 3 |
| 1 | C | 502/504 (100%) | 365 (73%) | 96 (19%) | 41 (8%) | 1 | 9 |
| 2 | D | 73/75 (97%) | 37 (51%) | 26 (36%) | 10 (14%) | 0 | 3 |
| 2 | E | 73/75 (97%) | 48 (66%) | 20 (27%) | 5 (7%) | 1 | 14 |
| 2 | F | 73/75 (97%) | 43 (59%) | 24 (33%) | 6 (8%) | 1 | 9 |
| All | All | 1725/1737 (99%) | 1156 (67%) | 393 (23%) | 176 (10%) | 1 | 6 |

All (176) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 36 | GLN |
| 1 | A | 132 | PRO |
| 1 | A | 322 | LEU |
| 1 | A | 323 | HIS |
| 1 | A | 357 | ARG |
| 1 | A | 359 | ILE |
| 1 | A | 465 | GLN |
| 1 | C | 37 | ASP |
| 1 | C | 66 | SER |
| 1 | C | 85 | GLN |
| 1 | C | 249 | HIS |
| 1 | C | 300 | LEU |
| 1 | C | 334 | GLY |
| 1 | C | 385 | SER |
| 1 | C | 433 | SER |
| 1 | C | 462 | TRP |
| 2 | D | 18 | THR |
| 1 | B | 7 | SER |
| 1 | B | 14 | GLY |
| 1 | B | 62 | GLU |
| 1 | B | 75 | PRO |
| 1 | B | 82 | LEU |
| 1 | B | 134 | ASN |
| 1 | B | 176 | ALA |
| 1 | B | 198 | PHE |
| 1 | B | 216 | GLU |
| 1 | B | 217 | TRP |
| 1 | B | 223 | LEU |
| 1 | B | 260 | SER |
| 1 | B | 303 | VAL |
| 1 | B | 310 | ALA |
| 2 | E | 55 | SER |
| 2 | E | 74 | TYR |
| 2 | F | 28 | HIS |
| 2 | F | 30 | ILE |
| 1 | A | 16 | SER |
| 1 | A | 23 | VAL |
| 1 | A | 75 | PRO |
| 1 | A | 151 | MET |
| 1 | A | 239 | LYS |
| 1 | A | 297 | LYS |
| 1 | A | 339 | CYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 374 | MET |
| 1 | A | 378 | LEU |
| 1 | A | 425 | GLY |
| 1 | C | 76 | THR |
| 1 | C | 88 | THR |
| 1 | C | 134 | ASN |
| 1 | C | 161 | ASP |
| 1 | C | 195 | GLY |
| 1 | C | 234 | PRO |
| 1 | C | 258 | LEU |
| 1 | C | 264 | ALA |
| 1 | C | 307 | LEU |
| 1 | C | 348 | ASP |
| 1 | C | 392 | GLY |
| 1 | C | 442 | GLY |
| 1 | C | 444 | GLY |
| 1 | C | 456 | LEU |
| 2 | D | 6 | SER |
| 2 | D | 20 | LEU |
| 2 | D | 22 | SER |
| 2 | D | 24 | GLU |
| 1 | B | 18 | GLY |
| 1 | B | 29 | GLY |
| 1 | B | 45 | LEU |
| 1 | B | 46 | VAL |
| 1 | B | 63 | ALA |
| 1 | B | 111 | GLY |
| 1 | B | 147 | GLN |
| 1 | B | 181 | GLY |
| 1 | B | 195 | GLY |
| 1 | B | 234 | PRO |
| 1 | B | 333 | ALA |
| 1 | B | 335 | THR |
| 1 | B | 352 | LEU |
| 1 | B | 367 | GLU |
| 1 | B | 397 | THR |
| 1 | B | 425 | GLY |
| 1 | B | 433 | SER |
| 1 | B | 434 | VAL |
| 1 | B | 462 | TRP |
| 1 | B | 476 | GLY |
| 1 | A | 8 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 154 | ASN |
| 1 | A | 157 | GLY |
| 1 | A | 216 | GLU |
| 1 | A | 266 | HIS |
| 1 | A | 344 | GLN |
| 1 | A | 352 | LEU |
| 1 | A | 377 | GLU |
| 1 | A | 481 | ASN |
| 1 | C | 2 | ARG |
| 1 | C | 9 | ARG |
| 1 | C | 262 | GLU |
| 1 | C | 337 | GLY |
| 1 | C | 380 | PRO |
| 2 | D | 5 | PRO |
| 2 | D | 12 | LEU |
| 2 | D | 48 | ALA |
| 2 | D | 49 | ILE |
| 1 | B | 15 | MET |
| 1 | B | 51 | SER |
| 1 | B | 83 | ASP |
| 1 | B | 136 | GLU |
| 1 | B | 152 | ILE |
| 1 | B | 153 | VAL |
| 1 | B | 182 | GLY |
| 1 | B | 224 | PRO |
| 1 | B | 239 | LYS |
| 1 | B | 269 | LEU |
| 1 | B | 286 | SER |
| 1 | B | 360 | THR |
| 1 | B | 361 | ALA |
| 1 | B | 371 | ASN |
| 1 | B | 387 | ILE |
| 1 | B | 427 | THR |
| 1 | B | 436 | GLY |
| 1 | B | 453 | PHE |
| 1 | A | 88 | THR |
| 1 | A | 150 | GLY |
| 1 | A | 262 | GLU |
| 1 | A | 318 | PRO |
| 1 | A | 338 | PRO |
| 1 | A | 355 | VAL |
| 1 | A | 361 | ALA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 426 | ASP |
| 1 | A | 436 | GLY |
| 1 | C | 382 | PHE |
| 1 | C | 485 | SER |
| 1 | B | 241 | ALA |
| 1 | B | 422 | ALA |
| 1 | B | 460 | MET |
| 1 | B | 483 | SER |
| 1 | B | 484 | ILE |
| 2 | E | 32 | VAL |
| 2 | F | 19 | TRP |
| 2 | F | 62 | ILE |
| 2 | F | 68 | LEU |
| 1 | A | 146 | SER |
| 1 | A | 200 | ASP |
| 1 | A | 390 | GLY |
| 1 | A | 471 | LEU |
| 1 | A | 498 | LEU |
| 1 | C | 4 | ILE |
| 1 | C | 132 | PRO |
| 1 | C | 168 | GLU |
| 1 | C | 222 | PRO |
| 1 | C | 352 | LEU |
| 1 | C | 425 | GLY |
| 1 | C | 458 | GLY |
| 2 | D | 42 | PHE |
| 1 | B | 39 | PRO |
| 1 | B | 396 | ILE |
| 1 | B | 452 | ALA |
| 2 | E | 2 | VAL |
| 2 | E | 11 | LYS |
| 2 | F | 22 | SER |
| 1 | A | 143 | VAL |
| 1 | A | 409 | LYS |
| 1 | A | 97 | VAL |
| 1 | A | 234 | PRO |
| 1 | A | 388 | VAL |
| 1 | C | 445 | ILE |
| 1 | B | 6 | VAL |
| 1 | B | 56 | VAL |
| 1 | A | 4 | ILE |
| 1 | A | 468 | ILE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 5 | GLY |
| 1 | C | 145 | GLY |
| 1 | B | 192 | PRO |
| 1 | C | 318 | PRO |
| 1 | B | 21 | VAL |
| 1 | B | 334 | GLY |
| 1 | B | 432 | GLY |
| 1 | B | 448 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|-----------|-------------|----|
| 1 | A | 410/410 (100%) | 335 (82%) | 75 (18%) | 1 | 8 |
| 1 | B | 410/410 (100%) | 343 (84%) | 67 (16%) | 2 | 12 |
| 1 | C | 410/410 (100%) | 349 (85%) | 61 (15%) | 2 | 15 |
| 2 | D | 64/64 (100%) | 53 (83%) | 11 (17%) | 1 | 11 |
| 2 | E | 64/64 (100%) | 52 (81%) | 12 (19%) | 1 | 8 |
| 2 | F | 64/64 (100%) | 55 (86%) | 9 (14%) | 3 | 17 |
| All | All | 1422/1422 (100%) | 1187 (84%) | 235 (16%) | 4 | 12 |

All (235) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 2 | ARG |
| 1 | A | 22 | ASP |
| 1 | A | 25 | LEU |
| 1 | A | 26 | GLU |
| 1 | A | 30 | CYS |
| 1 | A | 34 | MET |
| 1 | A | 38 | LYS |
| 1 | A | 42 | ASP |
| 1 | A | 43 | ILE |
| 1 | A | 58 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 74 | CYS |
| 1 | A | 83 | ASP |
| 1 | A | 92 | CYS |
| 1 | A | 96 | LEU |
| 1 | A | 99 | ARG |
| 1 | A | 101 | TRP |
| 1 | A | 113 | LEU |
| 1 | A | 119 | PHE |
| 1 | A | 124 | LYS |
| 1 | A | 132 | PRO |
| 1 | A | 135 | LEU |
| 1 | A | 148 | HIS |
| 1 | A | 152 | ILE |
| 1 | A | 161 | ASP |
| 1 | A | 162 | GLU |
| 1 | A | 163 | ASN |
| 1 | A | 167 | VAL |
| 1 | A | 177 | GLU |
| 1 | A | 180 | LEU |
| 1 | A | 186 | LEU |
| 1 | A | 188 | LEU |
| 1 | A | 189 | ASP |
| 1 | A | 193 | ARG |
| 1 | A | 204 | LEU |
| 1 | A | 205 | THR |
| 1 | A | 215 | LYS |
| 1 | A | 225 | TRP |
| 1 | A | 240 | GLU |
| 1 | A | 244 | GLU |
| 1 | A | 252 | ARG |
| 1 | A | 253 | GLN |
| 1 | A | 257 | VAL |
| 1 | A | 258 | LEU |
| 1 | A | 261 | GLN |
| 1 | A | 266 | HIS |
| 1 | A | 291 | CYS |
| 1 | A | 296 | ASP |
| 1 | A | 297 | LYS |
| 1 | A | 299 | ARG |
| 1 | A | 314 | PHE |
| 1 | A | 320 | GLU |
| 1 | A | 323 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 329 | GLU |
| 1 | A | 330 | VAL |
| 1 | A | 338 | PRO |
| 1 | A | 345 | MET |
| 1 | A | 348 | ASP |
| 1 | A | 349 | MET |
| 1 | A | 350 | GLN |
| 1 | A | 358 | LEU |
| 1 | A | 378 | LEU |
| 1 | A | 386 | TYR |
| 1 | A | 388 | VAL |
| 1 | A | 395 | LYS |
| 1 | A | 402 | ARG |
| 1 | A | 421 | MET |
| 1 | A | 438 | LEU |
| 1 | A | 439 | ASN |
| 1 | A | 443 | LYS |
| 1 | A | 446 | HIS |
| 1 | A | 454 | LYS |
| 1 | A | 456 | LEU |
| 1 | A | 464 | SER |
| 1 | A | 495 | LEU |
| 1 | A | 497 | PHE |
| 1 | C | 13 | GLU |
| 1 | C | 20 | TRP |
| 1 | C | 21 | VAL |
| 1 | C | 25 | LEU |
| 1 | C | 30 | CYS |
| 1 | C | 81 | TYR |
| 1 | C | 82 | LEU |
| 1 | C | 90 | TYR |
| 1 | C | 92 | CYS |
| 1 | C | 93 | LYS |
| 1 | C | 99 | ARG |
| 1 | C | 115 | THR |
| 1 | C | 118 | LYS |
| 1 | C | 124 | LYS |
| 1 | C | 125 | MET |
| 1 | C | 133 | GLU |
| 1 | C | 134 | ASN |
| 1 | C | 148 | HIS |
| 1 | C | 168 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 188 | LEU |
| 1 | C | 203 | TYR |
| 1 | C | 220 | ASP |
| 1 | C | 230 | ASP |
| 1 | C | 233 | THR |
| 1 | C | 234 | PRO |
| 1 | C | 240 | GLU |
| 1 | C | 253 | GLN |
| 1 | C | 260 | SER |
| 1 | C | 283 | ARG |
| 1 | C | 284 | LEU |
| 1 | C | 286 | SER |
| 1 | C | 292 | ARG |
| 1 | C | 293 | LEU |
| 1 | C | 296 | ASP |
| 1 | C | 299 | ARG |
| 1 | C | 300 | LEU |
| 1 | C | 301 | LYS |
| 1 | C | 308 | CYS |
| 1 | C | 316 | LYS |
| 1 | C | 318 | PRO |
| 1 | C | 327 | THR |
| 1 | C | 329 | GLU |
| 1 | C | 330 | VAL |
| 1 | C | 336 | ASP |
| 1 | C | 340 | LYS |
| 1 | C | 342 | PRO |
| 1 | C | 345 | MET |
| 1 | C | 351 | THR |
| 1 | C | 373 | LYS |
| 1 | C | 374 | MET |
| 1 | C | 375 | MET |
| 1 | C | 378 | LEU |
| 1 | C | 382 | PHE |
| 1 | C | 384 | ASP |
| 1 | C | 395 | LYS |
| 1 | C | 400 | TRP |
| 1 | C | 409 | LYS |
| 1 | C | 457 | PHE |
| 1 | C | 475 | LEU |
| 1 | C | 499 | SER |
| 1 | C | 500 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 3 | THR |
| 2 | D | 9 | THR |
| 2 | D | 10 | ARG |
| 2 | D | 12 | LEU |
| 2 | D | 18 | THR |
| 2 | D | 21 | GLU |
| 2 | D | 25 | TYR |
| 2 | D | 34 | ASN |
| 2 | D | 63 | TYR |
| 2 | D | 68 | LEU |
| 2 | D | 70 | ILE |
| 1 | B | 9 | ARG |
| 1 | B | 11 | PHE |
| 1 | B | 15 | MET |
| 1 | B | 19 | THR |
| 1 | B | 21 | VAL |
| 1 | B | 22 | ASP |
| 1 | B | 30 | CYS |
| 1 | B | 43 | ILE |
| 1 | B | 45 | LEU |
| 1 | B | 53 | MET |
| 1 | B | 76 | THR |
| 1 | B | 83 | ASP |
| 1 | B | 86 | SER |
| 1 | B | 88 | THR |
| 1 | B | 108 | PHE |
| 1 | B | 113 | LEU |
| 1 | B | 131 | GLN |
| 1 | B | 134 | ASN |
| 1 | B | 139 | ILE |
| 1 | B | 141 | LEU |
| 1 | B | 155 | ASP |
| 1 | B | 167 | VAL |
| 1 | B | 169 | ILE |
| 1 | B | 170 | THR |
| 1 | B | 174 | PRO |
| 1 | B | 175 | ARG |
| 1 | B | 180 | LEU |
| 1 | B | 196 | LEU |
| 1 | B | 201 | LEU |
| 1 | B | 210 | HIS |
| 1 | B | 211 | TRP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 216 | GLU |
| 1 | B | 221 | ILE |
| 1 | B | 225 | TRP |
| 1 | B | 226 | HIS |
| 1 | B | 230 | ASP |
| 1 | B | 237 | ASN |
| 1 | B | 240 | GLU |
| 1 | B | 258 | LEU |
| 1 | B | 269 | LEU |
| 1 | B | 281 | LYS |
| 1 | B | 283 | ARG |
| 1 | B | 284 | LEU |
| 1 | B | 288 | HIS |
| 1 | B | 289 | LEU |
| 1 | B | 307 | LEU |
| 1 | B | 318 | PRO |
| 1 | B | 325 | THR |
| 1 | B | 328 | VAL |
| 1 | B | 341 | VAL |
| 1 | B | 344 | GLN |
| 1 | B | 349 | MET |
| 1 | B | 352 | LEU |
| 1 | B | 353 | THR |
| 1 | B | 357 | ARG |
| 1 | B | 377 | GLU |
| 1 | B | 382 | PHE |
| 1 | B | 388 | VAL |
| 1 | B | 397 | THR |
| 1 | B | 414 | THR |
| 1 | B | 426 | ASP |
| 1 | B | 431 | PHE |
| 1 | B | 441 | LEU |
| 1 | B | 446 | HIS |
| 1 | B | 456 | LEU |
| 1 | B | 471 | LEU |
| 1 | B | 486 | LEU |
| 2 | E | 2 | VAL |
| 2 | E | 4 | LEU |
| 2 | E | 8 | SER |
| 2 | E | 10 | ARG |
| 2 | E | 12 | LEU |
| 2 | E | 17 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | E | 18 | THR |
| 2 | E | 19 | TRP |
| 2 | E | 20 | LEU |
| 2 | E | 38 | ARG |
| 2 | E | 49 | ILE |
| 2 | E | 53 | LEU |
| 2 | F | 2 | VAL |
| 2 | F | 12 | LEU |
| 2 | F | 20 | LEU |
| 2 | F | 34 | ASN |
| 2 | F | 38 | ARG |
| 2 | F | 61 | VAL |
| 2 | F | 62 | ILE |
| 2 | F | 63 | TYR |
| 2 | F | 66 | MET |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 8 | ASN |
| 1 | A | 85 | GLN |
| 1 | A | 89 | GLN |
| 1 | A | 131 | GLN |
| 1 | A | 134 | ASN |
| 1 | A | 147 | GLN |
| 1 | A | 207 | ASN |
| 1 | A | 253 | GLN |
| 1 | A | 261 | GLN |
| 1 | A | 331 | GLN |
| 1 | C | 85 | GLN |
| 1 | C | 134 | ASN |
| 1 | C | 144 | HIS |
| 1 | C | 207 | ASN |
| 1 | C | 210 | HIS |
| 1 | C | 237 | ASN |
| 1 | C | 253 | GLN |
| 1 | C | 261 | GLN |
| 1 | C | 344 | GLN |
| 1 | B | 27 | HIS |
| 1 | B | 77 | GLN |
| 1 | B | 103 | ASN |
| 1 | B | 134 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 144 | HIS |
| 1 | B | 147 | GLN |
| 1 | B | 158 | HIS |
| 1 | B | 208 | ASN |
| 1 | B | 261 | GLN |
| 1 | B | 323 | HIS |
| 1 | B | 362 | ASN |
| 1 | B | 439 | ASN |
| 2 | E | 7 | HIS |
| 2 | E | 28 | HIS |
| 2 | F | 34 | 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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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 | NAG | C | 601 | 1 | 14,14,15 | 1.12 | 2 (14%) | 17,19,21 | 0.91 | 0 |
| 3 | NAG | B | 601 | 1 | 14,14,15 | 0.67 | 0 | 17,19,21 | 0.66 | 0 |
| 3 | NAG | A | 601 | 1 | 14,14,15 | 1.04 | 0 | 17,19,21 | 0.96 | 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 | NAG | C | 601 | 1 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | B | 601 | 1 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | NAG | A | 601 | 1 | - | 4/6/23/26 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3 | C | 601 | NAG | C1-C2 | 2.95 | 1.56 | 1.52 |
| 3 | C | 601 | NAG | C3-C2 | 2.31 | 1.57 | 1.52 |

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 3 | A | 601 | NAG | C8-C7-N2-C2 |
| 3 | A | 601 | NAG | O7-C7-N2-C2 |
| 3 | C | 601 | NAG | C8-C7-N2-C2 |
| 3 | C | 601 | NAG | O7-C7-N2-C2 |
| 3 | B | 601 | NAG | C8-C7-N2-C2 |
| 3 | B | 601 | NAG | O7-C7-N2-C2 |
| 3 | C | 601 | NAG | O5-C5-C6-O6 |
| 3 | B | 601 | NAG | O5-C5-C6-O6 |
| 3 | A | 601 | NAG | O5-C5-C6-O6 |
| 3 | A | 601 | NAG | C4-C5-C6-O6 |
| 3 | C | 601 | NAG | C4-C5-C6-O6 |

There are no ring outliers.

3 monomers are involved in 10 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3 | C | 601 | NAG | 5 | 0 |
| 3 | B | 601 | NAG | 1 | 0 |
| 3 | A | 601 | NAG | 4 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

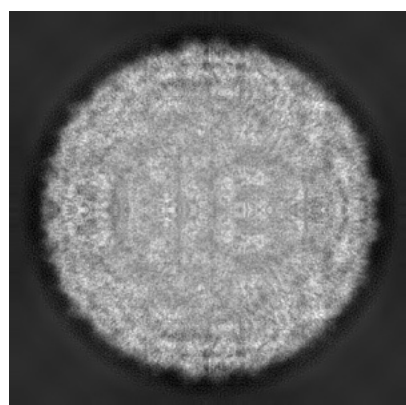
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8139. These allow visual inspection of the internal detail of the map and identification of artifacts.

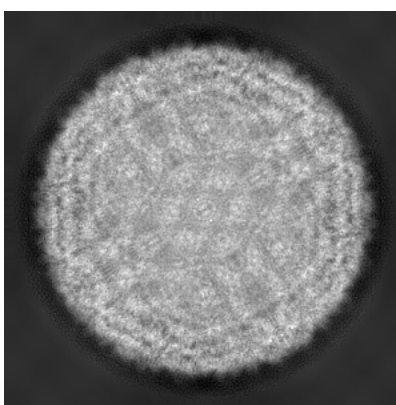
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

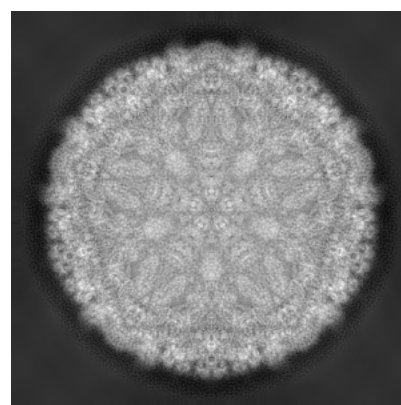
6.1.1 Primary map



X



Y

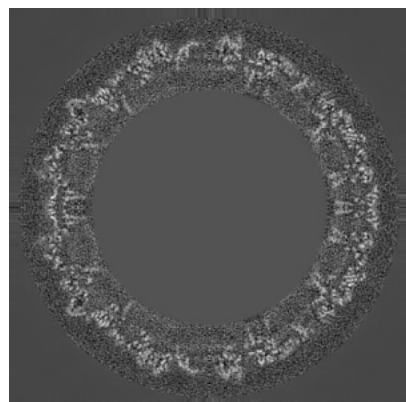


Z

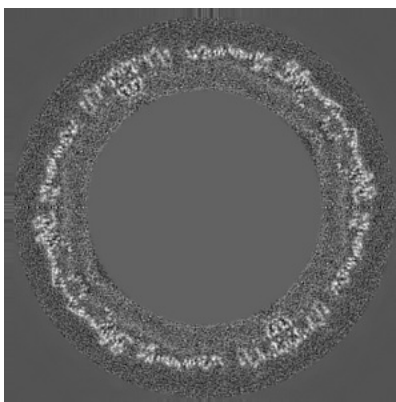
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

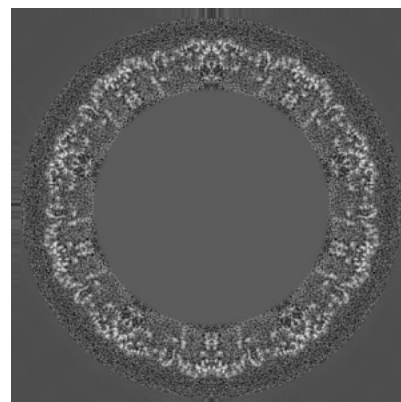
6.2.1 Primary map



X Index: 200



Y Index: 200

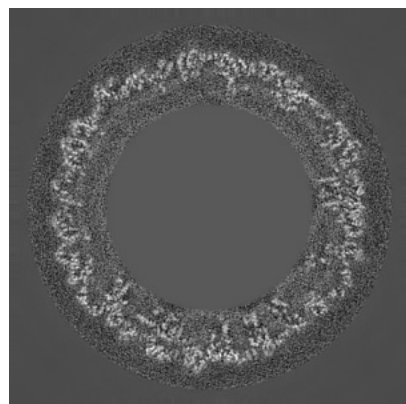


Z Index: 200

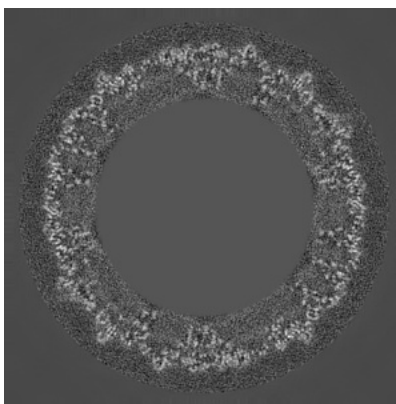
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

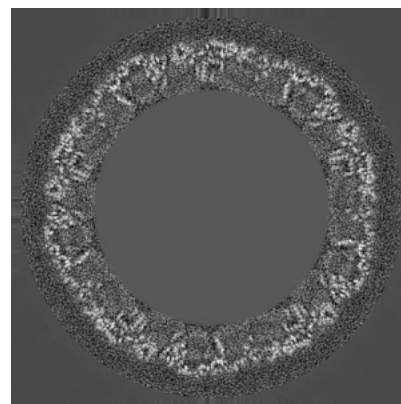
6.3.1 Primary map



X Index: 256



Y Index: 156

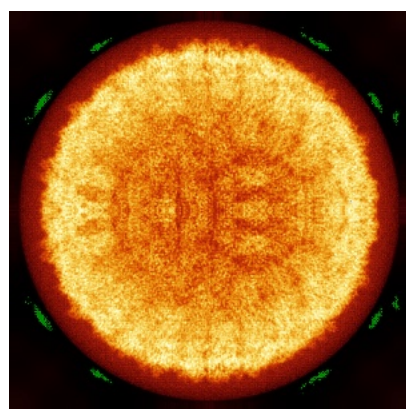


Z Index: 194

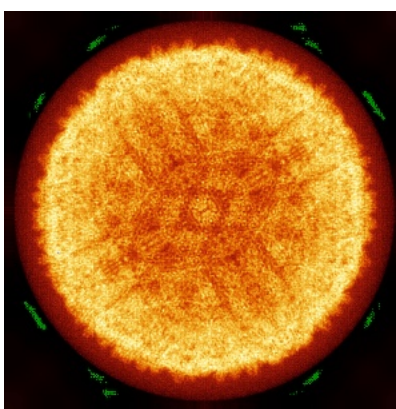
The images above show the largest variance slices of the map in three orthogonal directions.

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

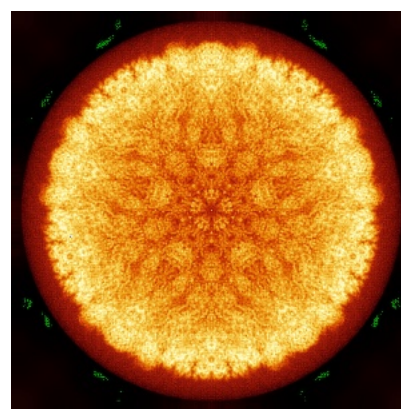
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

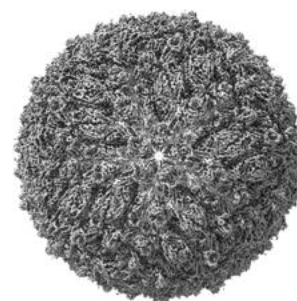
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

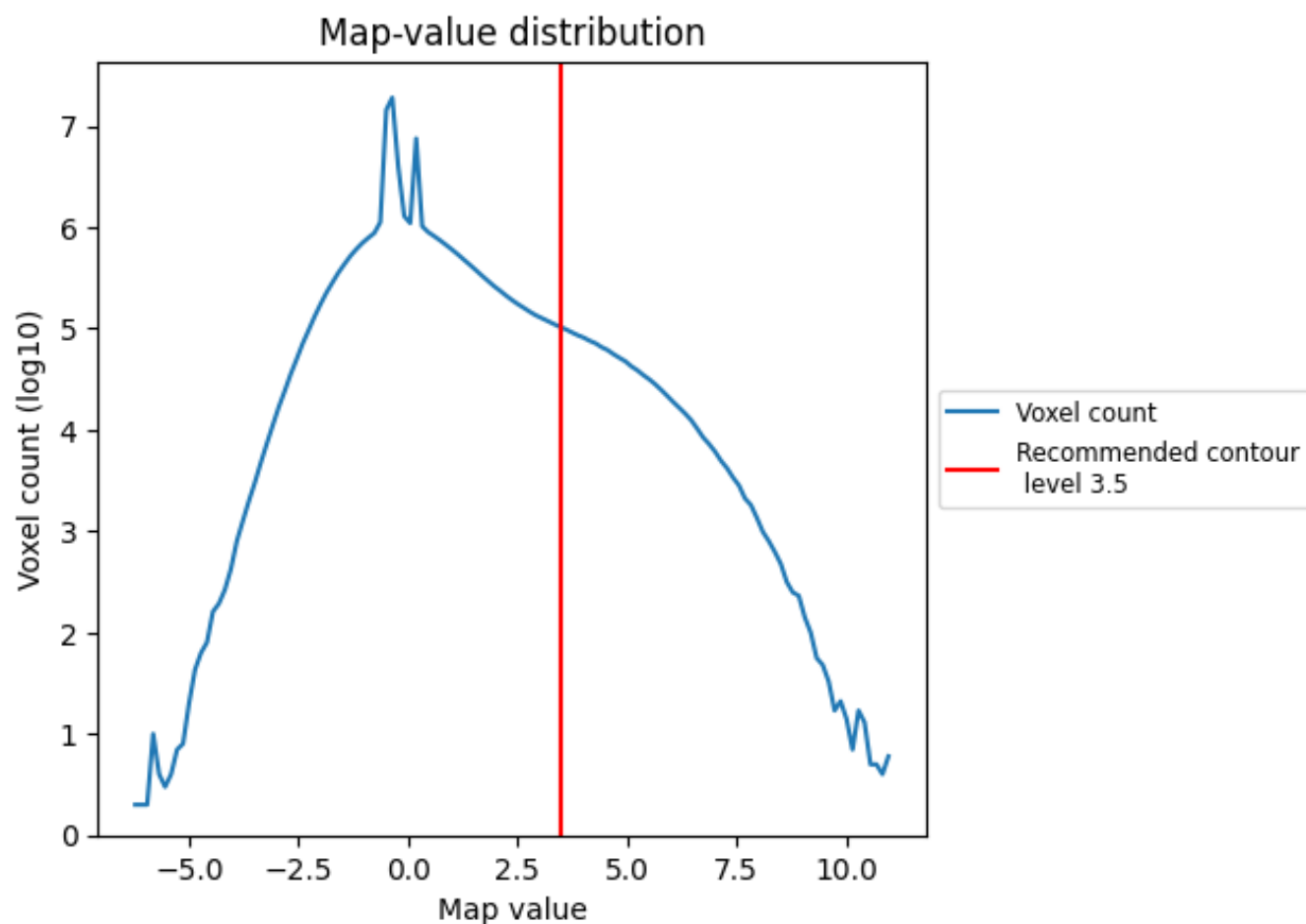
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

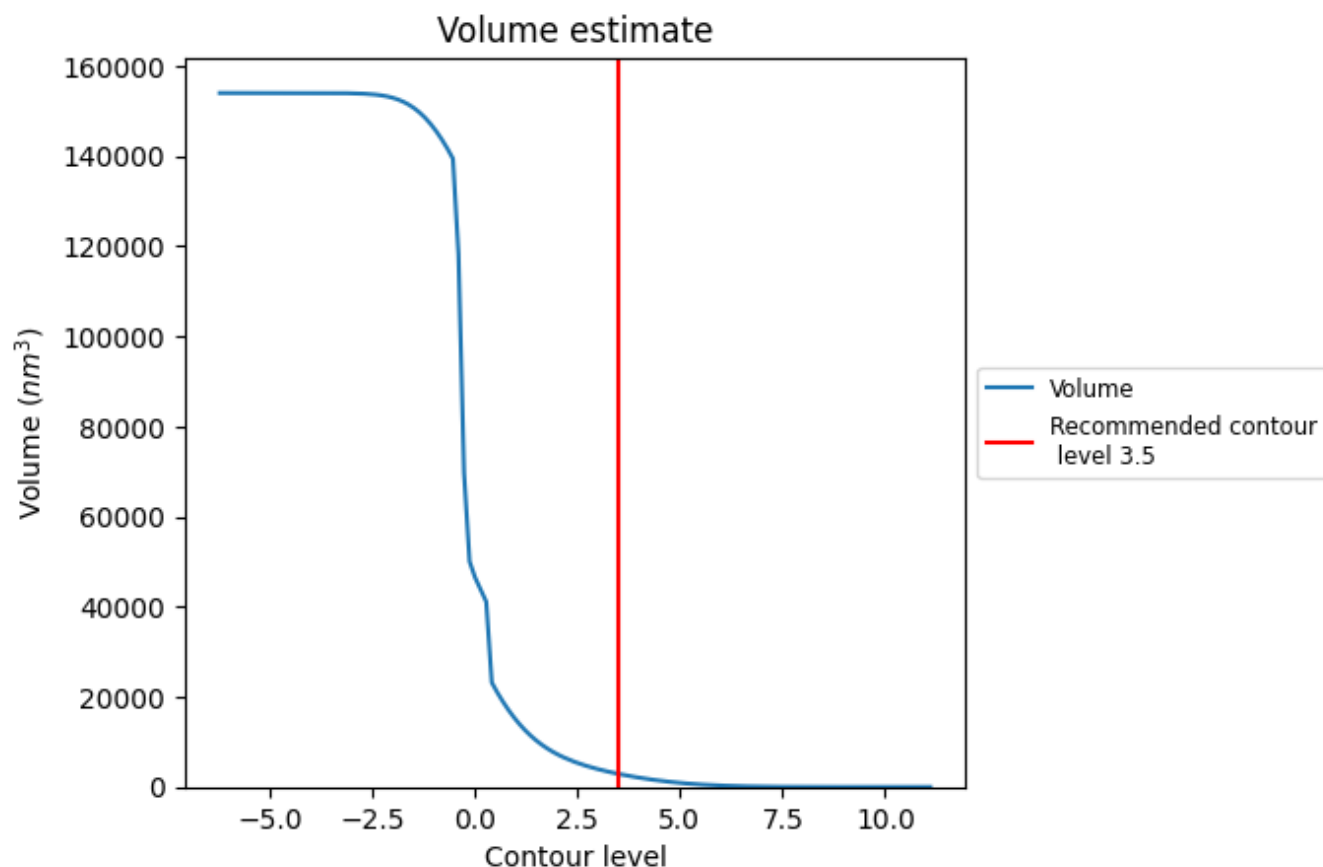
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

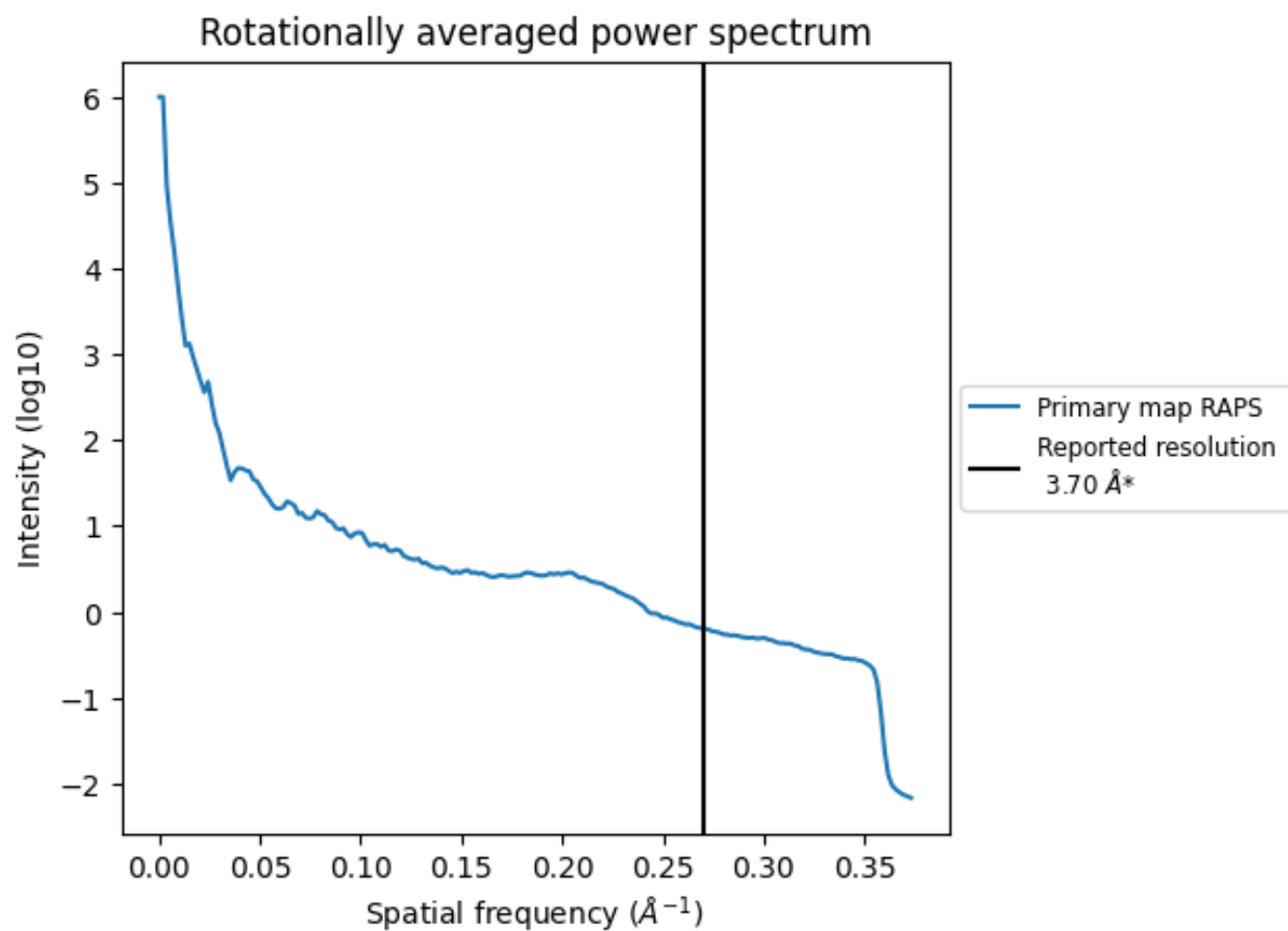
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2891 nm³; this corresponds to an approximate mass of 2612 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation ⓘ

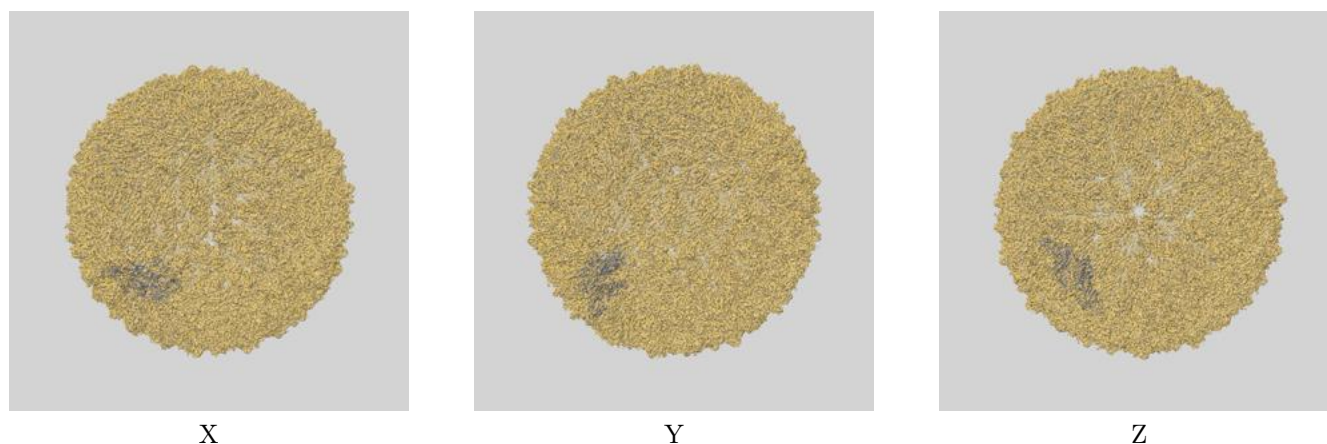
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

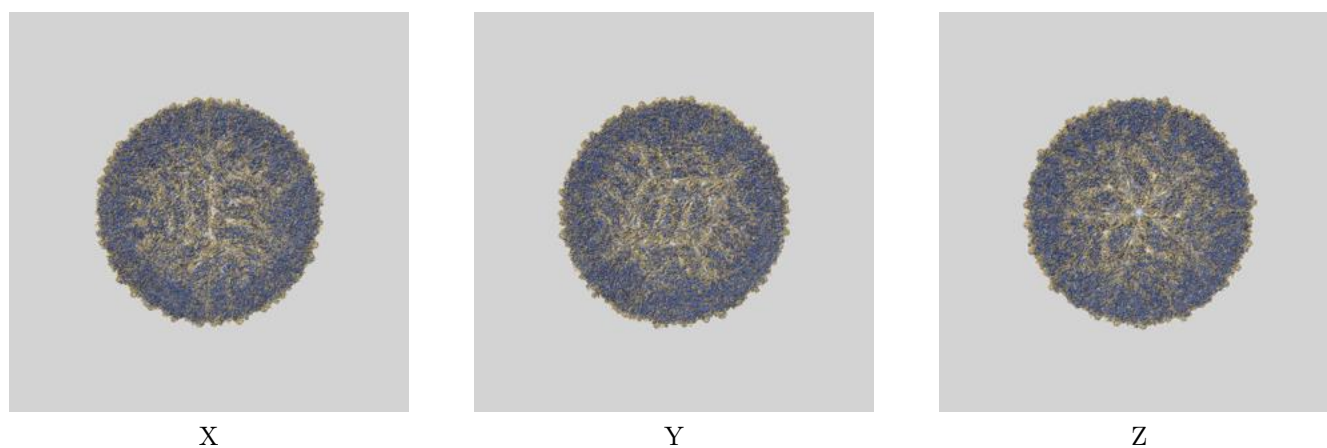
This section contains information regarding the fit between EMDB map EMD-8139 and PDB model 5IZ7. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

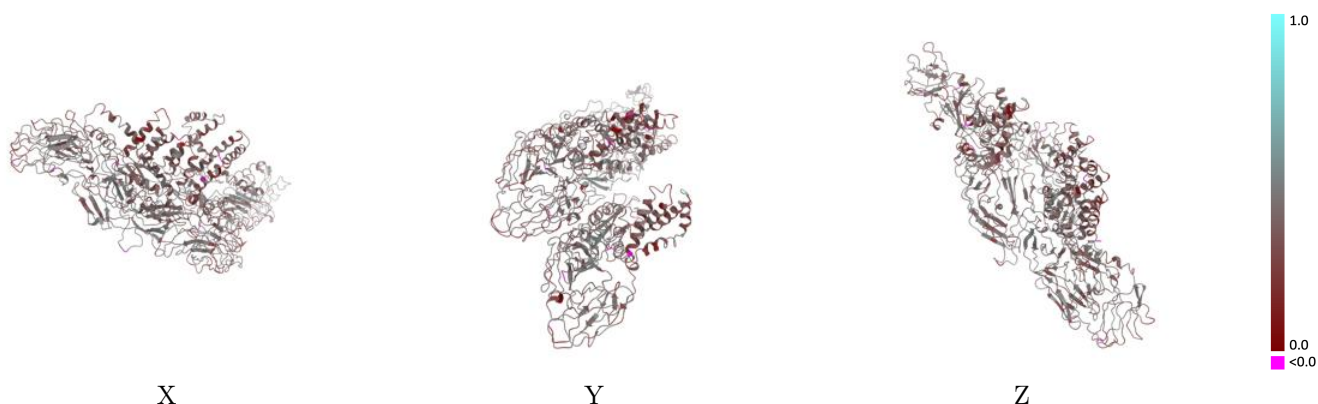


9.1.2 Map-model assembly overlay [i](#)



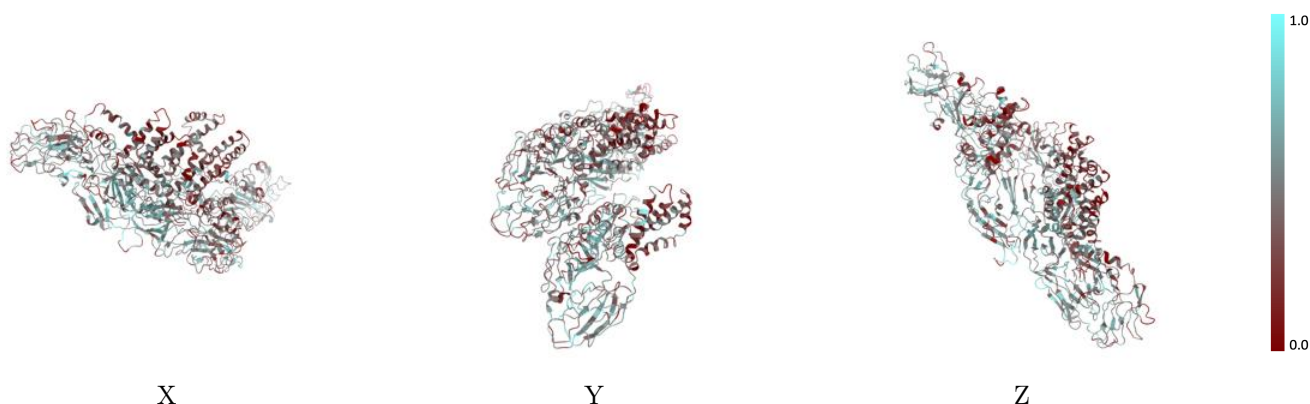
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



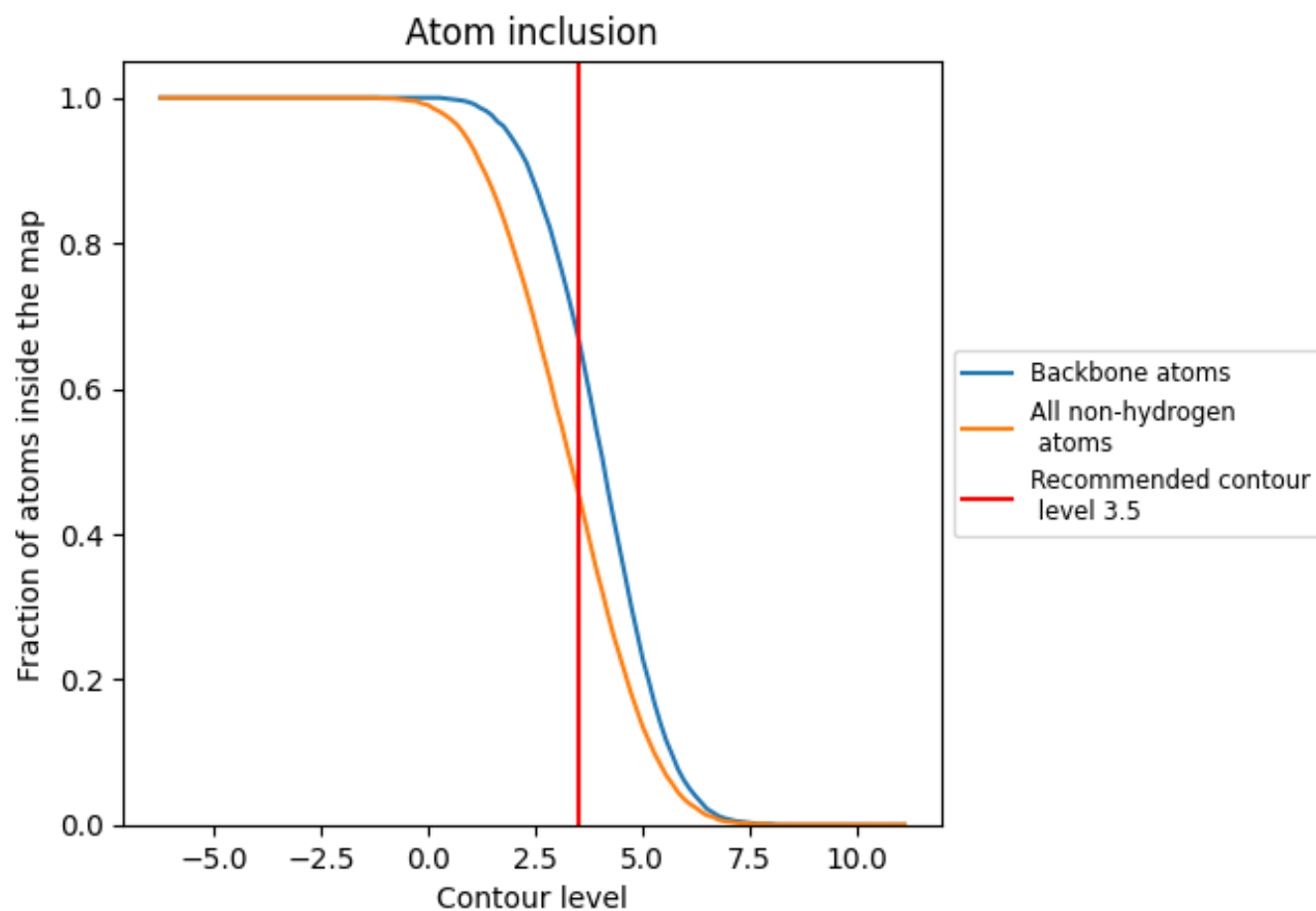
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|-------------------------------|-------------------------------|
| All | <div><div></div></div> 0.4580 | <div><div></div></div> 0.3870 |
| A | <div><div></div></div> 0.4700 | <div><div></div></div> 0.3950 |
| B | <div><div></div></div> 0.4880 | <div><div></div></div> 0.3910 |
| C | <div><div></div></div> 0.4510 | <div><div></div></div> 0.3860 |
| D | <div><div></div></div> 0.3920 | <div><div></div></div> 0.3770 |
| E | <div><div></div></div> 0.3750 | <div><div></div></div> 0.3420 |
| F | <div><div></div></div> 0.3960 | <div><div></div></div> 0.3710 |

1.0

0.0

<0.0