



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:11 AM GMT

PDB ID : 3HI8
Title : Crystal structure of proliferating cell nuclear antigen (PCNA) from *Haloferax volcanii*
Authors : Morgunova, E.; Gray, F.C.; MacNeill S.A.; Ladenstein, R.
Deposited on : 2009-05-19
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

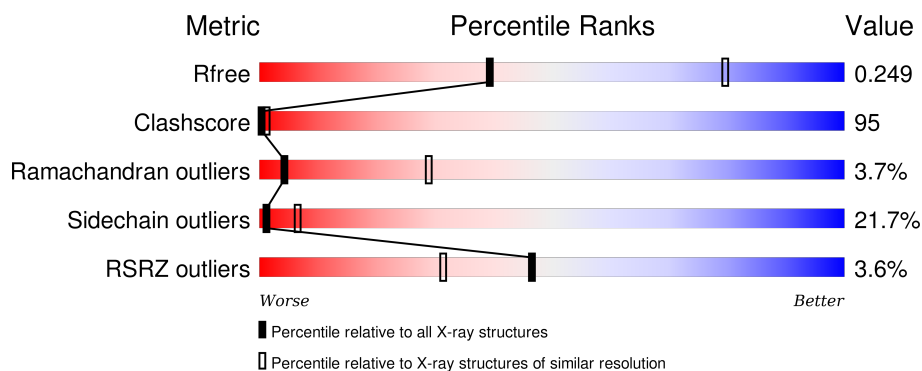
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1124 (3.24-3.16) |
| Clashscore | 102246 | 1024 (3.22-3.18) |
| Ramachandran outliers | 100387 | 1004 (3.22-3.18) |
| Sidechain outliers | 100360 | 1003 (3.22-3.18) |
| RSRZ outliers | 91569 | 1129 (3.24-3.16) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 247 | <div> <div>4%</div> <div>23%</div> <div>59%</div> <div>14%</div> <div>.</div> </div> |
| 1 | B | 247 | <div> <div>4%</div> <div>22%</div> <div>60%</div> <div>14%</div> <div>.</div> </div> |
| 1 | C | 247 | <div> <div>3%</div> <div>22%</div> <div>60%</div> <div>14%</div> <div>.</div> </div> |
| 1 | D | 247 | <div> <div>5%</div> <div>23%</div> <div>60%</div> <div>14%</div> <div>.</div> </div> |
| 1 | E | 247 | <div> <div>3%</div> <div>23%</div> <div>60%</div> <div>14%</div> <div>.</div> </div> |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | F | 247 | <div><div></div><div>2%</div><div>23%</div><div>59%</div><div>14%</div><div></div></div> |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11245 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proliferating cell nuclear antigen PcnA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 247 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1869 | 1167 | 308 | 386 | 8 | | | |
| 1 | B | 247 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1869 | 1167 | 308 | 386 | 8 | | | |
| 1 | C | 247 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1869 | 1167 | 308 | 386 | 8 | | | |
| 1 | D | 247 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1869 | 1167 | 308 | 386 | 8 | | | |
| 1 | E | 247 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1869 | 1167 | 308 | 386 | 8 | | | |
| 1 | F | 247 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1869 | 1167 | 308 | 386 | 8 | | | |

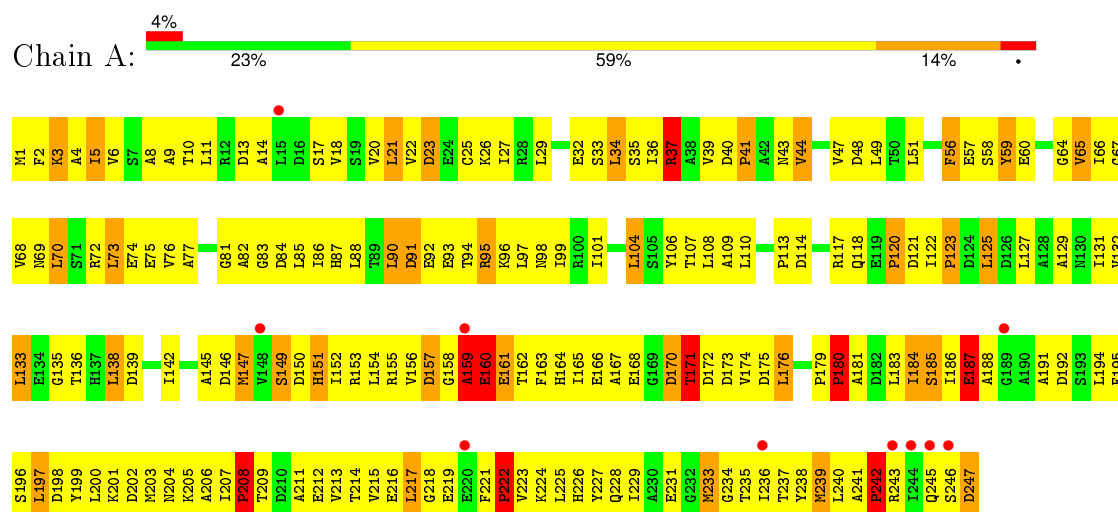
- Molecule 2 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 2 | A | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 2 | B | 3 | Total | O | 0 | 0 |
| | | | 3 | 3 | | |
| 2 | C | 2 | Total | O | 0 | 0 |
| | | | 2 | 2 | | |
| 2 | D | 7 | Total | O | 0 | 0 |
| | | | 7 | 7 | | |
| 2 | E | 5 | Total | O | 0 | 0 |
| | | | 5 | 5 | | |
| 2 | F | 9 | Total | O | 0 | 0 |
| | | | 9 | 9 | | |

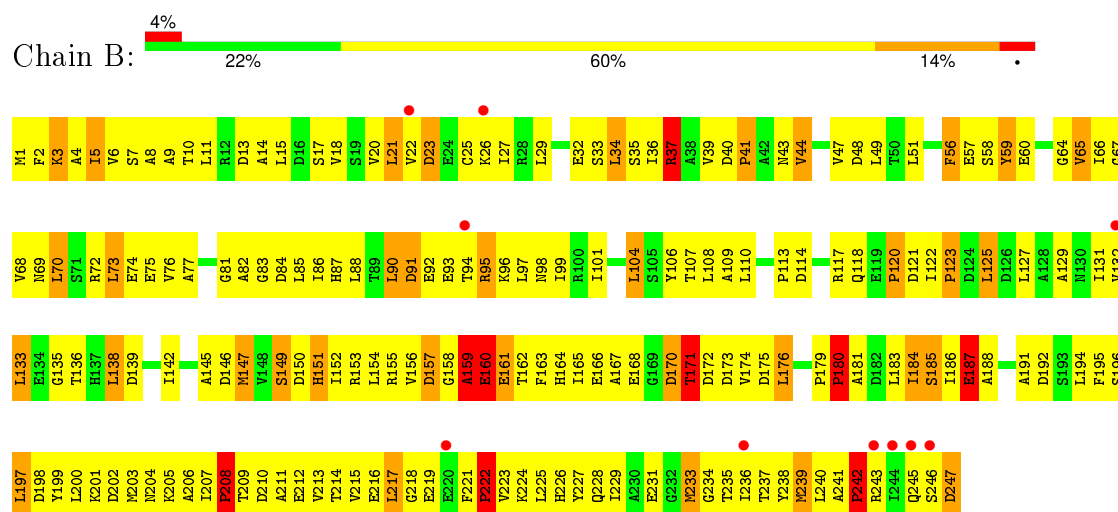
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Proliferating cell nuclear antigen PcnA

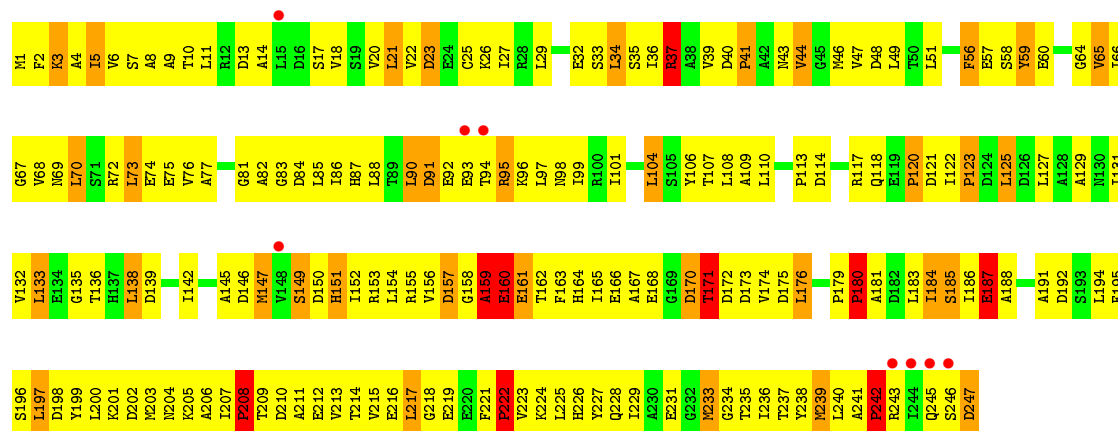


• Molecule 1: Proliferating cell nuclear antigen PcnA

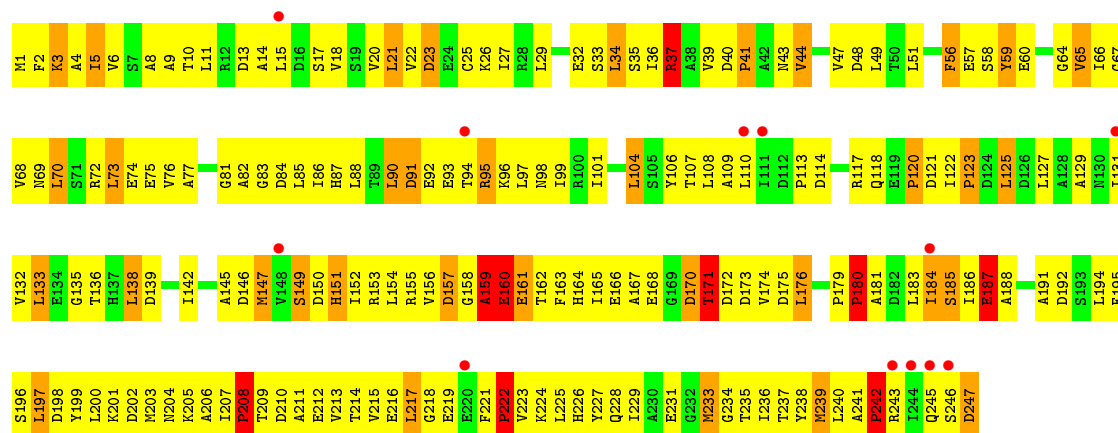


• Molecule 1: Proliferating cell nuclear antigen PcnA

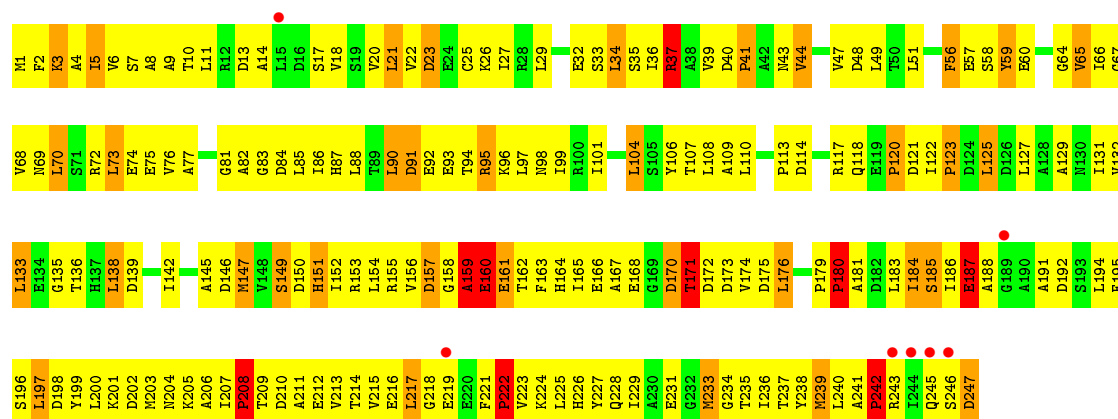




• Molecule 1: Proliferating cell nuclear antigen Pcna



• Molecule 1: Proliferating cell nuclear antigen Pcna



• Molecule 1: Proliferating cell nuclear antigen Pcna





4 Data and refinement statistics

| Property | Value | Source |
|---|--|------------------|
| Space group | C 1 2 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 174.44Å 123.24Å 123.26Å 90.00° 135.00° 90.00° | Depositor |
| Resolution (Å) | 32.95 – 3.20 32.96 – 3.20 | Depositor EDS |
| % Data completeness (in resolution range) | 86.6 (32.95-3.20) 86.5 (32.96-3.20) | Depositor EDS |
| R_{merge} | 0.12 | Depositor |
| R_{sym} | 0.12 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.19 (at 3.18Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, R_{free} | 0.237 , 0.250 0.236 , 0.249 | Depositor DCC |
| R_{free} test set | 1324 reflections (5.02%) | DCC |
| Wilson B-factor (Å ²) | 138.1 | Xtriage |
| Anisotropy | 0.037 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.23 , 88.6 | EDS |
| Estimated twinning fraction | 0.357 for -h-2*k,l,h+1 0.348 for k+1,h+1,-l 0.357 for -k+1,-h-1,-l 0.349 for -h-k-1,l,k 0.349 for -h+k-1,-l,-k 0.347 for -h-k-1,-l,h+1 0.347 for k+1,-h-1,-k 0.348 for -h+k-1,l,h+1 0.349 for -k+1,h+1,k 0.357 for -h,-k,h+1 0.358 for -h-2*k,-k,l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$ | Xtriage |
| Outliers | 0 of 26380 reflections | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 11245 | wwPDB-VP |
| Average B, all atoms (Å ²) | 139.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 | 0.71 | 0/1893 | 1.20 | 11/2572 (0.4%) |
| 1 | B | 0.71 | 0/1893 | 1.20 | 11/2572 (0.4%) |
| 1 | C | 0.71 | 0/1893 | 1.20 | 11/2572 (0.4%) |
| 1 | D | 0.71 | 0/1893 | 1.20 | 11/2572 (0.4%) |
| 1 | E | 0.71 | 0/1893 | 1.20 | 11/2572 (0.4%) |
| 1 | F | 0.71 | 0/1893 | 1.20 | 11/2572 (0.4%) |
| All | All | 0.71 | 0/11358 | 1.20 | 66/15432 (0.4%) |

There are no bond length outliers.

All (66) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | D | 180 | PRO | CA-N-CD | -14.39 | 91.35 | 111.50 |
| 1 | F | 180 | PRO | CA-N-CD | -14.37 | 91.38 | 111.50 |
| 1 | C | 180 | PRO | CA-N-CD | -14.37 | 91.39 | 111.50 |
| 1 | A | 180 | PRO | CA-N-CD | -14.36 | 91.39 | 111.50 |
| 1 | E | 180 | PRO | CA-N-CD | -14.35 | 91.41 | 111.50 |
| 1 | B | 180 | PRO | CA-N-CD | -14.35 | 91.41 | 111.50 |
| 1 | E | 120 | PRO | CA-N-CD | -13.38 | 92.77 | 111.50 |
| 1 | A | 120 | PRO | CA-N-CD | -13.36 | 92.80 | 111.50 |
| 1 | F | 120 | PRO | CA-N-CD | -13.35 | 92.81 | 111.50 |
| 1 | D | 120 | PRO | CA-N-CD | -13.35 | 92.81 | 111.50 |
| 1 | B | 120 | PRO | CA-N-CD | -13.35 | 92.82 | 111.50 |
| 1 | C | 120 | PRO | CA-N-CD | -13.33 | 92.83 | 111.50 |
| 1 | D | 242 | PRO | CA-N-CD | -10.54 | 96.75 | 111.50 |
| 1 | F | 242 | PRO | CA-N-CD | -10.53 | 96.76 | 111.50 |
| 1 | E | 242 | PRO | CA-N-CD | -10.53 | 96.76 | 111.50 |
| 1 | C | 242 | PRO | CA-N-CD | -10.52 | 96.78 | 111.50 |
| 1 | A | 242 | PRO | CA-N-CD | -10.51 | 96.79 | 111.50 |
| 1 | B | 242 | PRO | CA-N-CD | -10.51 | 96.79 | 111.50 |
| 1 | B | 171 | THR | CA-CB-OG1 | 10.40 | 130.84 | 109.00 |
| 1 | D | 171 | THR | CA-CB-OG1 | 10.40 | 130.83 | 109.00 |
| 1 | C | 171 | THR | CA-CB-OG1 | 10.39 | 130.82 | 109.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | E | 171 | THR | CA-CB-OG1 | 10.38 | 130.79 | 109.00 |
| 1 | F | 171 | THR | CA-CB-OG1 | 10.38 | 130.79 | 109.00 |
| 1 | A | 171 | THR | CA-CB-OG1 | 10.37 | 130.77 | 109.00 |
| 1 | E | 222 | PRO | CA-N-CD | -10.13 | 97.32 | 111.50 |
| 1 | B | 222 | PRO | CA-N-CD | -10.13 | 97.32 | 111.50 |
| 1 | F | 222 | PRO | CA-N-CD | -10.12 | 97.33 | 111.50 |
| 1 | D | 222 | PRO | CA-N-CD | -10.10 | 97.36 | 111.50 |
| 1 | A | 222 | PRO | CA-N-CD | -10.10 | 97.36 | 111.50 |
| 1 | C | 222 | PRO | CA-N-CD | -10.10 | 97.36 | 111.50 |
| 1 | F | 208 | PRO | CA-N-CD | -9.94 | 97.58 | 111.50 |
| 1 | D | 208 | PRO | CA-N-CD | -9.93 | 97.60 | 111.50 |
| 1 | C | 208 | PRO | CA-N-CD | -9.93 | 97.60 | 111.50 |
| 1 | B | 208 | PRO | CA-N-CD | -9.92 | 97.61 | 111.50 |
| 1 | A | 208 | PRO | CA-N-CD | -9.91 | 97.62 | 111.50 |
| 1 | E | 208 | PRO | CA-N-CD | -9.90 | 97.64 | 111.50 |
| 1 | F | 41 | PRO | CA-N-CD | -9.85 | 97.70 | 111.50 |
| 1 | E | 41 | PRO | CA-N-CD | -9.84 | 97.73 | 111.50 |
| 1 | D | 41 | PRO | CA-N-CD | -9.84 | 97.73 | 111.50 |
| 1 | A | 41 | PRO | CA-N-CD | -9.83 | 97.74 | 111.50 |
| 1 | C | 41 | PRO | CA-N-CD | -9.81 | 97.76 | 111.50 |
| 1 | B | 41 | PRO | CA-N-CD | -9.81 | 97.76 | 111.50 |
| 1 | E | 160 | GLU | CB-CA-C | 7.18 | 124.76 | 110.40 |
| 1 | C | 160 | GLU | CB-CA-C | 7.17 | 124.74 | 110.40 |
| 1 | A | 160 | GLU | CB-CA-C | 7.17 | 124.73 | 110.40 |
| 1 | F | 160 | GLU | CB-CA-C | 7.16 | 124.73 | 110.40 |
| 1 | B | 160 | GLU | CB-CA-C | 7.16 | 124.72 | 110.40 |
| 1 | D | 160 | GLU | CB-CA-C | 7.16 | 124.72 | 110.40 |
| 1 | B | 123 | PRO | CB-CA-C | 5.91 | 126.78 | 112.00 |
| 1 | A | 123 | PRO | CB-CA-C | 5.91 | 126.77 | 112.00 |
| 1 | D | 123 | PRO | CB-CA-C | 5.91 | 126.77 | 112.00 |
| 1 | C | 123 | PRO | CB-CA-C | 5.90 | 126.76 | 112.00 |
| 1 | E | 123 | PRO | CB-CA-C | 5.90 | 126.76 | 112.00 |
| 1 | F | 123 | PRO | CB-CA-C | 5.90 | 126.74 | 112.00 |
| 1 | D | 159 | ALA | O-C-N | 5.53 | 131.54 | 122.70 |
| 1 | A | 159 | ALA | O-C-N | 5.52 | 131.54 | 122.70 |
| 1 | C | 159 | ALA | O-C-N | 5.51 | 131.52 | 122.70 |
| 1 | F | 159 | ALA | O-C-N | 5.51 | 131.52 | 122.70 |
| 1 | E | 159 | ALA | O-C-N | 5.50 | 131.50 | 122.70 |
| 1 | B | 159 | ALA | O-C-N | 5.50 | 131.49 | 122.70 |
| 1 | E | 187 | GLU | N-CA-C | -5.26 | 96.80 | 111.00 |
| 1 | A | 187 | GLU | N-CA-C | -5.25 | 96.82 | 111.00 |
| 1 | D | 187 | GLU | N-CA-C | -5.25 | 96.82 | 111.00 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | F | 187 | GLU | N-CA-C | -5.25 | 96.83 | 111.00 |
| 1 | C | 187 | GLU | N-CA-C | -5.24 | 96.84 | 111.00 |
| 1 | B | 187 | GLU | N-CA-C | -5.24 | 96.86 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1869 | 0 | 1847 | 373 | 0 |
| 1 | B | 1869 | 0 | 1847 | 377 | 0 |
| 1 | C | 1869 | 0 | 1847 | 372 | 0 |
| 1 | D | 1869 | 0 | 1847 | 374 | 0 |
| 1 | E | 1869 | 0 | 1847 | 365 | 0 |
| 1 | F | 1869 | 0 | 1847 | 358 | 0 |
| 2 | A | 5 | 0 | 0 | 0 | 0 |
| 2 | B | 3 | 0 | 0 | 0 | 0 |
| 2 | C | 2 | 0 | 0 | 0 | 0 |
| 2 | D | 7 | 0 | 0 | 0 | 0 |
| 2 | E | 5 | 0 | 0 | 0 | 0 |
| 2 | F | 9 | 0 | 0 | 0 | 0 |
| All | All | 11245 | 0 | 11082 | 2123 | 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 95.

All (2123) 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:A:149:SER:CB | 1:A:167:ALA:HB1 | 1.53 | 1.38 |
| 1:B:149:SER:CB | 1:B:167:ALA:HB1 | 1.53 | 1.37 |
| 1:C:149:SER:CB | 1:C:167:ALA:HB1 | 1.53 | 1.36 |
| 1:F:149:SER:CB | 1:F:167:ALA:HB1 | 1.53 | 1.35 |
| 1:E:149:SER:CB | 1:E:167:ALA:HB1 | 1.53 | 1.35 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:149:SER:CB | 1:D:167:ALA:HB1 | 1.53 | 1.35 |
| 1:D:156:VAL:HB | 1:D:191:ALA:O | 1.25 | 1.33 |
| 1:A:150:ASP:O | 1:A:197:LEU:HD22 | 1.28 | 1.32 |
| 1:B:150:ASP:O | 1:B:197:LEU:HD22 | 1.28 | 1.31 |
| 1:C:156:VAL:HB | 1:C:191:ALA:O | 1.25 | 1.31 |
| 1:F:95:ARG:O | 1:F:109:ALA:HA | 1.29 | 1.30 |
| 1:C:150:ASP:O | 1:C:197:LEU:HD22 | 1.28 | 1.30 |
| 1:F:150:ASP:O | 1:F:197:LEU:HD22 | 1.28 | 1.29 |
| 1:A:156:VAL:HB | 1:A:191:ALA:O | 1.25 | 1.29 |
| 1:D:8:ALA:HB3 | 1:D:82:ALA:O | 1.32 | 1.29 |
| 1:E:95:ARG:O | 1:E:109:ALA:HA | 1.29 | 1.29 |
| 1:A:8:ALA:HB3 | 1:A:82:ALA:O | 1.32 | 1.29 |
| 1:E:156:VAL:HB | 1:E:191:ALA:O | 1.25 | 1.29 |
| 1:A:95:ARG:O | 1:A:109:ALA:HA | 1.29 | 1.28 |
| 1:D:150:ASP:O | 1:D:197:LEU:HD22 | 1.28 | 1.28 |
| 1:B:156:VAL:HB | 1:B:191:ALA:O | 1.25 | 1.27 |
| 1:E:8:ALA:HB3 | 1:E:82:ALA:O | 1.33 | 1.26 |
| 1:E:150:ASP:O | 1:E:197:LEU:HD22 | 1.28 | 1.26 |
| 1:D:95:ARG:O | 1:D:109:ALA:HA | 1.29 | 1.25 |
| 1:D:72:ARG:HH12 | 1:F:171:THR:CG2 | 1.48 | 1.25 |
| 1:B:47:VAL:HA | 1:B:237:THR:O | 1.36 | 1.25 |
| 1:C:8:ALA:HB3 | 1:C:82:ALA:O | 1.32 | 1.25 |
| 1:C:47:VAL:HA | 1:C:237:THR:O | 1.36 | 1.25 |
| 1:C:95:ARG:O | 1:C:109:ALA:HA | 1.29 | 1.25 |
| 1:F:8:ALA:HB3 | 1:F:82:ALA:O | 1.32 | 1.24 |
| 1:F:156:VAL:HB | 1:F:191:ALA:O | 1.25 | 1.24 |
| 1:B:8:ALA:HB3 | 1:B:82:ALA:O | 1.32 | 1.24 |
| 1:B:95:ARG:O | 1:B:109:ALA:HA | 1.29 | 1.24 |
| 1:D:47:VAL:HA | 1:D:237:THR:O | 1.36 | 1.23 |
| 1:B:171:THR:CG2 | 1:C:72:ARG:HH12 | 1.50 | 1.22 |
| 1:E:47:VAL:HA | 1:E:237:THR:O | 1.36 | 1.21 |
| 1:E:171:THR:CG2 | 1:F:72:ARG:HH12 | 1.54 | 1.20 |
| 1:A:23:ASP:O | 1:A:70:LEU:HB3 | 1.03 | 1.20 |
| 1:F:47:VAL:HA | 1:F:237:THR:O | 1.36 | 1.19 |
| 1:A:72:ARG:HH12 | 1:C:171:THR:CG2 | 1.55 | 1.18 |
| 1:A:47:VAL:HA | 1:A:237:THR:O | 1.36 | 1.18 |
| 1:C:195:PHE:CE2 | 1:C:242:PRO:HD3 | 1.79 | 1.18 |
| 1:C:23:ASP:O | 1:C:70:LEU:HB3 | 1.03 | 1.18 |
| 1:B:23:ASP:O | 1:B:70:LEU:HB3 | 1.03 | 1.18 |
| 1:E:23:ASP:O | 1:E:70:LEU:HB3 | 1.03 | 1.17 |
| 1:D:23:ASP:O | 1:D:70:LEU:HB3 | 1.03 | 1.17 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:195:PHE:CE2 | 1:A:242:PRO:HD3 | 1.79 | 1.17 |
| 1:F:23:ASP:O | 1:F:70:LEU:HB3 | 1.03 | 1.17 |
| 1:D:195:PHE:CE2 | 1:D:242:PRO:HD3 | 1.79 | 1.17 |
| 1:A:195:PHE:HE2 | 1:A:242:PRO:HD3 | 1.00 | 1.17 |
| 1:F:222:PRO:HD3 | 1:F:242:PRO:HG2 | 1.23 | 1.17 |
| 1:E:195:PHE:CE2 | 1:E:242:PRO:HD3 | 1.79 | 1.16 |
| 1:A:171:THR:CG2 | 1:B:72:ARG:HH12 | 1.57 | 1.16 |
| 1:A:222:PRO:HD3 | 1:A:242:PRO:CG | 1.75 | 1.16 |
| 1:F:195:PHE:CE2 | 1:F:242:PRO:HD3 | 1.79 | 1.16 |
| 1:F:222:PRO:HD3 | 1:F:242:PRO:CG | 1.75 | 1.16 |
| 1:D:171:THR:CG2 | 1:E:72:ARG:HH12 | 1.57 | 1.16 |
| 1:B:195:PHE:CE2 | 1:B:242:PRO:HD3 | 1.79 | 1.16 |
| 1:E:222:PRO:HD3 | 1:E:242:PRO:CG | 1.75 | 1.16 |
| 1:F:8:ALA:HB1 | 1:F:81:GLY:O | 1.46 | 1.16 |
| 1:B:222:PRO:HD3 | 1:B:242:PRO:CG | 1.75 | 1.15 |
| 1:C:222:PRO:HD3 | 1:C:242:PRO:CG | 1.75 | 1.15 |
| 1:A:8:ALA:HB1 | 1:A:81:GLY:O | 1.46 | 1.15 |
| 1:D:222:PRO:HD3 | 1:D:242:PRO:CG | 1.75 | 1.15 |
| 1:E:2:PHE:O | 1:E:88:LEU:O | 1.66 | 1.14 |
| 1:B:2:PHE:O | 1:B:88:LEU:O | 1.66 | 1.14 |
| 1:F:2:PHE:O | 1:F:88:LEU:O | 1.66 | 1.14 |
| 1:C:222:PRO:HD3 | 1:C:242:PRO:HG2 | 1.23 | 1.13 |
| 1:E:195:PHE:HE2 | 1:E:242:PRO:HD3 | 1.00 | 1.13 |
| 1:E:149:SER:HB2 | 1:E:167:ALA:HB1 | 1.15 | 1.13 |
| 1:F:23:ASP:O | 1:F:70:LEU:CB | 1.97 | 1.13 |
| 1:C:2:PHE:O | 1:C:88:LEU:O | 1.66 | 1.13 |
| 1:B:23:ASP:O | 1:B:70:LEU:CB | 1.97 | 1.13 |
| 1:A:23:ASP:O | 1:A:70:LEU:CB | 1.97 | 1.13 |
| 1:E:8:ALA:HB1 | 1:E:81:GLY:O | 1.46 | 1.12 |
| 1:D:23:ASP:O | 1:D:70:LEU:CB | 1.97 | 1.13 |
| 1:B:8:ALA:HB1 | 1:B:81:GLY:O | 1.46 | 1.12 |
| 1:D:222:PRO:HD3 | 1:D:242:PRO:HG2 | 1.23 | 1.12 |
| 1:C:8:ALA:HB1 | 1:C:81:GLY:O | 1.46 | 1.12 |
| 1:C:23:ASP:O | 1:C:70:LEU:CB | 1.97 | 1.12 |
| 1:B:149:SER:HB2 | 1:B:167:ALA:HB1 | 1.15 | 1.12 |
| 1:F:195:PHE:HE2 | 1:F:242:PRO:HD3 | 1.00 | 1.12 |
| 1:D:2:PHE:O | 1:D:88:LEU:O | 1.66 | 1.12 |
| 1:A:149:SER:HB3 | 1:A:167:ALA:HB1 | 1.32 | 1.12 |
| 1:B:222:PRO:HD3 | 1:B:242:PRO:HG2 | 1.23 | 1.12 |
| 1:C:152:ILE:HG23 | 1:C:165:ILE:CG2 | 1.80 | 1.12 |
| 1:D:8:ALA:HB1 | 1:D:81:GLY:O | 1.46 | 1.12 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:2:PHE:O | 1:A:88:LEU:O | 1.66 | 1.12 |
| 1:E:222:PRO:HD3 | 1:E:242:PRO:HG2 | 1.23 | 1.12 |
| 1:E:152:ILE:HG23 | 1:E:165:ILE:CG2 | 1.80 | 1.12 |
| 1:D:149:SER:HB2 | 1:D:167:ALA:HB1 | 1.15 | 1.11 |
| 1:D:27:ILE:N | 1:D:66:ILE:O | 1.83 | 1.11 |
| 1:B:152:ILE:HG23 | 1:B:165:ILE:CG2 | 1.80 | 1.11 |
| 1:E:23:ASP:O | 1:E:70:LEU:CB | 1.97 | 1.11 |
| 1:C:195:PHE:HE2 | 1:C:242:PRO:HD3 | 1.00 | 1.11 |
| 1:C:149:SER:HB2 | 1:C:167:ALA:HB1 | 1.15 | 1.11 |
| 1:F:27:ILE:N | 1:F:66:ILE:O | 1.83 | 1.11 |
| 1:A:152:ILE:HG23 | 1:A:165:ILE:CG2 | 1.80 | 1.10 |
| 1:F:152:ILE:HG23 | 1:F:165:ILE:CG2 | 1.80 | 1.10 |
| 1:D:152:ILE:HG23 | 1:D:165:ILE:CG2 | 1.80 | 1.10 |
| 1:B:195:PHE:HE2 | 1:B:242:PRO:HD3 | 1.00 | 1.10 |
| 1:F:149:SER:HB2 | 1:F:167:ALA:HB1 | 1.15 | 1.10 |
| 1:A:27:ILE:N | 1:A:66:ILE:O | 1.83 | 1.09 |
| 1:A:149:SER:HB2 | 1:A:167:ALA:HB1 | 1.15 | 1.09 |
| 1:B:149:SER:HB3 | 1:B:167:ALA:HB1 | 1.32 | 1.09 |
| 1:B:27:ILE:N | 1:B:66:ILE:O | 1.83 | 1.09 |
| 1:E:27:ILE:N | 1:E:66:ILE:O | 1.83 | 1.09 |
| 1:A:96:LYS:HA | 1:A:108:LEU:O | 1.52 | 1.09 |
| 1:C:27:ILE:N | 1:C:66:ILE:O | 1.83 | 1.09 |
| 1:B:96:LYS:HA | 1:B:108:LEU:O | 1.53 | 1.09 |
| 1:F:96:LYS:HA | 1:F:108:LEU:O | 1.52 | 1.09 |
| 1:D:96:LYS:HA | 1:D:108:LEU:O | 1.53 | 1.09 |
| 1:D:195:PHE:HE2 | 1:D:242:PRO:HD3 | 1.00 | 1.09 |
| 1:A:222:PRO:HD3 | 1:A:242:PRO:HG2 | 1.23 | 1.08 |
| 1:C:96:LYS:HA | 1:C:108:LEU:O | 1.52 | 1.08 |
| 1:E:149:SER:HB3 | 1:E:167:ALA:HB1 | 1.32 | 1.08 |
| 1:F:149:SER:HB3 | 1:F:167:ALA:HB1 | 1.32 | 1.08 |
| 1:E:96:LYS:HA | 1:E:108:LEU:O | 1.52 | 1.07 |
| 1:C:149:SER:HB3 | 1:C:167:ALA:HB1 | 1.32 | 1.05 |
| 1:C:228:GLN:HA | 1:C:234:GLY:O | 1.57 | 1.04 |
| 1:A:228:GLN:HA | 1:A:234:GLY:O | 1.58 | 1.03 |
| 1:D:149:SER:HB3 | 1:D:167:ALA:HB1 | 1.32 | 1.03 |
| 1:C:191:ALA:HB1 | 1:C:218:GLY:C | 1.80 | 1.02 |
| 1:E:191:ALA:HB1 | 1:E:218:GLY:C | 1.79 | 1.02 |
| 1:D:228:GLN:HA | 1:D:234:GLY:O | 1.58 | 1.02 |
| 1:B:191:ALA:HB1 | 1:B:218:GLY:C | 1.79 | 1.01 |
| 1:F:191:ALA:HB1 | 1:F:218:GLY:C | 1.79 | 1.01 |
| 1:A:191:ALA:HB1 | 1:A:218:GLY:C | 1.79 | 1.01 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:228:GLN:HA | 1:F:234:GLY:O | 1.58 | 1.01 |
| 1:B:228:GLN:HA | 1:B:234:GLY:O | 1.58 | 1.01 |
| 1:B:152:ILE:HG23 | 1:B:165:ILE:HG23 | 1.41 | 1.01 |
| 1:D:197:LEU:HD23 | 1:D:198:ASP:N | 1.76 | 1.01 |
| 1:E:228:GLN:HA | 1:E:234:GLY:O | 1.58 | 1.01 |
| 1:B:149:SER:HB2 | 1:B:167:ALA:CB | 1.91 | 1.01 |
| 1:F:149:SER:HB2 | 1:F:167:ALA:CB | 1.91 | 1.01 |
| 1:D:191:ALA:HB1 | 1:D:218:GLY:C | 1.79 | 1.01 |
| 1:E:149:SER:HB2 | 1:E:167:ALA:CB | 1.91 | 1.00 |
| 1:B:197:LEU:HD23 | 1:B:198:ASP:N | 1.76 | 1.00 |
| 1:B:171:THR:HG23 | 1:C:72:ARG:NH1 | 1.76 | 1.00 |
| 1:D:149:SER:HB2 | 1:D:167:ALA:CB | 1.91 | 1.00 |
| 1:C:197:LEU:HD23 | 1:C:198:ASP:N | 1.76 | 1.00 |
| 1:D:152:ILE:HG23 | 1:D:165:ILE:HG23 | 1.40 | 1.00 |
| 1:A:197:LEU:HD23 | 1:A:198:ASP:N | 1.76 | 1.00 |
| 1:F:152:ILE:HG23 | 1:F:165:ILE:HG23 | 1.40 | 1.00 |
| 1:D:72:ARG:HH12 | 1:F:171:THR:HG23 | 1.25 | 0.99 |
| 1:C:149:SER:HB2 | 1:C:167:ALA:CB | 1.91 | 0.99 |
| 1:F:197:LEU:HD23 | 1:F:198:ASP:N | 1.76 | 0.99 |
| 1:E:156:VAL:HG21 | 1:E:217:LEU:HG | 1.44 | 0.99 |
| 1:B:165:ILE:O | 1:B:176:LEU:HD23 | 1.63 | 0.99 |
| 1:C:165:ILE:O | 1:C:176:LEU:HD23 | 1.63 | 0.99 |
| 1:C:156:VAL:HG21 | 1:C:217:LEU:HG | 1.44 | 0.99 |
| 1:A:149:SER:HB2 | 1:A:167:ALA:CB | 1.91 | 0.99 |
| 1:D:171:THR:HG23 | 1:E:72:ARG:HH12 | 1.27 | 0.99 |
| 1:E:197:LEU:HD23 | 1:E:198:ASP:N | 1.76 | 0.99 |
| 1:E:165:ILE:O | 1:E:176:LEU:HD23 | 1.63 | 0.99 |
| 1:E:152:ILE:HG23 | 1:E:165:ILE:HG23 | 1.40 | 0.98 |
| 1:B:156:VAL:HG21 | 1:B:217:LEU:HG | 1.44 | 0.98 |
| 1:A:165:ILE:O | 1:A:176:LEU:HD23 | 1.63 | 0.98 |
| 1:D:165:ILE:O | 1:D:176:LEU:HD23 | 1.63 | 0.98 |
| 1:A:152:ILE:HG23 | 1:A:165:ILE:HG23 | 1.40 | 0.98 |
| 1:C:152:ILE:HG23 | 1:C:165:ILE:HG23 | 1.40 | 0.97 |
| 1:D:72:ARG:NH1 | 1:F:171:THR:HG23 | 1.78 | 0.97 |
| 1:F:156:VAL:HG21 | 1:F:217:LEU:HG | 1.44 | 0.97 |
| 1:E:171:THR:HG23 | 1:F:72:ARG:HH12 | 1.29 | 0.97 |
| 1:F:165:ILE:O | 1:F:176:LEU:HD23 | 1.63 | 0.97 |
| 1:C:8:ALA:HB3 | 1:C:82:ALA:C | 1.85 | 0.97 |
| 1:B:8:ALA:HB3 | 1:B:82:ALA:C | 1.85 | 0.97 |
| 1:C:156:VAL:CB | 1:C:191:ALA:O | 2.13 | 0.97 |
| 1:A:37:ARG:HG2 | 1:A:37:ARG:O | 1.65 | 0.97 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:171:THR:CG2 | 1:C:72:ARG:NH1 | 2.28 | 0.97 |
| 1:B:37:ARG:O | 1:B:37:ARG:HG2 | 1.65 | 0.97 |
| 1:F:8:ALA:HB3 | 1:F:82:ALA:C | 1.85 | 0.96 |
| 1:E:8:ALA:HB3 | 1:E:82:ALA:C | 1.85 | 0.96 |
| 1:D:72:ARG:NH1 | 1:F:171:THR:CG2 | 2.27 | 0.96 |
| 1:B:171:THR:HG23 | 1:C:72:ARG:HH12 | 1.23 | 0.96 |
| 1:A:156:VAL:CB | 1:A:191:ALA:O | 2.13 | 0.96 |
| 1:B:156:VAL:CB | 1:B:191:ALA:O | 2.13 | 0.96 |
| 1:A:8:ALA:HB3 | 1:A:82:ALA:C | 1.85 | 0.96 |
| 1:E:37:ARG:O | 1:E:37:ARG:HG2 | 1.65 | 0.96 |
| 1:C:222:PRO:HD3 | 1:C:242:PRO:CD | 1.95 | 0.95 |
| 1:A:222:PRO:HD3 | 1:A:242:PRO:CD | 1.95 | 0.95 |
| 1:B:222:PRO:HD3 | 1:B:242:PRO:CD | 1.95 | 0.95 |
| 1:E:156:VAL:CB | 1:E:191:ALA:O | 2.13 | 0.95 |
| 1:E:222:PRO:HD3 | 1:E:242:PRO:CD | 1.95 | 0.95 |
| 1:D:37:ARG:O | 1:D:37:ARG:HG2 | 1.65 | 0.95 |
| 1:F:156:VAL:CB | 1:F:191:ALA:O | 2.13 | 0.95 |
| 1:D:156:VAL:HG21 | 1:D:217:LEU:HG | 1.44 | 0.95 |
| 1:D:156:VAL:CB | 1:D:191:ALA:O | 2.13 | 0.95 |
| 1:F:222:PRO:HD3 | 1:F:242:PRO:CD | 1.95 | 0.95 |
| 1:F:37:ARG:O | 1:F:37:ARG:HG2 | 1.65 | 0.95 |
| 1:A:156:VAL:HG21 | 1:A:217:LEU:HG | 1.44 | 0.95 |
| 1:D:8:ALA:HB3 | 1:D:82:ALA:C | 1.85 | 0.95 |
| 1:E:222:PRO:CD | 1:E:242:PRO:HG2 | 1.97 | 0.94 |
| 1:C:222:PRO:CD | 1:C:242:PRO:HG2 | 1.97 | 0.94 |
| 1:D:222:PRO:HD3 | 1:D:242:PRO:CD | 1.95 | 0.94 |
| 1:C:37:ARG:O | 1:C:37:ARG:HG2 | 1.65 | 0.94 |
| 1:A:222:PRO:CD | 1:A:242:PRO:HG2 | 1.97 | 0.94 |
| 1:F:150:ASP:O | 1:F:197:LEU:CD2 | 2.16 | 0.94 |
| 1:E:171:THR:HG23 | 1:F:72:ARG:NH1 | 1.82 | 0.94 |
| 1:F:156:VAL:CG2 | 1:F:217:LEU:HG | 1.98 | 0.94 |
| 1:F:222:PRO:CD | 1:F:242:PRO:HG2 | 1.97 | 0.94 |
| 1:E:133:LEU:HG | 1:E:183:LEU:HD11 | 1.50 | 0.94 |
| 1:C:150:ASP:O | 1:C:197:LEU:CD2 | 2.16 | 0.94 |
| 1:D:222:PRO:CD | 1:D:242:PRO:HG2 | 1.97 | 0.93 |
| 1:B:133:LEU:HG | 1:B:183:LEU:HD11 | 1.50 | 0.93 |
| 1:D:156:VAL:CG2 | 1:D:217:LEU:HG | 1.98 | 0.93 |
| 1:C:156:VAL:CG2 | 1:C:217:LEU:HG | 1.98 | 0.93 |
| 1:A:156:VAL:CG2 | 1:A:217:LEU:HG | 1.98 | 0.93 |
| 1:B:150:ASP:O | 1:B:197:LEU:CD2 | 2.16 | 0.93 |
| 1:B:222:PRO:CD | 1:B:242:PRO:HG2 | 1.97 | 0.93 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:194:LEU:HD23 | 1:F:245:GLN:HG3 | 1.51 | 0.93 |
| 1:A:72:ARG:NH1 | 1:C:171:THR:HG23 | 1.83 | 0.93 |
| 1:E:171:THR:CG2 | 1:F:72:ARG:NH1 | 2.32 | 0.93 |
| 1:D:171:THR:HG23 | 1:E:72:ARG:NH1 | 1.83 | 0.93 |
| 1:A:133:LEU:HG | 1:A:183:LEU:HD11 | 1.50 | 0.93 |
| 1:A:146:ASP:HA | 1:A:197:LEU:HD11 | 1.51 | 0.93 |
| 1:A:72:ARG:NH1 | 1:C:171:THR:CG2 | 2.32 | 0.93 |
| 1:C:133:LEU:HG | 1:C:183:LEU:HD11 | 1.50 | 0.93 |
| 1:A:150:ASP:O | 1:A:197:LEU:CD2 | 2.16 | 0.93 |
| 1:E:156:VAL:CG2 | 1:E:217:LEU:HG | 1.98 | 0.93 |
| 1:C:194:LEU:HD23 | 1:C:245:GLN:HG3 | 1.51 | 0.92 |
| 1:B:227:TYR:O | 1:B:235:THR:HA | 1.69 | 0.92 |
| 1:C:227:TYR:O | 1:C:235:THR:HA | 1.69 | 0.92 |
| 1:A:227:TYR:O | 1:A:235:THR:HA | 1.69 | 0.92 |
| 1:D:227:TYR:O | 1:D:235:THR:HA | 1.70 | 0.92 |
| 1:A:171:THR:HG23 | 1:B:72:ARG:HH12 | 1.33 | 0.92 |
| 1:D:194:LEU:HD23 | 1:D:245:GLN:HG3 | 1.51 | 0.92 |
| 1:F:95:ARG:O | 1:F:109:ALA:CA | 2.18 | 0.92 |
| 1:B:156:VAL:CG2 | 1:B:217:LEU:HG | 1.98 | 0.92 |
| 1:E:95:ARG:O | 1:E:109:ALA:CA | 2.18 | 0.92 |
| 1:A:72:ARG:HH12 | 1:C:171:THR:HG23 | 1.31 | 0.91 |
| 1:F:133:LEU:HG | 1:F:183:LEU:HD11 | 1.50 | 0.91 |
| 1:A:95:ARG:O | 1:A:109:ALA:CA | 2.18 | 0.91 |
| 1:E:194:LEU:HD23 | 1:E:245:GLN:HG3 | 1.51 | 0.91 |
| 1:F:227:TYR:O | 1:F:235:THR:HA | 1.69 | 0.91 |
| 1:C:95:ARG:O | 1:C:109:ALA:CA | 2.18 | 0.91 |
| 1:A:194:LEU:HD23 | 1:A:245:GLN:HG3 | 1.51 | 0.91 |
| 1:B:194:LEU:HD23 | 1:B:245:GLN:HG3 | 1.51 | 0.91 |
| 1:E:150:ASP:O | 1:E:197:LEU:CD2 | 2.16 | 0.91 |
| 1:B:33:SER:CB | 1:B:51:LEU:O | 2.19 | 0.91 |
| 1:D:150:ASP:O | 1:D:197:LEU:CD2 | 2.16 | 0.91 |
| 1:D:146:ASP:HA | 1:D:197:LEU:HD11 | 1.51 | 0.91 |
| 1:C:33:SER:CB | 1:C:51:LEU:O | 2.19 | 0.91 |
| 1:C:146:ASP:HA | 1:C:197:LEU:HD11 | 1.51 | 0.91 |
| 1:D:33:SER:CB | 1:D:51:LEU:O | 2.19 | 0.91 |
| 1:E:146:ASP:HA | 1:E:197:LEU:HD11 | 1.51 | 0.90 |
| 1:E:227:TYR:O | 1:E:235:THR:HA | 1.69 | 0.90 |
| 1:D:133:LEU:HG | 1:D:183:LEU:HD11 | 1.50 | 0.90 |
| 1:A:171:THR:HG23 | 1:B:72:ARG:NH1 | 1.85 | 0.90 |
| 1:D:21:LEU:HB3 | 1:D:40:ASP:HB3 | 1.54 | 0.90 |
| 1:E:33:SER:CB | 1:E:51:LEU:O | 2.19 | 0.90 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:153:ARG:O | 1:E:165:ILE:HA | 1.72 | 0.90 |
| 1:A:33:SER:CB | 1:A:51:LEU:O | 2.19 | 0.90 |
| 1:B:146:ASP:HA | 1:B:197:LEU:HD11 | 1.51 | 0.90 |
| 1:A:153:ARG:O | 1:A:165:ILE:HA | 1.72 | 0.90 |
| 1:A:108:LEU:HD22 | 1:A:110:LEU:HD23 | 1.54 | 0.90 |
| 1:D:133:LEU:HG | 1:D:183:LEU:CD1 | 2.02 | 0.90 |
| 1:B:153:ARG:O | 1:B:165:ILE:HA | 1.72 | 0.90 |
| 1:C:108:LEU:HD22 | 1:C:110:LEU:HD23 | 1.54 | 0.90 |
| 1:F:146:ASP:HA | 1:F:197:LEU:HD11 | 1.51 | 0.89 |
| 1:E:6:VAL:HG22 | 1:E:56:PHE:HD2 | 1.38 | 0.89 |
| 1:A:21:LEU:HB3 | 1:A:40:ASP:HB3 | 1.54 | 0.89 |
| 1:A:6:VAL:HG22 | 1:A:56:PHE:HD2 | 1.37 | 0.89 |
| 1:A:171:THR:CG2 | 1:B:72:ARG:NH1 | 2.34 | 0.89 |
| 1:E:133:LEU:HG | 1:E:183:LEU:CD1 | 2.02 | 0.89 |
| 1:F:21:LEU:HB3 | 1:F:40:ASP:HB3 | 1.54 | 0.89 |
| 1:E:21:LEU:HB3 | 1:E:40:ASP:HB3 | 1.54 | 0.89 |
| 1:F:133:LEU:HG | 1:F:183:LEU:CD1 | 2.02 | 0.89 |
| 1:C:6:VAL:HG22 | 1:C:56:PHE:HD2 | 1.37 | 0.89 |
| 1:A:133:LEU:HG | 1:A:183:LEU:CD1 | 2.02 | 0.89 |
| 1:F:33:SER:CB | 1:F:51:LEU:O | 2.19 | 0.89 |
| 1:F:108:LEU:HD22 | 1:F:110:LEU:HD23 | 1.54 | 0.89 |
| 1:D:95:ARG:O | 1:D:109:ALA:CA | 2.18 | 0.89 |
| 1:D:72:ARG:HH12 | 1:F:171:THR:HG21 | 1.35 | 0.88 |
| 1:F:8:ALA:N | 1:F:84:ASP:O | 2.06 | 0.88 |
| 1:C:153:ARG:O | 1:C:165:ILE:HA | 1.72 | 0.88 |
| 1:A:173:ASP:HB2 | 1:B:107:THR:CG2 | 2.02 | 0.88 |
| 1:D:153:ARG:O | 1:D:165:ILE:HA | 1.72 | 0.88 |
| 1:C:133:LEU:HG | 1:C:183:LEU:CD1 | 2.02 | 0.88 |
| 1:B:6:VAL:HG22 | 1:B:56:PHE:HD2 | 1.37 | 0.88 |
| 1:B:142:ILE:HD13 | 1:B:152:ILE:HD12 | 1.56 | 0.88 |
| 1:F:153:ARG:O | 1:F:165:ILE:HA | 1.72 | 0.88 |
| 1:D:171:THR:CG2 | 1:E:72:ARG:NH1 | 2.35 | 0.88 |
| 1:B:173:ASP:HB2 | 1:C:107:THR:CG2 | 2.03 | 0.88 |
| 1:D:8:ALA:N | 1:D:84:ASP:O | 2.06 | 0.88 |
| 1:E:108:LEU:HD22 | 1:E:110:LEU:HD23 | 1.54 | 0.88 |
| 1:B:133:LEU:HG | 1:B:183:LEU:CD1 | 2.02 | 0.88 |
| 1:F:213:VAL:HG22 | 1:F:227:TYR:CZ | 2.09 | 0.88 |
| 1:D:170:ASP:O | 1:D:171:THR:HG22 | 1.74 | 0.88 |
| 1:D:6:VAL:HG22 | 1:D:56:PHE:HD2 | 1.38 | 0.88 |
| 1:C:170:ASP:O | 1:C:171:THR:HG22 | 1.74 | 0.88 |
| 1:C:213:VAL:HG22 | 1:C:227:TYR:CZ | 2.09 | 0.88 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:8:ALA:N | 1:B:84:ASP:O | 2.06 | 0.88 |
| 1:B:95:ARG:O | 1:B:109:ALA:CA | 2.18 | 0.87 |
| 1:B:21:LEU:HB3 | 1:B:40:ASP:HB3 | 1.54 | 0.87 |
| 1:F:142:ILE:HD13 | 1:F:152:ILE:HD12 | 1.56 | 0.87 |
| 1:D:108:LEU:HD22 | 1:D:110:LEU:HD23 | 1.54 | 0.87 |
| 1:A:107:THR:CG2 | 1:C:173:ASP:HB2 | 2.04 | 0.87 |
| 1:A:213:VAL:HG22 | 1:A:227:TYR:CZ | 2.09 | 0.87 |
| 1:C:142:ILE:HD13 | 1:C:152:ILE:HD12 | 1.56 | 0.87 |
| 1:E:213:VAL:HG22 | 1:E:227:TYR:CZ | 2.09 | 0.87 |
| 1:A:8:ALA:N | 1:A:84:ASP:O | 2.06 | 0.87 |
| 1:E:152:ILE:CG2 | 1:E:165:ILE:HG23 | 2.05 | 0.87 |
| 1:B:213:VAL:HG22 | 1:B:227:TYR:CZ | 2.09 | 0.87 |
| 1:C:8:ALA:N | 1:C:84:ASP:O | 2.06 | 0.87 |
| 1:B:170:ASP:O | 1:B:171:THR:HG22 | 1.74 | 0.87 |
| 1:F:152:ILE:CG2 | 1:F:165:ILE:HG23 | 2.05 | 0.87 |
| 1:A:170:ASP:O | 1:A:171:THR:HG22 | 1.74 | 0.87 |
| 1:E:8:ALA:N | 1:E:84:ASP:O | 2.06 | 0.86 |
| 1:C:152:ILE:CG2 | 1:C:165:ILE:HG23 | 2.05 | 0.86 |
| 1:E:142:ILE:HD13 | 1:E:152:ILE:HD12 | 1.56 | 0.86 |
| 1:E:146:ASP:HA | 1:E:197:LEU:CD1 | 2.05 | 0.86 |
| 1:D:213:VAL:HG22 | 1:D:227:TYR:CZ | 2.09 | 0.86 |
| 1:B:152:ILE:CG2 | 1:B:165:ILE:HG23 | 2.05 | 0.86 |
| 1:C:146:ASP:HA | 1:C:197:LEU:CD1 | 2.05 | 0.86 |
| 1:B:146:ASP:HA | 1:B:197:LEU:CD1 | 2.05 | 0.86 |
| 1:B:108:LEU:HD22 | 1:B:110:LEU:HD23 | 1.54 | 0.86 |
| 1:A:152:ILE:CG2 | 1:A:165:ILE:HG23 | 2.05 | 0.86 |
| 1:F:222:PRO:HD3 | 1:F:242:PRO:HD2 | 1.58 | 0.86 |
| 1:D:173:ASP:HB2 | 1:E:107:THR:CG2 | 2.05 | 0.86 |
| 1:A:222:PRO:HD3 | 1:A:242:PRO:HD2 | 1.58 | 0.86 |
| 1:D:146:ASP:HA | 1:D:197:LEU:CD1 | 2.05 | 0.86 |
| 1:C:21:LEU:HB3 | 1:C:40:ASP:HB3 | 1.54 | 0.86 |
| 1:F:6:VAL:HG22 | 1:F:56:PHE:HD2 | 1.37 | 0.86 |
| 1:D:152:ILE:CG2 | 1:D:165:ILE:HG23 | 2.05 | 0.86 |
| 1:A:146:ASP:HA | 1:A:197:LEU:CD1 | 2.05 | 0.86 |
| 1:C:152:ILE:CG2 | 1:C:165:ILE:CG2 | 2.54 | 0.86 |
| 1:F:170:ASP:O | 1:F:171:THR:HG22 | 1.74 | 0.85 |
| 1:C:222:PRO:HD3 | 1:C:242:PRO:HD2 | 1.58 | 0.85 |
| 1:B:152:ILE:CG2 | 1:B:165:ILE:CG2 | 2.54 | 0.85 |
| 1:E:170:ASP:O | 1:E:171:THR:HG22 | 1.74 | 0.85 |
| 1:D:142:ILE:HD13 | 1:D:152:ILE:HD12 | 1.56 | 0.85 |
| 1:D:152:ILE:CG2 | 1:D:165:ILE:CG2 | 2.54 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:146:ASP:HA | 1:F:197:LEU:CD1 | 2.05 | 0.85 |
| 1:E:173:ASP:HB2 | 1:F:107:THR:CG2 | 2.06 | 0.85 |
| 1:A:152:ILE:CG2 | 1:A:165:ILE:CG2 | 2.54 | 0.84 |
| 1:F:152:ILE:CG2 | 1:F:165:ILE:CG2 | 2.54 | 0.84 |
| 1:E:129:ALA:HB1 | 1:E:156:VAL:HG11 | 1.59 | 0.84 |
| 1:A:142:ILE:HD13 | 1:A:152:ILE:HD12 | 1.56 | 0.84 |
| 1:E:152:ILE:CG2 | 1:E:165:ILE:CG2 | 2.54 | 0.84 |
| 1:F:135:GLY:N | 1:F:211:ALA:O | 2.10 | 0.84 |
| 1:B:129:ALA:HB1 | 1:B:156:VAL:HG11 | 1.59 | 0.84 |
| 1:C:135:GLY:N | 1:C:211:ALA:O | 2.10 | 0.84 |
| 1:E:135:GLY:N | 1:E:211:ALA:O | 2.10 | 0.84 |
| 1:A:129:ALA:HB1 | 1:A:156:VAL:HG11 | 1.59 | 0.84 |
| 1:C:34:LEU:O | 1:C:51:LEU:HB2 | 1.78 | 0.84 |
| 1:A:34:LEU:O | 1:A:51:LEU:HB2 | 1.78 | 0.84 |
| 1:F:34:LEU:O | 1:F:51:LEU:HB2 | 1.78 | 0.83 |
| 1:E:222:PRO:HD3 | 1:E:242:PRO:HD2 | 1.58 | 0.83 |
| 1:A:135:GLY:N | 1:A:211:ALA:O | 2.10 | 0.83 |
| 1:B:222:PRO:HD3 | 1:B:242:PRO:HD2 | 1.58 | 0.83 |
| 1:D:8:ALA:CB | 1:D:81:GLY:O | 2.27 | 0.83 |
| 1:D:34:LEU:O | 1:D:51:LEU:HB2 | 1.78 | 0.83 |
| 1:E:33:SER:HB2 | 1:E:51:LEU:O | 1.79 | 0.83 |
| 1:D:135:GLY:N | 1:D:211:ALA:O | 2.10 | 0.83 |
| 1:B:135:GLY:N | 1:B:211:ALA:O | 2.10 | 0.83 |
| 1:A:72:ARG:HH12 | 1:C:171:THR:HG21 | 1.42 | 0.83 |
| 1:D:129:ALA:HB1 | 1:D:156:VAL:HG11 | 1.59 | 0.82 |
| 1:B:8:ALA:CB | 1:B:81:GLY:O | 2.27 | 0.82 |
| 1:C:8:ALA:CB | 1:C:81:GLY:O | 2.27 | 0.82 |
| 1:D:213:VAL:HG22 | 1:D:227:TYR:OH | 1.80 | 0.82 |
| 1:A:213:VAL:HG22 | 1:A:227:TYR:OH | 1.80 | 0.82 |
| 1:D:222:PRO:HD3 | 1:D:242:PRO:HD2 | 1.58 | 0.82 |
| 1:E:8:ALA:CB | 1:E:81:GLY:O | 2.27 | 0.82 |
| 1:B:33:SER:HB2 | 1:B:51:LEU:O | 1.79 | 0.82 |
| 1:C:129:ALA:HB1 | 1:C:156:VAL:HG11 | 1.59 | 0.82 |
| 1:F:129:ALA:HB1 | 1:F:156:VAL:HG11 | 1.59 | 0.82 |
| 1:A:8:ALA:CB | 1:A:81:GLY:O | 2.27 | 0.82 |
| 1:E:34:LEU:O | 1:E:51:LEU:HB2 | 1.78 | 0.82 |
| 1:C:213:VAL:HG22 | 1:C:227:TYR:OH | 1.80 | 0.81 |
| 1:B:34:LEU:O | 1:B:51:LEU:HB2 | 1.78 | 0.81 |
| 1:D:9:ALA:HB2 | 1:D:82:ALA:HB1 | 1.63 | 0.81 |
| 1:B:222:PRO:HB3 | 1:B:239:MET:HG2 | 1.61 | 0.81 |
| 1:C:222:PRO:HB3 | 1:C:239:MET:HG2 | 1.61 | 0.81 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:222:PRO:HB3 | 1:A:239:MET:HG2 | 1.61 | 0.81 |
| 1:F:33:SER:HB2 | 1:F:51:LEU:O | 1.79 | 0.81 |
| 1:C:166:GLU:HB3 | 1:C:175:ASP:HA | 1.63 | 0.81 |
| 1:F:213:VAL:HG22 | 1:F:227:TYR:OH | 1.80 | 0.81 |
| 1:F:9:ALA:HB2 | 1:F:82:ALA:HB1 | 1.63 | 0.81 |
| 1:B:213:VAL:HG22 | 1:B:227:TYR:OH | 1.80 | 0.81 |
| 1:E:171:THR:HG21 | 1:F:72:ARG:HH12 | 1.42 | 0.81 |
| 1:F:166:GLU:HB3 | 1:F:175:ASP:HA | 1.63 | 0.81 |
| 1:D:151:HIS:HA | 1:D:197:LEU:H | 1.46 | 0.81 |
| 1:A:171:THR:HG21 | 1:B:72:ARG:HH12 | 1.46 | 0.81 |
| 1:B:152:ILE:HG23 | 1:B:165:ILE:HG22 | 1.63 | 0.81 |
| 1:F:222:PRO:HB3 | 1:F:239:MET:HG2 | 1.61 | 0.81 |
| 1:E:222:PRO:HB3 | 1:E:239:MET:HG2 | 1.61 | 0.81 |
| 1:D:33:SER:HB2 | 1:D:51:LEU:O | 1.79 | 0.81 |
| 1:C:136:THR:HB | 1:C:209:THR:HA | 1.63 | 0.81 |
| 1:E:213:VAL:HG22 | 1:E:227:TYR:OH | 1.80 | 0.80 |
| 1:E:166:GLU:HB3 | 1:E:175:ASP:HA | 1.63 | 0.80 |
| 1:D:107:THR:CG2 | 1:F:173:ASP:HB2 | 2.12 | 0.80 |
| 1:C:33:SER:HB2 | 1:C:51:LEU:O | 1.79 | 0.80 |
| 1:B:171:THR:HG21 | 1:C:72:ARG:HH12 | 1.43 | 0.80 |
| 1:A:33:SER:HB2 | 1:A:51:LEU:O | 1.79 | 0.80 |
| 1:E:152:ILE:HG23 | 1:E:165:ILE:HG22 | 1.63 | 0.80 |
| 1:C:229:ILE:HD11 | 1:C:236:ILE:HD11 | 1.63 | 0.80 |
| 1:F:152:ILE:HG23 | 1:F:165:ILE:HG22 | 1.63 | 0.80 |
| 1:E:136:THR:HB | 1:E:209:THR:HA | 1.63 | 0.80 |
| 1:D:222:PRO:HB3 | 1:D:239:MET:HG2 | 1.61 | 0.80 |
| 1:E:195:PHE:HB3 | 1:E:240:LEU:HD22 | 1.64 | 0.80 |
| 1:F:8:ALA:CB | 1:F:81:GLY:O | 2.27 | 0.80 |
| 1:C:195:PHE:HB3 | 1:C:240:LEU:HD22 | 1.64 | 0.80 |
| 1:D:166:GLU:HB3 | 1:D:175:ASP:HA | 1.63 | 0.80 |
| 1:F:229:ILE:HD11 | 1:F:236:ILE:HD11 | 1.63 | 0.79 |
| 1:D:195:PHE:HB3 | 1:D:240:LEU:HD22 | 1.64 | 0.79 |
| 1:B:9:ALA:HB2 | 1:B:82:ALA:HB1 | 1.63 | 0.79 |
| 1:A:229:ILE:HD11 | 1:A:236:ILE:HD11 | 1.63 | 0.79 |
| 1:F:195:PHE:HB3 | 1:F:240:LEU:HD22 | 1.64 | 0.79 |
| 1:D:152:ILE:HG23 | 1:D:165:ILE:HG22 | 1.63 | 0.79 |
| 1:F:4:ALA:O | 1:F:87:HIS:HA | 1.83 | 0.79 |
| 1:B:166:GLU:HB3 | 1:B:175:ASP:HA | 1.63 | 0.79 |
| 1:B:136:THR:HB | 1:B:209:THR:HA | 1.63 | 0.79 |
| 1:E:9:ALA:HB2 | 1:E:82:ALA:HB1 | 1.63 | 0.79 |
| 1:E:4:ALA:O | 1:E:87:HIS:HA | 1.83 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:152:ILE:HG23 | 1:C:165:ILE:HG22 | 1.63 | 0.79 |
| 1:A:152:ILE:HG23 | 1:A:165:ILE:HG22 | 1.63 | 0.79 |
| 1:A:9:ALA:HB2 | 1:A:82:ALA:HB1 | 1.63 | 0.79 |
| 1:C:9:ALA:HB2 | 1:C:82:ALA:HB1 | 1.63 | 0.79 |
| 1:D:136:THR:HB | 1:D:209:THR:HA | 1.63 | 0.79 |
| 1:B:151:HIS:HA | 1:B:197:LEU:H | 1.46 | 0.79 |
| 1:C:4:ALA:O | 1:C:87:HIS:HA | 1.83 | 0.79 |
| 1:D:229:ILE:HD11 | 1:D:236:ILE:HD11 | 1.63 | 0.79 |
| 1:C:151:HIS:HA | 1:C:197:LEU:H | 1.46 | 0.79 |
| 1:F:136:THR:HB | 1:F:209:THR:HA | 1.63 | 0.79 |
| 1:F:151:HIS:HA | 1:F:197:LEU:H | 1.46 | 0.78 |
| 1:B:4:ALA:O | 1:B:87:HIS:HA | 1.83 | 0.78 |
| 1:D:4:ALA:O | 1:D:87:HIS:HA | 1.83 | 0.78 |
| 1:A:151:HIS:HA | 1:A:197:LEU:H | 1.46 | 0.78 |
| 1:B:204:ASN:HA | 1:B:207:ILE:HD13 | 1.65 | 0.78 |
| 1:A:4:ALA:O | 1:A:87:HIS:HA | 1.83 | 0.78 |
| 1:A:166:GLU:HB3 | 1:A:175:ASP:HA | 1.63 | 0.78 |
| 1:A:136:THR:HB | 1:A:209:THR:HA | 1.63 | 0.78 |
| 1:B:229:ILE:HD11 | 1:B:236:ILE:HD11 | 1.63 | 0.78 |
| 1:A:195:PHE:HB3 | 1:A:240:LEU:HD22 | 1.64 | 0.78 |
| 1:B:195:PHE:HB3 | 1:B:240:LEU:HD22 | 1.64 | 0.78 |
| 1:D:171:THR:HG21 | 1:E:72:ARG:HH12 | 1.47 | 0.78 |
| 1:B:171:THR:O | 1:B:172:ASP:OD1 | 2.02 | 0.78 |
| 1:D:204:ASN:HA | 1:D:207:ILE:HD13 | 1.66 | 0.78 |
| 1:F:204:ASN:HA | 1:F:207:ILE:HD13 | 1.66 | 0.78 |
| 1:C:149:SER:CB | 1:C:167:ALA:CB | 2.49 | 0.78 |
| 1:C:171:THR:O | 1:C:172:ASP:OD1 | 2.02 | 0.78 |
| 1:F:171:THR:O | 1:F:172:ASP:OD1 | 2.02 | 0.78 |
| 1:A:171:THR:O | 1:A:172:ASP:OD1 | 2.02 | 0.78 |
| 1:E:1:MET:HG3 | 1:E:91:ASP:CB | 2.14 | 0.77 |
| 1:E:151:HIS:HA | 1:E:197:LEU:H | 1.46 | 0.77 |
| 1:E:229:ILE:HD11 | 1:E:236:ILE:HD11 | 1.63 | 0.77 |
| 1:F:1:MET:HG3 | 1:F:91:ASP:CB | 2.14 | 0.77 |
| 1:D:157:ASP:O | 1:D:157:ASP:CG | 2.23 | 0.77 |
| 1:A:1:MET:HG3 | 1:A:91:ASP:CB | 2.14 | 0.77 |
| 1:C:204:ASN:HA | 1:C:207:ILE:HD13 | 1.66 | 0.77 |
| 1:D:1:MET:HG3 | 1:D:91:ASP:CB | 2.14 | 0.77 |
| 1:B:1:MET:HG3 | 1:B:91:ASP:CB | 2.14 | 0.77 |
| 1:D:20:VAL:HG13 | 1:D:202:ASP:HB3 | 1.67 | 0.77 |
| 1:C:1:MET:HG3 | 1:C:91:ASP:CB | 2.14 | 0.77 |
| 1:A:39:VAL:CG1 | 1:A:43:ASN:HA | 2.15 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:157:ASP:O | 1:C:157:ASP:CG | 2.23 | 0.77 |
| 1:A:20:VAL:HG13 | 1:A:202:ASP:HB3 | 1.67 | 0.77 |
| 1:C:39:VAL:CG1 | 1:C:43:ASN:HA | 2.15 | 0.77 |
| 1:F:151:HIS:HB3 | 1:F:196:SER:HA | 1.67 | 0.77 |
| 1:E:20:VAL:HG13 | 1:E:202:ASP:HB3 | 1.67 | 0.76 |
| 1:E:157:ASP:O | 1:E:157:ASP:CG | 2.23 | 0.76 |
| 1:D:171:THR:O | 1:D:172:ASP:OD1 | 2.02 | 0.76 |
| 1:E:204:ASN:HA | 1:E:207:ILE:HD13 | 1.66 | 0.76 |
| 1:E:39:VAL:CG1 | 1:E:43:ASN:HA | 2.15 | 0.76 |
| 1:E:171:THR:O | 1:E:172:ASP:OD1 | 2.02 | 0.76 |
| 1:A:151:HIS:HB3 | 1:A:196:SER:HA | 1.67 | 0.76 |
| 1:A:8:ALA:CB | 1:A:82:ALA:O | 2.25 | 0.76 |
| 1:A:204:ASN:HA | 1:A:207:ILE:HD13 | 1.65 | 0.76 |
| 1:B:3:LYS:O | 1:B:58:SER:O | 2.04 | 0.76 |
| 1:B:39:VAL:CG1 | 1:B:43:ASN:HA | 2.15 | 0.76 |
| 1:F:3:LYS:O | 1:F:58:SER:O | 2.04 | 0.76 |
| 1:F:39:VAL:CG1 | 1:F:43:ASN:HA | 2.15 | 0.76 |
| 1:F:157:ASP:CG | 1:F:157:ASP:O | 2.23 | 0.76 |
| 1:D:39:VAL:CG1 | 1:D:43:ASN:HA | 2.15 | 0.76 |
| 1:B:157:ASP:O | 1:B:157:ASP:CG | 2.23 | 0.76 |
| 1:E:3:LYS:O | 1:E:58:SER:O | 2.04 | 0.76 |
| 1:E:25:CYS:SG | 1:E:70:LEU:HG | 2.26 | 0.75 |
| 1:E:151:HIS:HB3 | 1:E:196:SER:HA | 1.68 | 0.75 |
| 1:C:3:LYS:O | 1:C:58:SER:O | 2.04 | 0.75 |
| 1:A:25:CYS:SG | 1:A:70:LEU:HG | 2.26 | 0.75 |
| 1:E:8:ALA:CB | 1:E:82:ALA:O | 2.26 | 0.75 |
| 1:B:8:ALA:CB | 1:B:82:ALA:O | 2.25 | 0.75 |
| 1:D:5:ILE:HG22 | 1:D:85:LEU:HB3 | 1.68 | 0.75 |
| 1:C:20:VAL:HG13 | 1:C:202:ASP:HB3 | 1.67 | 0.75 |
| 1:B:151:HIS:HB3 | 1:B:196:SER:HA | 1.67 | 0.75 |
| 1:F:20:VAL:HG13 | 1:F:202:ASP:HB3 | 1.67 | 0.75 |
| 1:C:151:HIS:HB3 | 1:C:196:SER:HA | 1.67 | 0.75 |
| 1:C:5:ILE:HG22 | 1:C:85:LEU:HB3 | 1.68 | 0.75 |
| 1:F:26:LYS:HE2 | 1:F:113:PRO:O | 1.87 | 0.75 |
| 1:C:214:THR:OG1 | 1:C:226:HIS:HB2 | 1.87 | 0.75 |
| 1:F:191:ALA:CB | 1:F:218:GLY:HA2 | 2.17 | 0.75 |
| 1:B:20:VAL:HG13 | 1:B:202:ASP:HB3 | 1.67 | 0.75 |
| 1:D:240:LEU:HD23 | 1:D:241:ALA:O | 1.87 | 0.75 |
| 1:C:29:LEU:HD23 | 1:C:34:LEU:HD13 | 1.69 | 0.75 |
| 1:A:3:LYS:O | 1:A:58:SER:O | 2.04 | 0.75 |
| 1:F:29:LEU:HD23 | 1:F:34:LEU:HD13 | 1.69 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:5:ILE:HG22 | 1:B:85:LEU:HB3 | 1.68 | 0.75 |
| 1:F:5:ILE:HG22 | 1:F:85:LEU:HB3 | 1.68 | 0.75 |
| 1:B:240:LEU:HD23 | 1:B:241:ALA:O | 1.87 | 0.74 |
| 1:F:25:CYS:SG | 1:F:70:LEU:HG | 2.26 | 0.74 |
| 1:A:108:LEU:HD22 | 1:A:110:LEU:CD2 | 2.17 | 0.74 |
| 1:D:25:CYS:SG | 1:D:70:LEU:HG | 2.26 | 0.74 |
| 1:F:214:THR:OG1 | 1:F:226:HIS:HB2 | 1.87 | 0.74 |
| 1:D:29:LEU:HD23 | 1:D:34:LEU:HD13 | 1.69 | 0.74 |
| 1:D:3:LYS:O | 1:D:58:SER:O | 2.04 | 0.74 |
| 1:C:240:LEU:HD23 | 1:C:241:ALA:O | 1.87 | 0.74 |
| 1:C:191:ALA:CB | 1:C:218:GLY:HA2 | 2.17 | 0.74 |
| 1:C:26:LYS:HE2 | 1:C:113:PRO:O | 1.87 | 0.74 |
| 1:A:157:ASP:O | 1:A:157:ASP:CG | 2.23 | 0.74 |
| 1:D:214:THR:OG1 | 1:D:226:HIS:HB2 | 1.87 | 0.74 |
| 1:D:149:SER:CB | 1:D:167:ALA:CB | 2.49 | 0.74 |
| 1:E:108:LEU:HD22 | 1:E:110:LEU:CD2 | 2.17 | 0.74 |
| 1:E:240:LEU:HD23 | 1:E:241:ALA:O | 1.87 | 0.74 |
| 1:D:191:ALA:CB | 1:D:218:GLY:HA2 | 2.17 | 0.74 |
| 1:E:26:LYS:HE2 | 1:E:113:PRO:O | 1.87 | 0.74 |
| 1:D:197:LEU:HA | 1:D:200:LEU:HD12 | 1.70 | 0.74 |
| 1:B:25:CYS:SG | 1:B:70:LEU:HG | 2.26 | 0.74 |
| 1:E:29:LEU:HD23 | 1:E:34:LEU:HD13 | 1.69 | 0.74 |
| 1:F:108:LEU:HD22 | 1:F:110:LEU:CD2 | 2.17 | 0.74 |
| 1:A:96:LYS:CA | 1:A:108:LEU:O | 2.35 | 0.74 |
| 1:C:25:CYS:SG | 1:C:70:LEU:HG | 2.26 | 0.74 |
| 1:A:197:LEU:HA | 1:A:200:LEU:HD12 | 1.70 | 0.74 |
| 1:C:197:LEU:HA | 1:C:200:LEU:HD12 | 1.70 | 0.74 |
| 1:F:240:LEU:HD23 | 1:F:241:ALA:O | 1.87 | 0.74 |
| 1:C:6:VAL:HG22 | 1:C:56:PHE:CD2 | 2.23 | 0.74 |
| 1:B:108:LEU:HD22 | 1:B:110:LEU:CD2 | 2.17 | 0.74 |
| 1:E:214:THR:OG1 | 1:E:226:HIS:HB2 | 1.87 | 0.74 |
| 1:A:29:LEU:HD23 | 1:A:34:LEU:HD13 | 1.69 | 0.74 |
| 1:D:108:LEU:HD22 | 1:D:110:LEU:CD2 | 2.17 | 0.74 |
| 1:D:6:VAL:HG22 | 1:D:56:PHE:CD2 | 2.23 | 0.74 |
| 1:B:197:LEU:HA | 1:B:200:LEU:HD12 | 1.70 | 0.73 |
| 1:A:191:ALA:CB | 1:A:218:GLY:HA2 | 2.17 | 0.73 |
| 1:B:214:THR:OG1 | 1:B:226:HIS:HB2 | 1.87 | 0.73 |
| 1:E:191:ALA:CB | 1:E:218:GLY:HA2 | 2.17 | 0.73 |
| 1:D:151:HIS:HB3 | 1:D:196:SER:HA | 1.68 | 0.73 |
| 1:B:191:ALA:CB | 1:B:218:GLY:HA2 | 2.17 | 0.73 |
| 1:E:5:ILE:HG22 | 1:E:85:LEU:HB3 | 1.68 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:26:LYS:HE2 | 1:B:113:PRO:O | 1.87 | 0.73 |
| 1:D:96:LYS:CA | 1:D:108:LEU:O | 2.35 | 0.73 |
| 1:D:26:LYS:HE2 | 1:D:113:PRO:O | 1.87 | 0.73 |
| 1:A:6:VAL:HG22 | 1:A:56:PHE:CD2 | 2.23 | 0.73 |
| 1:A:26:LYS:HE2 | 1:A:113:PRO:O | 1.87 | 0.73 |
| 1:E:1:MET:HG3 | 1:E:91:ASP:HB3 | 1.70 | 0.73 |
| 1:A:214:THR:OG1 | 1:A:226:HIS:HB2 | 1.87 | 0.73 |
| 1:B:1:MET:HG3 | 1:B:91:ASP:HB3 | 1.70 | 0.73 |
| 1:D:8:ALA:CB | 1:D:82:ALA:O | 2.26 | 0.73 |
| 1:C:8:ALA:CB | 1:C:82:ALA:O | 2.25 | 0.73 |
| 1:A:240:LEU:HD23 | 1:A:241:ALA:O | 1.87 | 0.72 |
| 1:F:197:LEU:HA | 1:F:200:LEU:HD12 | 1.70 | 0.72 |
| 1:C:108:LEU:HD22 | 1:C:110:LEU:CD2 | 2.17 | 0.72 |
| 1:F:8:ALA:CB | 1:F:82:ALA:O | 2.25 | 0.72 |
| 1:E:101:ILE:HD11 | 1:E:104:LEU:HD12 | 1.71 | 0.72 |
| 1:E:197:LEU:HA | 1:E:200:LEU:HD12 | 1.70 | 0.72 |
| 1:E:6:VAL:HG22 | 1:E:56:PHE:CD2 | 2.23 | 0.72 |
| 1:B:96:LYS:CA | 1:B:108:LEU:O | 2.35 | 0.72 |
| 1:B:29:LEU:HD23 | 1:B:34:LEU:HD13 | 1.69 | 0.72 |
| 1:A:5:ILE:HG22 | 1:A:85:LEU:HB3 | 1.68 | 0.72 |
| 1:A:104:LEU:HD21 | 1:C:174:VAL:HG23 | 1.72 | 0.72 |
| 1:D:101:ILE:HD11 | 1:D:104:LEU:HD12 | 1.71 | 0.72 |
| 1:C:1:MET:HG3 | 1:C:91:ASP:HB3 | 1.70 | 0.72 |
| 1:B:101:ILE:HD11 | 1:B:104:LEU:HD12 | 1.71 | 0.72 |
| 1:F:96:LYS:CA | 1:F:108:LEU:O | 2.35 | 0.72 |
| 1:D:1:MET:HG3 | 1:D:91:ASP:HB3 | 1.70 | 0.72 |
| 1:A:101:ILE:HD11 | 1:A:104:LEU:HD12 | 1.71 | 0.72 |
| 1:E:96:LYS:CA | 1:E:108:LEU:O | 2.35 | 0.72 |
| 1:A:1:MET:HG3 | 1:A:91:ASP:HB3 | 1.70 | 0.72 |
| 1:A:197:LEU:HD23 | 1:A:198:ASP:H | 1.55 | 0.71 |
| 1:B:197:LEU:HD23 | 1:B:198:ASP:H | 1.55 | 0.71 |
| 1:C:104:LEU:HD13 | 1:C:104:LEU:O | 1.90 | 0.71 |
| 1:E:104:LEU:HD13 | 1:E:104:LEU:O | 1.90 | 0.71 |
| 1:C:29:LEU:HA | 1:C:34:LEU:HB3 | 1.73 | 0.71 |
| 1:C:101:ILE:HD11 | 1:C:104:LEU:HD12 | 1.71 | 0.71 |
| 1:C:191:ALA:CB | 1:C:218:GLY:CA | 2.69 | 0.71 |
| 1:F:197:LEU:HD23 | 1:F:198:ASP:H | 1.55 | 0.71 |
| 1:B:142:ILE:HD13 | 1:B:152:ILE:CD1 | 2.21 | 0.71 |
| 1:D:142:ILE:HD13 | 1:D:152:ILE:CD1 | 2.21 | 0.71 |
| 1:D:29:LEU:HA | 1:D:34:LEU:HB3 | 1.73 | 0.71 |
| 1:B:104:LEU:HD13 | 1:B:104:LEU:O | 1.91 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:142:ILE:HD13 | 1:C:152:ILE:CD1 | 2.21 | 0.71 |
| 1:D:197:LEU:HD23 | 1:D:198:ASP:H | 1.55 | 0.71 |
| 1:F:191:ALA:HB1 | 1:F:218:GLY:CA | 2.21 | 0.71 |
| 1:D:191:ALA:HB1 | 1:D:218:GLY:CA | 2.21 | 0.71 |
| 1:E:191:ALA:HB1 | 1:E:218:GLY:CA | 2.21 | 0.71 |
| 1:F:101:ILE:HD11 | 1:F:104:LEU:HD12 | 1.71 | 0.71 |
| 1:A:142:ILE:HD13 | 1:A:152:ILE:CD1 | 2.21 | 0.71 |
| 1:B:6:VAL:HG22 | 1:B:56:PHE:CD2 | 2.23 | 0.71 |
| 1:B:29:LEU:HA | 1:B:34:LEU:HB3 | 1.73 | 0.71 |
| 1:D:191:ALA:CB | 1:D:218:GLY:CA | 2.69 | 0.71 |
| 1:A:191:ALA:HB1 | 1:A:218:GLY:CA | 2.21 | 0.71 |
| 1:D:229:ILE:HD11 | 1:D:236:ILE:CD1 | 2.21 | 0.71 |
| 1:C:229:ILE:HD11 | 1:C:236:ILE:CD1 | 2.21 | 0.71 |
| 1:E:29:LEU:HA | 1:E:34:LEU:HB3 | 1.73 | 0.71 |
| 1:B:191:ALA:HB1 | 1:B:218:GLY:CA | 2.21 | 0.70 |
| 1:B:155:ARG:HA | 1:B:192:ASP:HB2 | 1.73 | 0.70 |
| 1:E:142:ILE:HD13 | 1:E:152:ILE:CD1 | 2.21 | 0.70 |
| 1:F:104:LEU:O | 1:F:104:LEU:HD13 | 1.90 | 0.70 |
| 1:F:155:ARG:HA | 1:F:192:ASP:HB2 | 1.73 | 0.70 |
| 1:F:229:ILE:HD11 | 1:F:236:ILE:CD1 | 2.21 | 0.70 |
| 1:A:104:LEU:HD13 | 1:A:104:LEU:O | 1.90 | 0.70 |
| 1:B:191:ALA:CB | 1:B:218:GLY:CA | 2.69 | 0.70 |
| 1:F:191:ALA:CB | 1:F:218:GLY:CA | 2.69 | 0.70 |
| 1:A:29:LEU:HA | 1:A:34:LEU:HB3 | 1.73 | 0.70 |
| 1:C:125:LEU:HD12 | 1:C:224:LYS:HE3 | 1.74 | 0.70 |
| 1:F:142:ILE:HD13 | 1:F:152:ILE:CD1 | 2.21 | 0.70 |
| 1:C:155:ARG:HA | 1:C:192:ASP:HB2 | 1.73 | 0.70 |
| 1:B:229:ILE:HD11 | 1:B:236:ILE:CD1 | 2.21 | 0.70 |
| 1:A:174:VAL:HG23 | 1:B:104:LEU:HD21 | 1.73 | 0.70 |
| 1:F:138:LEU:HG | 1:F:213:VAL:HG11 | 1.74 | 0.70 |
| 1:E:155:ARG:HA | 1:E:192:ASP:HB2 | 1.73 | 0.70 |
| 1:E:191:ALA:CB | 1:E:218:GLY:CA | 2.69 | 0.70 |
| 1:A:229:ILE:HD11 | 1:A:236:ILE:CD1 | 2.21 | 0.70 |
| 1:D:138:LEU:HG | 1:D:213:VAL:HG11 | 1.74 | 0.70 |
| 1:F:125:LEU:HD12 | 1:F:224:LYS:HE3 | 1.73 | 0.70 |
| 1:F:1:MET:HG3 | 1:F:91:ASP:HB3 | 1.70 | 0.70 |
| 1:D:104:LEU:O | 1:D:104:LEU:HD13 | 1.90 | 0.70 |
| 1:E:229:ILE:HD11 | 1:E:236:ILE:CD1 | 2.21 | 0.70 |
| 1:B:138:LEU:HG | 1:B:213:VAL:HG11 | 1.74 | 0.70 |
| 1:F:29:LEU:HA | 1:F:34:LEU:HB3 | 1.73 | 0.70 |
| 1:A:155:ARG:HA | 1:A:192:ASP:HB2 | 1.73 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:138:LEU:HG | 1:C:213:VAL:HG11 | 1.74 | 0.70 |
| 1:F:6:VAL:HG22 | 1:F:56:PHE:CD2 | 2.23 | 0.70 |
| 1:A:191:ALA:CB | 1:A:218:GLY:CA | 2.69 | 0.69 |
| 1:A:125:LEU:HD12 | 1:A:224:LYS:HE3 | 1.74 | 0.69 |
| 1:E:197:LEU:HD23 | 1:E:198:ASP:H | 1.55 | 0.69 |
| 1:B:125:LEU:HD12 | 1:B:224:LYS:HE3 | 1.74 | 0.69 |
| 1:C:191:ALA:HB1 | 1:C:218:GLY:CA | 2.21 | 0.69 |
| 1:F:25:CYS:O | 1:F:67:GLY:HA2 | 1.93 | 0.69 |
| 1:B:107:THR:HG23 | 1:B:107:THR:O | 1.92 | 0.69 |
| 1:A:33:SER:HB3 | 1:A:51:LEU:O | 1.92 | 0.69 |
| 1:A:25:CYS:O | 1:A:68:VAL:N | 2.26 | 0.69 |
| 1:D:155:ARG:HA | 1:D:192:ASP:HB2 | 1.73 | 0.69 |
| 1:C:197:LEU:HD23 | 1:C:198:ASP:H | 1.55 | 0.69 |
| 1:F:215:VAL:HG12 | 1:F:223:VAL:HG21 | 1.75 | 0.69 |
| 1:E:107:THR:O | 1:E:107:THR:HG23 | 1.92 | 0.69 |
| 1:E:215:VAL:HG12 | 1:E:223:VAL:HG21 | 1.75 | 0.69 |
| 1:D:107:THR:HG23 | 1:D:107:THR:O | 1.92 | 0.69 |
| 1:C:33:SER:HB3 | 1:C:51:LEU:O | 1.92 | 0.69 |
| 1:B:174:VAL:HG23 | 1:C:104:LEU:HD21 | 1.75 | 0.69 |
| 1:E:138:LEU:HG | 1:E:213:VAL:HG11 | 1.74 | 0.69 |
| 1:B:215:VAL:HG12 | 1:B:223:VAL:HG21 | 1.75 | 0.69 |
| 1:F:107:THR:HG23 | 1:F:107:THR:O | 1.92 | 0.69 |
| 1:D:104:LEU:HD21 | 1:F:174:VAL:HG23 | 1.73 | 0.69 |
| 1:A:25:CYS:O | 1:A:67:GLY:HA2 | 1.93 | 0.69 |
| 1:D:25:CYS:O | 1:D:67:GLY:HA2 | 1.93 | 0.69 |
| 1:C:107:THR:O | 1:C:107:THR:HG23 | 1.92 | 0.69 |
| 1:C:25:CYS:O | 1:C:68:VAL:N | 2.26 | 0.69 |
| 1:E:33:SER:HB3 | 1:E:51:LEU:O | 1.92 | 0.69 |
| 1:A:138:LEU:HG | 1:A:213:VAL:HG11 | 1.73 | 0.69 |
| 1:E:20:VAL:HG21 | 1:E:202:ASP:O | 1.93 | 0.69 |
| 1:C:20:VAL:HG21 | 1:C:202:ASP:O | 1.93 | 0.69 |
| 1:F:98:ASN:HA | 1:F:106:TYR:O | 1.93 | 0.69 |
| 1:A:98:ASN:HA | 1:A:106:TYR:O | 1.93 | 0.69 |
| 1:B:25:CYS:O | 1:B:67:GLY:HA2 | 1.93 | 0.69 |
| 1:A:20:VAL:HG21 | 1:A:202:ASP:O | 1.93 | 0.69 |
| 1:F:33:SER:HB3 | 1:F:51:LEU:O | 1.92 | 0.69 |
| 1:A:215:VAL:HG12 | 1:A:223:VAL:HG21 | 1.75 | 0.68 |
| 1:F:25:CYS:O | 1:F:68:VAL:N | 2.26 | 0.68 |
| 1:C:98:ASN:HA | 1:C:106:TYR:O | 1.93 | 0.68 |
| 1:E:125:LEU:HD12 | 1:E:224:LYS:HE3 | 1.73 | 0.68 |
| 1:D:153:ARG:HG2 | 1:D:194:LEU:CD2 | 2.24 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:96:LYS:CA | 1:C:108:LEU:O | 2.35 | 0.68 |
| 1:D:125:LEU:HD12 | 1:D:224:LYS:HE3 | 1.73 | 0.68 |
| 1:D:20:VAL:HG21 | 1:D:202:ASP:O | 1.93 | 0.68 |
| 1:C:25:CYS:O | 1:C:67:GLY:HA2 | 1.93 | 0.68 |
| 1:D:215:VAL:HG12 | 1:D:223:VAL:HG21 | 1.75 | 0.68 |
| 1:B:3:LYS:O | 1:B:59:TYR:HA | 1.94 | 0.68 |
| 1:D:33:SER:HB3 | 1:D:51:LEU:O | 1.92 | 0.68 |
| 1:C:153:ARG:HG2 | 1:C:194:LEU:CD2 | 2.24 | 0.68 |
| 1:E:191:ALA:HB1 | 1:E:218:GLY:O | 1.94 | 0.68 |
| 1:F:191:ALA:HB1 | 1:F:218:GLY:O | 1.94 | 0.68 |
| 1:F:20:VAL:HG21 | 1:F:202:ASP:O | 1.93 | 0.68 |
| 1:F:149:SER:CB | 1:F:167:ALA:CB | 2.49 | 0.68 |
| 1:A:153:ARG:HG2 | 1:A:194:LEU:CD2 | 2.24 | 0.68 |
| 1:F:153:ARG:HG2 | 1:F:194:LEU:CD2 | 2.24 | 0.68 |
| 1:E:25:CYS:O | 1:E:67:GLY:HA2 | 1.93 | 0.67 |
| 1:B:20:VAL:HG21 | 1:B:202:ASP:O | 1.93 | 0.67 |
| 1:C:191:ALA:HB1 | 1:C:218:GLY:O | 1.94 | 0.67 |
| 1:E:25:CYS:O | 1:E:68:VAL:N | 2.26 | 0.67 |
| 1:A:107:THR:HG23 | 1:A:107:THR:O | 1.92 | 0.67 |
| 1:A:3:LYS:O | 1:A:59:TYR:HA | 1.94 | 0.67 |
| 1:D:222:PRO:CD | 1:D:242:PRO:CG | 2.64 | 0.67 |
| 1:E:174:VAL:HG23 | 1:F:104:LEU:HD21 | 1.75 | 0.67 |
| 1:C:3:LYS:O | 1:C:59:TYR:HA | 1.94 | 0.67 |
| 1:E:3:LYS:O | 1:E:59:TYR:HA | 1.94 | 0.67 |
| 1:E:161:GLU:HB3 | 1:E:188:ALA:HB1 | 1.76 | 0.67 |
| 1:E:153:ARG:HG2 | 1:E:194:LEU:CD2 | 2.24 | 0.67 |
| 1:D:191:ALA:HB1 | 1:D:218:GLY:O | 1.94 | 0.67 |
| 1:C:215:VAL:HG12 | 1:C:223:VAL:HG21 | 1.75 | 0.67 |
| 1:A:191:ALA:HB1 | 1:A:218:GLY:O | 1.94 | 0.67 |
| 1:C:136:THR:HB | 1:C:209:THR:HG22 | 1.77 | 0.67 |
| 1:B:136:THR:HB | 1:B:209:THR:HG22 | 1.77 | 0.67 |
| 1:B:153:ARG:HG2 | 1:B:194:LEU:CD2 | 2.24 | 0.67 |
| 1:A:73:LEU:HD22 | 1:A:77:ALA:HB2 | 1.77 | 0.67 |
| 1:A:180:PRO:HA | 1:A:186:ILE:HD11 | 1.77 | 0.67 |
| 1:B:191:ALA:HB1 | 1:B:218:GLY:O | 1.94 | 0.67 |
| 1:B:4:ALA:O | 1:B:86:ILE:O | 2.13 | 0.67 |
| 1:C:161:GLU:HB3 | 1:C:188:ALA:HB1 | 1.76 | 0.67 |
| 1:D:98:ASN:HA | 1:D:106:TYR:O | 1.93 | 0.67 |
| 1:A:47:VAL:CA | 1:A:237:THR:O | 2.30 | 0.67 |
| 1:F:3:LYS:O | 1:F:59:TYR:HA | 1.94 | 0.67 |
| 1:E:136:THR:HB | 1:E:209:THR:HG22 | 1.77 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:87:HIS:HE1 | 1:D:185:SER:HA | 1.60 | 0.67 |
| 1:D:180:PRO:HA | 1:D:186:ILE:HD11 | 1.77 | 0.67 |
| 1:F:231:GLU:HB2 | 1:F:233:MET:CE | 2.25 | 0.67 |
| 1:F:180:PRO:HA | 1:F:186:ILE:HD11 | 1.77 | 0.67 |
| 1:F:207:ILE:HD12 | 1:F:207:ILE:N | 2.10 | 0.67 |
| 1:A:161:GLU:HB3 | 1:A:188:ALA:HB1 | 1.76 | 0.67 |
| 1:E:47:VAL:CA | 1:E:237:THR:O | 2.30 | 0.67 |
| 1:B:33:SER:HB3 | 1:B:51:LEU:O | 1.92 | 0.67 |
| 1:E:98:ASN:HA | 1:E:106:TYR:O | 1.93 | 0.66 |
| 1:A:207:ILE:N | 1:A:207:ILE:HD12 | 2.10 | 0.66 |
| 1:D:47:VAL:CA | 1:D:237:THR:O | 2.30 | 0.66 |
| 1:C:180:PRO:HA | 1:C:186:ILE:HD11 | 1.77 | 0.66 |
| 1:B:161:GLU:HB3 | 1:B:188:ALA:HB1 | 1.76 | 0.66 |
| 1:C:236:ILE:O | 1:C:236:ILE:HG13 | 1.95 | 0.66 |
| 1:B:236:ILE:O | 1:B:236:ILE:HG13 | 1.95 | 0.66 |
| 1:D:3:LYS:O | 1:D:59:TYR:HA | 1.94 | 0.66 |
| 1:F:4:ALA:O | 1:F:86:ILE:O | 2.13 | 0.66 |
| 1:B:39:VAL:HG13 | 1:B:43:ASN:HA | 1.78 | 0.66 |
| 1:E:231:GLU:HB2 | 1:E:233:MET:CE | 2.25 | 0.66 |
| 1:B:149:SER:CB | 1:B:167:ALA:CB | 2.49 | 0.66 |
| 1:F:236:ILE:HG13 | 1:F:236:ILE:O | 1.96 | 0.66 |
| 1:D:236:ILE:O | 1:D:236:ILE:HG13 | 1.96 | 0.66 |
| 1:B:98:ASN:HA | 1:B:106:TYR:O | 1.93 | 0.66 |
| 1:A:231:GLU:HB2 | 1:A:233:MET:CE | 2.25 | 0.66 |
| 1:A:236:ILE:O | 1:A:236:ILE:HG13 | 1.96 | 0.66 |
| 1:E:180:PRO:HA | 1:E:186:ILE:HD11 | 1.77 | 0.66 |
| 1:D:231:GLU:HB2 | 1:D:233:MET:CE | 2.25 | 0.66 |
| 1:D:170:ASP:O | 1:D:171:THR:CG2 | 2.44 | 0.66 |
| 1:A:4:ALA:O | 1:A:86:ILE:O | 2.13 | 0.66 |
| 1:F:136:THR:HB | 1:F:209:THR:HG22 | 1.77 | 0.66 |
| 1:D:161:GLU:HB3 | 1:D:188:ALA:HB1 | 1.76 | 0.66 |
| 1:E:207:ILE:HD12 | 1:E:207:ILE:N | 2.10 | 0.66 |
| 1:C:39:VAL:HG13 | 1:C:43:ASN:HA | 1.78 | 0.66 |
| 1:D:25:CYS:O | 1:D:68:VAL:N | 2.26 | 0.66 |
| 1:C:73:LEU:HD22 | 1:C:77:ALA:HB2 | 1.77 | 0.66 |
| 1:B:73:LEU:HD22 | 1:B:77:ALA:HB2 | 1.77 | 0.66 |
| 1:E:39:VAL:HG13 | 1:E:43:ASN:HA | 1.78 | 0.66 |
| 1:D:73:LEU:HD22 | 1:D:77:ALA:HB2 | 1.77 | 0.66 |
| 1:D:136:THR:HB | 1:D:209:THR:HG22 | 1.77 | 0.66 |
| 1:C:4:ALA:O | 1:C:86:ILE:O | 2.13 | 0.66 |
| 1:B:47:VAL:CA | 1:B:237:THR:O | 2.30 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:207:ILE:N | 1:B:207:ILE:HD12 | 2.10 | 0.66 |
| 1:B:25:CYS:O | 1:B:68:VAL:N | 2.26 | 0.66 |
| 1:D:32:GLU:N | 1:D:32:GLU:OE1 | 2.29 | 0.65 |
| 1:F:170:ASP:O | 1:F:171:THR:CG2 | 2.44 | 0.65 |
| 1:F:161:GLU:HB3 | 1:F:188:ALA:HB1 | 1.76 | 0.65 |
| 1:B:231:GLU:HB2 | 1:B:233:MET:CE | 2.25 | 0.65 |
| 1:C:231:GLU:HB2 | 1:C:233:MET:CE | 2.25 | 0.65 |
| 1:C:170:ASP:O | 1:C:171:THR:CG2 | 2.44 | 0.65 |
| 1:E:4:ALA:O | 1:E:86:ILE:O | 2.13 | 0.65 |
| 1:A:29:LEU:CD2 | 1:A:34:LEU:HD13 | 2.26 | 0.65 |
| 1:D:207:ILE:HD12 | 1:D:207:ILE:N | 2.10 | 0.65 |
| 1:C:29:LEU:CD2 | 1:C:34:LEU:HD13 | 2.26 | 0.65 |
| 1:D:4:ALA:O | 1:D:86:ILE:O | 2.13 | 0.65 |
| 1:C:136:THR:HB | 1:C:209:THR:CA | 2.27 | 0.65 |
| 1:A:39:VAL:HG13 | 1:A:43:ASN:HA | 1.78 | 0.65 |
| 1:F:73:LEU:HD22 | 1:F:77:ALA:HB2 | 1.77 | 0.65 |
| 1:E:73:LEU:HD22 | 1:E:77:ALA:HB2 | 1.77 | 0.65 |
| 1:E:200:LEU:HA | 1:E:203:MET:HE2 | 1.77 | 0.65 |
| 1:C:207:ILE:HD12 | 1:C:207:ILE:N | 2.10 | 0.65 |
| 1:B:136:THR:HB | 1:B:209:THR:CA | 2.27 | 0.65 |
| 1:A:200:LEU:HA | 1:A:203:MET:HE2 | 1.78 | 0.65 |
| 1:D:29:LEU:CD2 | 1:D:34:LEU:HD13 | 2.26 | 0.65 |
| 1:F:39:VAL:HG13 | 1:F:43:ASN:HA | 1.78 | 0.65 |
| 1:B:180:PRO:HA | 1:B:186:ILE:HD11 | 1.77 | 0.65 |
| 1:B:170:ASP:O | 1:B:171:THR:CG2 | 2.44 | 0.65 |
| 1:A:170:ASP:O | 1:A:171:THR:CG2 | 2.44 | 0.65 |
| 1:C:32:GLU:OE1 | 1:C:32:GLU:N | 2.30 | 0.65 |
| 1:E:29:LEU:CD2 | 1:E:34:LEU:HD13 | 2.26 | 0.65 |
| 1:D:39:VAL:HG13 | 1:D:43:ASN:HA | 1.77 | 0.65 |
| 1:A:149:SER:CB | 1:A:167:ALA:CB | 2.49 | 0.65 |
| 1:D:154:LEU:O | 1:D:156:VAL:HG23 | 1.97 | 0.65 |
| 1:C:222:PRO:CD | 1:C:242:PRO:CG | 2.64 | 0.65 |
| 1:B:154:LEU:O | 1:B:156:VAL:HG23 | 1.97 | 0.65 |
| 1:F:29:LEU:CD2 | 1:F:34:LEU:HD13 | 2.26 | 0.65 |
| 1:A:195:PHE:CE2 | 1:A:240:LEU:O | 2.50 | 0.65 |
| 1:B:157:ASP:HA | 1:B:160:GLU:O | 1.97 | 0.65 |
| 1:B:136:THR:CB | 1:B:209:THR:HG22 | 2.27 | 0.65 |
| 1:D:136:THR:HB | 1:D:209:THR:CA | 2.27 | 0.65 |
| 1:F:136:THR:HB | 1:F:209:THR:CA | 2.27 | 0.65 |
| 1:E:157:ASP:HA | 1:E:160:GLU:O | 1.97 | 0.65 |
| 1:E:73:LEU:CD2 | 1:E:77:ALA:HB2 | 2.27 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:87:HIS:CE1 | 1:D:185:SER:HA | 2.31 | 0.64 |
| 1:E:136:THR:CB | 1:E:209:THR:HG22 | 2.28 | 0.64 |
| 1:A:136:THR:HB | 1:A:209:THR:HG22 | 1.77 | 0.64 |
| 1:A:154:LEU:O | 1:A:156:VAL:HG23 | 1.97 | 0.64 |
| 1:E:236:ILE:HG13 | 1:E:236:ILE:O | 1.95 | 0.64 |
| 1:D:196:SER:H | 1:D:240:LEU:HD21 | 1.62 | 0.64 |
| 1:A:136:THR:CB | 1:A:209:THR:HG22 | 2.28 | 0.64 |
| 1:C:157:ASP:HA | 1:C:160:GLU:O | 1.97 | 0.64 |
| 1:A:73:LEU:CD2 | 1:A:77:ALA:HB2 | 2.27 | 0.64 |
| 1:D:108:LEU:CD2 | 1:D:110:LEU:HD23 | 2.28 | 0.64 |
| 1:A:136:THR:HB | 1:A:209:THR:CA | 2.27 | 0.64 |
| 1:B:73:LEU:CD2 | 1:B:77:ALA:HB2 | 2.27 | 0.64 |
| 1:E:32:GLU:OE1 | 1:E:32:GLU:N | 2.29 | 0.64 |
| 1:B:215:VAL:HG12 | 1:B:223:VAL:CG2 | 2.28 | 0.64 |
| 1:D:195:PHE:CE2 | 1:D:240:LEU:O | 2.50 | 0.64 |
| 1:D:200:LEU:HA | 1:D:203:MET:HE2 | 1.78 | 0.64 |
| 1:F:158:GLY:H | 1:F:162:THR:HB | 1.62 | 0.64 |
| 1:F:136:THR:CB | 1:F:209:THR:HG22 | 2.27 | 0.64 |
| 1:C:195:PHE:CE2 | 1:C:240:LEU:O | 2.50 | 0.64 |
| 1:C:200:LEU:HA | 1:C:203:MET:HE2 | 1.80 | 0.64 |
| 1:D:215:VAL:HG12 | 1:D:223:VAL:CG2 | 2.28 | 0.64 |
| 1:E:195:PHE:CE2 | 1:E:240:LEU:O | 2.50 | 0.64 |
| 1:F:32:GLU:N | 1:F:32:GLU:OE1 | 2.30 | 0.64 |
| 1:E:136:THR:HB | 1:E:209:THR:CB | 2.28 | 0.64 |
| 1:D:157:ASP:HA | 1:D:160:GLU:O | 1.97 | 0.64 |
| 1:A:108:LEU:CD2 | 1:A:110:LEU:HD23 | 2.28 | 0.64 |
| 1:D:73:LEU:CD2 | 1:D:77:ALA:HB2 | 2.27 | 0.64 |
| 1:C:73:LEU:CD2 | 1:C:77:ALA:HB2 | 2.27 | 0.64 |
| 1:C:136:THR:CB | 1:C:209:THR:HG22 | 2.27 | 0.64 |
| 1:E:136:THR:HB | 1:E:209:THR:CA | 2.27 | 0.64 |
| 1:B:136:THR:HB | 1:B:209:THR:CB | 2.28 | 0.64 |
| 1:B:195:PHE:CE2 | 1:B:240:LEU:O | 2.50 | 0.64 |
| 1:F:215:VAL:HG12 | 1:F:223:VAL:CG2 | 2.28 | 0.64 |
| 1:E:215:VAL:HG12 | 1:E:223:VAL:CG2 | 2.28 | 0.64 |
| 1:A:136:THR:HB | 1:A:209:THR:CB | 2.28 | 0.64 |
| 1:D:158:GLY:H | 1:D:162:THR:HB | 1.62 | 0.64 |
| 1:A:215:VAL:HG12 | 1:A:223:VAL:CG2 | 2.28 | 0.64 |
| 1:E:170:ASP:O | 1:E:171:THR:CG2 | 2.44 | 0.64 |
| 1:F:157:ASP:HA | 1:F:160:GLU:O | 1.97 | 0.64 |
| 1:A:32:GLU:OE1 | 1:A:32:GLU:N | 2.30 | 0.64 |
| 1:E:2:PHE:HZ | 1:E:64:GLY:HA3 | 1.64 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:136:THR:CB | 1:D:209:THR:HG22 | 2.27 | 0.64 |
| 1:A:231:GLU:HB2 | 1:A:233:MET:HE2 | 1.80 | 0.64 |
| 1:B:196:SER:H | 1:B:240:LEU:HD21 | 1.62 | 0.63 |
| 1:D:174:VAL:HG23 | 1:E:104:LEU:HD21 | 1.79 | 0.63 |
| 1:B:158:GLY:H | 1:B:162:THR:HB | 1.62 | 0.63 |
| 1:B:29:LEU:CD2 | 1:B:34:LEU:HD13 | 2.26 | 0.63 |
| 1:C:158:GLY:O | 1:C:159:ALA:HB3 | 1.98 | 0.63 |
| 1:E:158:GLY:H | 1:E:162:THR:HB | 1.62 | 0.63 |
| 1:E:196:SER:H | 1:E:240:LEU:HD21 | 1.62 | 0.63 |
| 1:A:157:ASP:HA | 1:A:160:GLU:O | 1.97 | 0.63 |
| 1:E:158:GLY:O | 1:E:159:ALA:HB3 | 1.98 | 0.63 |
| 1:B:158:GLY:O | 1:B:159:ALA:HB3 | 1.98 | 0.63 |
| 1:F:154:LEU:O | 1:F:156:VAL:HG23 | 1.97 | 0.63 |
| 1:F:73:LEU:CD2 | 1:F:77:ALA:HB2 | 2.27 | 0.63 |
| 1:A:158:GLY:H | 1:A:162:THR:HB | 1.62 | 0.63 |
| 1:D:136:THR:HB | 1:D:209:THR:CB | 2.28 | 0.63 |
| 1:C:158:GLY:H | 1:C:162:THR:HB | 1.62 | 0.63 |
| 1:C:215:VAL:HG12 | 1:C:223:VAL:CG2 | 2.28 | 0.63 |
| 1:C:2:PHE:HZ | 1:C:64:GLY:HA3 | 1.64 | 0.63 |
| 1:D:158:GLY:O | 1:D:159:ALA:HB3 | 1.98 | 0.63 |
| 1:E:154:LEU:O | 1:E:156:VAL:HG23 | 1.97 | 0.63 |
| 1:F:47:VAL:CA | 1:F:237:THR:O | 2.30 | 0.63 |
| 1:B:32:GLU:N | 1:B:32:GLU:OE1 | 2.29 | 0.63 |
| 1:F:136:THR:HB | 1:F:209:THR:CB | 2.28 | 0.63 |
| 1:C:154:LEU:O | 1:C:156:VAL:HG23 | 1.97 | 0.63 |
| 1:F:2:PHE:HZ | 1:F:64:GLY:HA3 | 1.63 | 0.63 |
| 1:F:195:PHE:CE2 | 1:F:240:LEU:O | 2.50 | 0.63 |
| 1:A:158:GLY:O | 1:A:159:ALA:HB3 | 1.98 | 0.63 |
| 1:D:231:GLU:HB2 | 1:D:233:MET:HE3 | 1.80 | 0.63 |
| 1:F:94:THR:O | 1:F:110:LEU:HB2 | 1.99 | 0.63 |
| 1:C:172:ASP:O | 1:C:173:ASP:OD1 | 2.17 | 0.63 |
| 1:C:136:THR:HB | 1:C:209:THR:CB | 2.28 | 0.63 |
| 1:E:149:SER:CB | 1:E:167:ALA:CB | 2.49 | 0.62 |
| 1:D:2:PHE:HZ | 1:D:64:GLY:HA3 | 1.64 | 0.62 |
| 1:F:158:GLY:O | 1:F:159:ALA:HB3 | 1.98 | 0.62 |
| 1:D:154:LEU:O | 1:D:155:ARG:C | 2.38 | 0.62 |
| 1:D:172:ASP:O | 1:D:173:ASP:OD1 | 2.17 | 0.62 |
| 1:E:108:LEU:CD2 | 1:E:110:LEU:HD23 | 2.28 | 0.62 |
| 1:C:196:SER:H | 1:C:240:LEU:HD21 | 1.62 | 0.62 |
| 1:E:154:LEU:O | 1:E:155:ARG:C | 2.38 | 0.62 |
| 1:B:94:THR:O | 1:B:110:LEU:HB2 | 1.99 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:108:LEU:CD2 | 1:F:110:LEU:HD23 | 2.28 | 0.62 |
| 1:F:153:ARG:HG2 | 1:F:194:LEU:HD21 | 1.82 | 0.62 |
| 1:D:73:LEU:HA | 1:D:76:VAL:CG1 | 2.29 | 0.62 |
| 1:B:97:LEU:HD12 | 1:B:110:LEU:HD21 | 1.81 | 0.62 |
| 1:F:195:PHE:HZ | 1:F:221:PHE:O | 1.83 | 0.62 |
| 1:B:2:PHE:HZ | 1:B:64:GLY:HA3 | 1.64 | 0.62 |
| 1:A:196:SER:H | 1:A:240:LEU:HD21 | 1.62 | 0.62 |
| 1:F:196:SER:H | 1:F:240:LEU:HD21 | 1.62 | 0.62 |
| 1:E:195:PHE:HZ | 1:E:221:PHE:O | 1.83 | 0.62 |
| 1:F:154:LEU:O | 1:F:155:ARG:C | 2.38 | 0.62 |
| 1:E:94:THR:O | 1:E:110:LEU:HB2 | 1.99 | 0.62 |
| 1:E:73:LEU:HA | 1:E:76:VAL:CG1 | 2.29 | 0.62 |
| 1:F:172:ASP:O | 1:F:173:ASP:OD1 | 2.17 | 0.62 |
| 1:A:154:LEU:O | 1:A:155:ARG:C | 2.38 | 0.62 |
| 1:C:108:LEU:CD2 | 1:C:110:LEU:HD23 | 2.28 | 0.62 |
| 1:A:2:PHE:HZ | 1:A:64:GLY:HA3 | 1.64 | 0.62 |
| 1:D:153:ARG:HG2 | 1:D:194:LEU:HD21 | 1.81 | 0.62 |
| 1:C:73:LEU:HA | 1:C:76:VAL:CG1 | 2.29 | 0.62 |
| 1:C:94:THR:O | 1:C:110:LEU:HB2 | 1.99 | 0.62 |
| 1:A:172:ASP:O | 1:A:173:ASP:OD1 | 2.17 | 0.62 |
| 1:A:222:PRO:CD | 1:A:242:PRO:CG | 2.64 | 0.62 |
| 1:C:153:ARG:HG2 | 1:C:194:LEU:HD21 | 1.82 | 0.62 |
| 1:E:153:ARG:HG2 | 1:E:194:LEU:HD21 | 1.82 | 0.61 |
| 1:B:108:LEU:CD2 | 1:B:110:LEU:HD23 | 2.28 | 0.61 |
| 1:B:73:LEU:HA | 1:B:76:VAL:CG1 | 2.29 | 0.61 |
| 1:A:153:ARG:HG2 | 1:A:194:LEU:HD21 | 1.82 | 0.61 |
| 1:E:172:ASP:O | 1:E:173:ASP:OD1 | 2.17 | 0.61 |
| 1:F:73:LEU:HA | 1:F:76:VAL:CG1 | 2.29 | 0.61 |
| 1:A:73:LEU:HA | 1:A:76:VAL:CG1 | 2.29 | 0.61 |
| 1:B:213:VAL:CG2 | 1:B:227:TYR:OH | 2.48 | 0.61 |
| 1:A:195:PHE:HZ | 1:A:221:PHE:O | 1.83 | 0.61 |
| 1:D:213:VAL:CG2 | 1:D:227:TYR:OH | 2.48 | 0.61 |
| 1:B:172:ASP:O | 1:B:173:ASP:OD1 | 2.17 | 0.61 |
| 1:F:200:LEU:HA | 1:F:203:MET:HE2 | 1.80 | 0.61 |
| 1:F:156:VAL:HG21 | 1:F:217:LEU:CG | 2.27 | 0.61 |
| 1:B:176:LEU:HD13 | 1:C:104:LEU:HB2 | 1.81 | 0.61 |
| 1:C:154:LEU:O | 1:C:155:ARG:C | 2.38 | 0.61 |
| 1:F:179:PRO:O | 1:F:183:LEU:HD22 | 2.01 | 0.61 |
| 1:A:213:VAL:CG2 | 1:A:227:TYR:OH | 2.48 | 0.61 |
| 1:D:195:PHE:HZ | 1:D:221:PHE:O | 1.83 | 0.61 |
| 1:C:231:GLU:HB2 | 1:C:233:MET:HE2 | 1.82 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:195:PHE:HZ | 1:B:221:PHE:O | 1.83 | 0.61 |
| 1:E:179:PRO:O | 1:E:183:LEU:HD22 | 2.01 | 0.61 |
| 1:C:195:PHE:HZ | 1:C:221:PHE:O | 1.83 | 0.61 |
| 1:E:97:LEU:HD12 | 1:E:110:LEU:HD21 | 1.82 | 0.61 |
| 1:D:94:THR:O | 1:D:110:LEU:HB2 | 1.99 | 0.61 |
| 1:E:156:VAL:HG23 | 1:E:217:LEU:HG | 1.83 | 0.61 |
| 1:A:94:THR:O | 1:A:110:LEU:HB2 | 1.99 | 0.61 |
| 1:B:185:SER:HA | 1:E:87:HIS:CE1 | 2.35 | 0.61 |
| 1:C:97:LEU:HD12 | 1:C:110:LEU:HD21 | 1.82 | 0.61 |
| 1:B:153:ARG:HG2 | 1:B:194:LEU:HD21 | 1.82 | 0.61 |
| 1:B:154:LEU:O | 1:B:155:ARG:C | 2.38 | 0.61 |
| 1:B:185:SER:HA | 1:E:87:HIS:HE1 | 1.66 | 0.61 |
| 1:F:133:LEU:HG | 1:F:183:LEU:HD12 | 1.83 | 0.61 |
| 1:D:8:ALA:HB2 | 1:D:84:ASP:O | 2.01 | 0.61 |
| 1:E:27:ILE:O | 1:E:65:VAL:HG23 | 2.01 | 0.61 |
| 1:A:179:PRO:O | 1:A:183:LEU:HD22 | 2.01 | 0.60 |
| 1:B:8:ALA:HB2 | 1:B:84:ASP:O | 2.01 | 0.60 |
| 1:C:191:ALA:CB | 1:C:218:GLY:C | 2.66 | 0.60 |
| 1:F:198:ASP:O | 1:F:201:LYS:HB2 | 2.01 | 0.60 |
| 1:A:97:LEU:HD12 | 1:A:110:LEU:HD21 | 1.81 | 0.60 |
| 1:B:179:PRO:O | 1:B:183:LEU:HD22 | 2.01 | 0.60 |
| 1:C:156:VAL:HG23 | 1:C:217:LEU:HG | 1.83 | 0.60 |
| 1:B:156:VAL:HG21 | 1:B:217:LEU:CG | 2.27 | 0.60 |
| 1:E:198:ASP:O | 1:E:201:LYS:HB2 | 2.01 | 0.60 |
| 1:B:27:ILE:O | 1:B:65:VAL:HG23 | 2.01 | 0.60 |
| 1:E:133:LEU:HG | 1:E:183:LEU:HD12 | 1.83 | 0.60 |
| 1:D:156:VAL:H | 1:D:192:ASP:CB | 2.15 | 0.60 |
| 1:F:213:VAL:CG2 | 1:F:227:TYR:OH | 2.48 | 0.60 |
| 1:A:133:LEU:HG | 1:A:183:LEU:HD12 | 1.83 | 0.60 |
| 1:B:156:VAL:H | 1:B:192:ASP:CB | 2.15 | 0.60 |
| 1:B:133:LEU:HG | 1:B:183:LEU:HD12 | 1.83 | 0.60 |
| 1:D:133:LEU:HG | 1:D:183:LEU:HD12 | 1.83 | 0.60 |
| 1:D:72:ARG:NH1 | 1:F:171:THR:HG21 | 2.08 | 0.60 |
| 1:F:231:GLU:HB2 | 1:F:233:MET:HE3 | 1.83 | 0.60 |
| 1:F:27:ILE:O | 1:F:65:VAL:HG23 | 2.01 | 0.60 |
| 1:A:156:VAL:H | 1:A:192:ASP:CB | 2.15 | 0.60 |
| 1:A:8:ALA:HB2 | 1:A:84:ASP:O | 2.01 | 0.60 |
| 1:A:27:ILE:O | 1:A:65:VAL:HG23 | 2.01 | 0.60 |
| 1:D:27:ILE:O | 1:D:65:VAL:HG23 | 2.01 | 0.60 |
| 1:B:198:ASP:O | 1:B:201:LYS:HB2 | 2.01 | 0.60 |
| 1:D:97:LEU:HD12 | 1:D:110:LEU:HD21 | 1.81 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:47:VAL:CA | 1:C:237:THR:O | 2.30 | 0.60 |
| 1:E:156:VAL:H | 1:E:192:ASP:CB | 2.15 | 0.60 |
| 1:C:198:ASP:O | 1:C:201:LYS:HB2 | 2.01 | 0.60 |
| 1:F:97:LEU:HD12 | 1:F:110:LEU:HD21 | 1.81 | 0.60 |
| 1:B:161:GLU:O | 1:B:162:THR:OG1 | 2.20 | 0.60 |
| 1:C:179:PRO:O | 1:C:183:LEU:HD22 | 2.01 | 0.60 |
| 1:D:179:PRO:O | 1:D:183:LEU:HD22 | 2.01 | 0.60 |
| 1:C:213:VAL:CG2 | 1:C:227:TYR:OH | 2.48 | 0.60 |
| 1:C:27:ILE:O | 1:C:65:VAL:HG23 | 2.01 | 0.59 |
| 1:F:8:ALA:HB2 | 1:F:84:ASP:O | 2.01 | 0.59 |
| 1:D:198:ASP:O | 1:D:201:LYS:HB2 | 2.01 | 0.59 |
| 1:B:179:PRO:HG2 | 1:D:179:PRO:HG2 | 1.83 | 0.59 |
| 1:F:156:VAL:HG23 | 1:F:217:LEU:HG | 1.83 | 0.59 |
| 1:C:8:ALA:HB2 | 1:C:84:ASP:O | 2.01 | 0.59 |
| 1:F:156:VAL:H | 1:F:192:ASP:CB | 2.15 | 0.59 |
| 1:E:213:VAL:CG2 | 1:E:227:TYR:OH | 2.48 | 0.59 |
| 1:B:175:ASP:O | 1:C:104:LEU:HD22 | 2.03 | 0.59 |
| 1:A:198:ASP:O | 1:A:201:LYS:HB2 | 2.01 | 0.59 |
| 1:B:195:PHE:CB | 1:B:240:LEU:HD22 | 2.33 | 0.59 |
| 1:F:194:LEU:CD2 | 1:F:245:GLN:HG3 | 2.30 | 0.59 |
| 1:E:8:ALA:HB2 | 1:E:84:ASP:O | 2.01 | 0.59 |
| 1:A:195:PHE:CB | 1:A:240:LEU:HD22 | 2.33 | 0.59 |
| 1:C:195:PHE:CB | 1:C:240:LEU:HD22 | 2.33 | 0.59 |
| 1:F:35:SER:O | 1:F:36:ILE:HD13 | 2.03 | 0.59 |
| 1:A:157:ASP:HB2 | 1:A:160:GLU:O | 2.03 | 0.59 |
| 1:A:156:VAL:HG23 | 1:A:217:LEU:HG | 1.83 | 0.59 |
| 1:D:222:PRO:CD | 1:D:242:PRO:HD2 | 2.32 | 0.59 |
| 1:E:222:PRO:CD | 1:E:242:PRO:CG | 2.64 | 0.59 |
| 1:D:87:HIS:O | 1:D:99:ILE:HG13 | 2.03 | 0.59 |
| 1:D:157:ASP:HB2 | 1:D:160:GLU:O | 2.03 | 0.59 |
| 1:E:231:GLU:HB2 | 1:E:233:MET:HE3 | 1.85 | 0.59 |
| 1:E:35:SER:O | 1:E:36:ILE:HD13 | 2.03 | 0.59 |
| 1:B:200:LEU:HA | 1:B:203:MET:HE2 | 1.83 | 0.59 |
| 1:A:87:HIS:O | 1:A:99:ILE:HG13 | 2.03 | 0.59 |
| 1:E:157:ASP:HB2 | 1:E:160:GLU:O | 2.03 | 0.59 |
| 1:C:156:VAL:H | 1:C:192:ASP:CB | 2.15 | 0.58 |
| 1:B:157:ASP:HB2 | 1:B:160:GLU:O | 2.03 | 0.58 |
| 1:F:157:ASP:HB2 | 1:F:160:GLU:O | 2.03 | 0.58 |
| 1:B:101:ILE:CD1 | 1:B:104:LEU:HD12 | 2.34 | 0.58 |
| 1:C:216:GLU:OE1 | 1:C:224:LYS:HD2 | 2.03 | 0.58 |
| 1:F:216:GLU:OE1 | 1:F:224:LYS:HD2 | 2.03 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:101:ILE:CD1 | 1:C:104:LEU:HD12 | 2.34 | 0.58 |
| 1:C:157:ASP:HB2 | 1:C:160:GLU:O | 2.03 | 0.58 |
| 1:A:101:ILE:CD1 | 1:A:104:LEU:HD12 | 2.34 | 0.58 |
| 1:C:222:PRO:CD | 1:C:242:PRO:HD2 | 2.32 | 0.58 |
| 1:C:6:VAL:CG2 | 1:C:56:PHE:HD2 | 2.14 | 0.58 |
| 1:C:73:LEU:HA | 1:C:76:VAL:HG12 | 1.86 | 0.58 |
| 1:A:216:GLU:OE1 | 1:A:224:LYS:HD2 | 2.03 | 0.58 |
| 1:D:156:VAL:HG23 | 1:D:217:LEU:HG | 1.83 | 0.58 |
| 1:F:133:LEU:CG | 1:F:183:LEU:CD1 | 2.80 | 0.58 |
| 1:E:216:GLU:OE1 | 1:E:224:LYS:HD2 | 2.03 | 0.58 |
| 1:A:191:ALA:CB | 1:A:218:GLY:C | 2.66 | 0.58 |
| 1:A:176:LEU:HD13 | 1:B:104:LEU:HB2 | 1.85 | 0.58 |
| 1:E:161:GLU:O | 1:E:162:THR:OG1 | 2.20 | 0.58 |
| 1:A:73:LEU:HA | 1:A:76:VAL:HG12 | 1.86 | 0.58 |
| 1:D:216:GLU:OE1 | 1:D:224:LYS:HD2 | 2.03 | 0.58 |
| 1:E:97:LEU:HB3 | 1:E:108:LEU:HB3 | 1.86 | 0.58 |
| 1:B:131:ILE:HD11 | 1:B:217:LEU:HB2 | 1.86 | 0.58 |
| 1:B:35:SER:O | 1:B:36:ILE:HD13 | 2.03 | 0.58 |
| 1:C:87:HIS:O | 1:C:99:ILE:HG13 | 2.03 | 0.58 |
| 1:E:195:PHE:CB | 1:E:240:LEU:HD22 | 2.33 | 0.58 |
| 1:C:6:VAL:N | 1:C:86:ILE:O | 2.37 | 0.58 |
| 1:D:35:SER:O | 1:D:36:ILE:HD13 | 2.03 | 0.58 |
| 1:B:87:HIS:O | 1:B:99:ILE:HG13 | 2.03 | 0.58 |
| 1:A:131:ILE:HD11 | 1:A:217:LEU:HB2 | 1.86 | 0.58 |
| 1:E:11:LEU:HD11 | 1:E:77:ALA:HB1 | 1.86 | 0.58 |
| 1:E:191:ALA:CB | 1:E:218:GLY:C | 2.66 | 0.58 |
| 1:E:87:HIS:O | 1:E:99:ILE:HG13 | 2.03 | 0.58 |
| 1:F:87:HIS:O | 1:F:99:ILE:HG13 | 2.03 | 0.58 |
| 1:F:222:PRO:CD | 1:F:242:PRO:HD2 | 2.32 | 0.57 |
| 1:E:101:ILE:CD1 | 1:E:104:LEU:HD12 | 2.34 | 0.57 |
| 1:E:194:LEU:CD2 | 1:E:245:GLN:HG3 | 2.30 | 0.57 |
| 1:D:97:LEU:HB3 | 1:D:108:LEU:HB3 | 1.86 | 0.57 |
| 1:D:73:LEU:HA | 1:D:76:VAL:HG12 | 1.86 | 0.57 |
| 1:E:6:VAL:CG2 | 1:E:56:PHE:HD2 | 2.14 | 0.57 |
| 1:B:214:THR:O | 1:B:225:LEU:HA | 2.04 | 0.57 |
| 1:E:133:LEU:CG | 1:E:183:LEU:CD1 | 2.80 | 0.57 |
| 1:B:216:GLU:OE1 | 1:B:224:LYS:HD2 | 2.03 | 0.57 |
| 1:F:97:LEU:HB3 | 1:F:108:LEU:HB3 | 1.86 | 0.57 |
| 1:F:73:LEU:HA | 1:F:76:VAL:HG12 | 1.86 | 0.57 |
| 1:E:131:ILE:HD11 | 1:E:217:LEU:HB2 | 1.86 | 0.57 |
| 1:A:186:ILE:HG22 | 1:A:187:GLU:N | 2.19 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:35:SER:O | 1:A:36:ILE:HD13 | 2.03 | 0.57 |
| 1:B:191:ALA:CB | 1:B:218:GLY:C | 2.66 | 0.57 |
| 1:B:186:ILE:HG22 | 1:B:187:GLU:N | 2.19 | 0.57 |
| 1:E:214:THR:O | 1:E:225:LEU:HA | 2.04 | 0.57 |
| 1:D:186:ILE:HG22 | 1:D:187:GLU:N | 2.19 | 0.57 |
| 1:C:35:SER:O | 1:C:36:ILE:HD13 | 2.03 | 0.57 |
| 1:F:214:THR:O | 1:F:225:LEU:HA | 2.04 | 0.57 |
| 1:A:214:THR:O | 1:A:225:LEU:HA | 2.04 | 0.57 |
| 1:E:73:LEU:HA | 1:E:76:VAL:HG12 | 1.86 | 0.57 |
| 1:D:195:PHE:CB | 1:D:240:LEU:HD22 | 2.33 | 0.57 |
| 1:C:214:THR:O | 1:C:225:LEU:HA | 2.04 | 0.57 |
| 1:C:133:LEU:HG | 1:C:183:LEU:HD12 | 1.83 | 0.57 |
| 1:B:73:LEU:HA | 1:B:76:VAL:HG12 | 1.86 | 0.57 |
| 1:D:157:ASP:O | 1:D:157:ASP:OD1 | 2.23 | 0.57 |
| 1:A:104:LEU:HB2 | 1:C:176:LEU:HD13 | 1.87 | 0.57 |
| 1:D:195:PHE:CE1 | 1:D:223:VAL:HB | 2.40 | 0.57 |
| 1:F:101:ILE:CD1 | 1:F:104:LEU:HD12 | 2.34 | 0.57 |
| 1:F:6:VAL:N | 1:F:86:ILE:O | 2.37 | 0.57 |
| 1:B:195:PHE:CE1 | 1:B:223:VAL:HB | 2.40 | 0.57 |
| 1:C:194:LEU:CD2 | 1:C:245:GLN:HG3 | 2.30 | 0.57 |
| 1:F:152:ILE:HG13 | 1:F:197:LEU:HB2 | 1.87 | 0.57 |
| 1:B:157:ASP:O | 1:B:157:ASP:OD1 | 2.23 | 0.57 |
| 1:E:152:ILE:HG13 | 1:E:197:LEU:HB2 | 1.87 | 0.57 |
| 1:C:97:LEU:HB3 | 1:C:108:LEU:HB3 | 1.86 | 0.57 |
| 1:C:145:ALA:O | 1:C:197:LEU:CD1 | 2.53 | 0.57 |
| 1:D:101:ILE:CD1 | 1:D:104:LEU:HD12 | 2.34 | 0.57 |
| 1:F:195:PHE:CB | 1:F:240:LEU:HD22 | 2.33 | 0.57 |
| 1:A:157:ASP:OD1 | 1:A:157:ASP:O | 2.23 | 0.57 |
| 1:A:194:LEU:CD2 | 1:A:245:GLN:HG3 | 2.30 | 0.57 |
| 1:F:186:ILE:HG22 | 1:F:187:GLU:N | 2.19 | 0.57 |
| 1:A:11:LEU:HD11 | 1:A:77:ALA:HB1 | 1.86 | 0.57 |
| 1:C:11:LEU:HD11 | 1:C:77:ALA:HB1 | 1.86 | 0.57 |
| 1:C:131:ILE:HD11 | 1:C:217:LEU:HB2 | 1.86 | 0.57 |
| 1:C:157:ASP:OD1 | 1:C:157:ASP:O | 2.23 | 0.57 |
| 1:A:6:VAL:CG2 | 1:A:56:PHE:HD2 | 2.14 | 0.57 |
| 1:B:194:LEU:CD2 | 1:B:245:GLN:HG3 | 2.30 | 0.56 |
| 1:A:222:PRO:CD | 1:A:242:PRO:HD2 | 2.32 | 0.56 |
| 1:F:68:VAL:O | 1:F:70:LEU:N | 2.38 | 0.56 |
| 1:C:195:PHE:CE1 | 1:C:223:VAL:HB | 2.40 | 0.56 |
| 1:A:156:VAL:H | 1:A:192:ASP:HB3 | 1.71 | 0.56 |
| 1:D:68:VAL:O | 1:D:70:LEU:N | 2.38 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:186:ILE:HG22 | 1:E:187:GLU:N | 2.19 | 0.56 |
| 1:D:149:SER:HB3 | 1:D:167:ALA:CB | 2.22 | 0.56 |
| 1:D:156:VAL:H | 1:D:192:ASP:HB3 | 1.71 | 0.56 |
| 1:D:131:ILE:HD11 | 1:D:217:LEU:HB2 | 1.86 | 0.56 |
| 1:A:152:ILE:HG13 | 1:A:197:LEU:HB2 | 1.87 | 0.56 |
| 1:F:195:PHE:CE1 | 1:F:223:VAL:HB | 2.40 | 0.56 |
| 1:F:145:ALA:O | 1:F:197:LEU:CD1 | 2.53 | 0.56 |
| 1:A:156:VAL:HG21 | 1:A:217:LEU:CG | 2.27 | 0.56 |
| 1:A:97:LEU:HB3 | 1:A:108:LEU:HB3 | 1.86 | 0.56 |
| 1:A:70:LEU:O | 1:A:74:GLU:HB2 | 2.06 | 0.56 |
| 1:D:145:ALA:O | 1:D:197:LEU:CD1 | 2.53 | 0.56 |
| 1:E:145:ALA:O | 1:E:197:LEU:CD1 | 2.53 | 0.56 |
| 1:B:97:LEU:HB3 | 1:B:108:LEU:HB3 | 1.86 | 0.56 |
| 1:B:70:LEU:O | 1:B:74:GLU:HB2 | 2.06 | 0.56 |
| 1:B:231:GLU:HB2 | 1:B:233:MET:HE2 | 1.87 | 0.56 |
| 1:D:92:GLU:O | 1:D:93:GLU:HG2 | 2.05 | 0.56 |
| 1:B:222:PRO:CB | 1:B:239:MET:HG2 | 2.34 | 0.56 |
| 1:C:152:ILE:HG13 | 1:C:197:LEU:HB2 | 1.87 | 0.56 |
| 1:C:133:LEU:CG | 1:C:183:LEU:CD1 | 2.80 | 0.56 |
| 1:C:186:ILE:HG22 | 1:C:187:GLU:N | 2.19 | 0.56 |
| 1:D:214:THR:O | 1:D:225:LEU:HA | 2.04 | 0.56 |
| 1:E:92:GLU:O | 1:E:93:GLU:HG2 | 2.06 | 0.56 |
| 1:C:222:PRO:CB | 1:C:239:MET:HG2 | 2.34 | 0.56 |
| 1:F:131:ILE:HD11 | 1:F:217:LEU:HB2 | 1.86 | 0.56 |
| 1:F:157:ASP:OD1 | 1:F:157:ASP:O | 2.23 | 0.56 |
| 1:B:11:LEU:HD11 | 1:B:77:ALA:HB1 | 1.86 | 0.56 |
| 1:D:6:VAL:CG2 | 1:D:56:PHE:HD2 | 2.14 | 0.56 |
| 1:D:6:VAL:N | 1:D:86:ILE:O | 2.37 | 0.56 |
| 1:E:157:ASP:O | 1:E:157:ASP:OD1 | 2.23 | 0.56 |
| 1:A:195:PHE:CE1 | 1:A:223:VAL:HB | 2.40 | 0.56 |
| 1:B:145:ALA:O | 1:B:197:LEU:CD1 | 2.53 | 0.56 |
| 1:C:201:LYS:O | 1:C:205:LYS:HB2 | 2.06 | 0.56 |
| 1:B:156:VAL:H | 1:B:192:ASP:HB3 | 1.71 | 0.56 |
| 1:E:6:VAL:N | 1:E:86:ILE:O | 2.37 | 0.56 |
| 1:A:145:ALA:O | 1:A:197:LEU:CD1 | 2.53 | 0.56 |
| 1:A:201:LYS:O | 1:A:205:LYS:HB2 | 2.06 | 0.56 |
| 1:B:195:PHE:HE2 | 1:B:240:LEU:O | 1.89 | 0.56 |
| 1:D:200:LEU:HG | 1:D:240:LEU:HD13 | 1.88 | 0.56 |
| 1:E:222:PRO:CD | 1:E:242:PRO:HD2 | 2.33 | 0.56 |
| 1:B:6:VAL:N | 1:B:86:ILE:O | 2.37 | 0.56 |
| 1:B:117:ARG:HG3 | 1:B:118:GLN:N | 2.21 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:161:GLU:O | 1:D:162:THR:OG1 | 2.20 | 0.56 |
| 1:D:127:LEU:HD22 | 1:D:218:GLY:HA3 | 1.88 | 0.56 |
| 1:B:200:LEU:HG | 1:B:240:LEU:HD13 | 1.88 | 0.56 |
| 1:C:161:GLU:O | 1:C:162:THR:OG1 | 2.20 | 0.56 |
| 1:F:11:LEU:HD11 | 1:F:77:ALA:HB1 | 1.86 | 0.56 |
| 1:F:222:PRO:CD | 1:F:242:PRO:CG | 2.64 | 0.56 |
| 1:D:201:LYS:O | 1:D:205:LYS:HB2 | 2.06 | 0.56 |
| 1:B:222:PRO:CD | 1:B:242:PRO:HD2 | 2.33 | 0.56 |
| 1:C:156:VAL:H | 1:C:192:ASP:HB3 | 1.70 | 0.56 |
| 1:C:70:LEU:O | 1:C:74:GLU:HB2 | 2.06 | 0.56 |
| 1:F:225:LEU:O | 1:F:237:THR:HA | 2.06 | 0.56 |
| 1:E:136:THR:HA | 1:E:208:PRO:O | 2.06 | 0.56 |
| 1:B:136:THR:HA | 1:B:208:PRO:O | 2.06 | 0.56 |
| 1:A:200:LEU:HG | 1:A:240:LEU:HD13 | 1.88 | 0.56 |
| 1:C:200:LEU:HG | 1:C:240:LEU:HD13 | 1.88 | 0.56 |
| 1:F:201:LYS:O | 1:F:205:LYS:HB2 | 2.06 | 0.56 |
| 1:D:11:LEU:HD11 | 1:D:77:ALA:HB1 | 1.86 | 0.56 |
| 1:E:225:LEU:O | 1:E:237:THR:HA | 2.06 | 0.56 |
| 1:B:231:GLU:HB2 | 1:B:233:MET:HE3 | 1.88 | 0.56 |
| 1:B:92:GLU:O | 1:B:93:GLU:HG2 | 2.05 | 0.56 |
| 1:F:149:SER:HB3 | 1:F:167:ALA:CB | 2.22 | 0.55 |
| 1:B:201:LYS:O | 1:B:205:LYS:HB2 | 2.06 | 0.55 |
| 1:F:49:LEU:HD21 | 1:F:236:ILE:HG22 | 1.88 | 0.55 |
| 1:D:104:LEU:HB2 | 1:F:176:LEU:HD13 | 1.88 | 0.55 |
| 1:D:152:ILE:HG13 | 1:D:197:LEU:HB2 | 1.87 | 0.55 |
| 1:E:195:PHE:HE2 | 1:E:240:LEU:O | 1.89 | 0.55 |
| 1:E:195:PHE:CE1 | 1:E:223:VAL:HB | 2.40 | 0.55 |
| 1:C:97:LEU:N | 1:C:108:LEU:O | 2.40 | 0.55 |
| 1:F:92:GLU:O | 1:F:93:GLU:HG2 | 2.05 | 0.55 |
| 1:B:152:ILE:HG13 | 1:B:197:LEU:HB2 | 1.87 | 0.55 |
| 1:E:70:LEU:O | 1:E:74:GLU:HB2 | 2.06 | 0.55 |
| 1:E:222:PRO:CB | 1:E:239:MET:HG2 | 2.34 | 0.55 |
| 1:B:49:LEU:HD21 | 1:B:236:ILE:HG22 | 1.88 | 0.55 |
| 1:B:97:LEU:N | 1:B:108:LEU:O | 2.40 | 0.55 |
| 1:F:5:ILE:HA | 1:F:86:ILE:O | 2.07 | 0.55 |
| 1:C:136:THR:HA | 1:C:208:PRO:O | 2.06 | 0.55 |
| 1:A:92:GLU:O | 1:A:93:GLU:HG2 | 2.05 | 0.55 |
| 1:D:156:VAL:HG21 | 1:D:217:LEU:CG | 2.27 | 0.55 |
| 1:F:70:LEU:O | 1:F:74:GLU:HB2 | 2.06 | 0.55 |
| 1:F:146:ASP:HA | 1:F:197:LEU:HD12 | 1.87 | 0.55 |
| 1:E:156:VAL:H | 1:E:192:ASP:HB3 | 1.71 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:68:VAL:O | 1:A:70:LEU:N | 2.37 | 0.55 |
| 1:A:97:LEU:N | 1:A:108:LEU:O | 2.40 | 0.55 |
| 1:E:201:LYS:O | 1:E:205:LYS:HB2 | 2.06 | 0.55 |
| 1:F:161:GLU:O | 1:F:162:THR:OG1 | 2.20 | 0.55 |
| 1:A:222:PRO:CB | 1:A:239:MET:HG2 | 2.34 | 0.55 |
| 1:A:161:GLU:O | 1:A:162:THR:OG1 | 2.20 | 0.55 |
| 1:E:97:LEU:N | 1:E:108:LEU:O | 2.40 | 0.55 |
| 1:D:136:THR:HA | 1:D:208:PRO:O | 2.06 | 0.55 |
| 1:A:117:ARG:HG3 | 1:A:118:GLN:N | 2.21 | 0.55 |
| 1:F:97:LEU:N | 1:F:108:LEU:O | 2.40 | 0.55 |
| 1:D:176:LEU:HD13 | 1:E:104:LEU:HB2 | 1.88 | 0.55 |
| 1:F:8:ALA:CB | 1:F:84:ASP:O | 2.55 | 0.55 |
| 1:F:156:VAL:H | 1:F:192:ASP:HB3 | 1.71 | 0.55 |
| 1:A:225:LEU:O | 1:A:237:THR:HA | 2.06 | 0.55 |
| 1:D:1:MET:HG3 | 1:D:91:ASP:HB2 | 1.89 | 0.55 |
| 1:F:117:ARG:HG3 | 1:F:118:GLN:N | 2.21 | 0.55 |
| 1:A:127:LEU:HD22 | 1:A:218:GLY:HA3 | 1.88 | 0.55 |
| 1:E:127:LEU:HD22 | 1:E:218:GLY:HA3 | 1.88 | 0.55 |
| 1:B:127:LEU:HD22 | 1:B:218:GLY:HA3 | 1.88 | 0.55 |
| 1:D:70:LEU:O | 1:D:74:GLU:HB2 | 2.06 | 0.55 |
| 1:F:136:THR:HB | 1:F:209:THR:CG2 | 2.37 | 0.55 |
| 1:E:138:LEU:HD12 | 1:E:204:ASN:ND2 | 2.22 | 0.55 |
| 1:A:49:LEU:HD21 | 1:A:236:ILE:HG22 | 1.88 | 0.55 |
| 1:B:156:VAL:HG23 | 1:B:217:LEU:HG | 1.83 | 0.55 |
| 1:E:8:ALA:CB | 1:E:84:ASP:O | 2.55 | 0.55 |
| 1:D:97:LEU:N | 1:D:108:LEU:O | 2.40 | 0.55 |
| 1:B:138:LEU:HD12 | 1:B:204:ASN:ND2 | 2.22 | 0.55 |
| 1:B:68:VAL:O | 1:B:70:LEU:N | 2.38 | 0.55 |
| 1:A:6:VAL:N | 1:A:86:ILE:O | 2.37 | 0.55 |
| 1:A:136:THR:HA | 1:A:208:PRO:O | 2.06 | 0.55 |
| 1:B:1:MET:HG3 | 1:B:91:ASP:HB2 | 1.89 | 0.55 |
| 1:D:117:ARG:HG3 | 1:D:118:GLN:N | 2.21 | 0.55 |
| 1:C:127:LEU:HD22 | 1:C:218:GLY:HA3 | 1.88 | 0.55 |
| 1:C:5:ILE:HA | 1:C:86:ILE:O | 2.07 | 0.55 |
| 1:D:138:LEU:HD12 | 1:D:204:ASN:ND2 | 2.22 | 0.55 |
| 1:C:225:LEU:O | 1:C:237:THR:HA | 2.06 | 0.55 |
| 1:F:136:THR:HA | 1:F:208:PRO:O | 2.06 | 0.55 |
| 1:A:216:GLU:HB2 | 1:A:224:LYS:HB2 | 1.89 | 0.55 |
| 1:D:216:GLU:HB2 | 1:D:224:LYS:HB2 | 1.89 | 0.55 |
| 1:D:8:ALA:CB | 1:D:84:ASP:O | 2.55 | 0.55 |
| 1:E:49:LEU:HD21 | 1:E:236:ILE:HG22 | 1.88 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:49:LEU:HD21 | 1:D:236:ILE:HG22 | 1.88 | 0.55 |
| 1:A:5:ILE:HA | 1:A:86:ILE:O | 2.07 | 0.55 |
| 1:E:20:VAL:CG1 | 1:E:202:ASP:HB3 | 2.36 | 0.55 |
| 1:D:5:ILE:HA | 1:D:86:ILE:O | 2.07 | 0.55 |
| 1:B:20:VAL:CG1 | 1:B:202:ASP:HB3 | 2.36 | 0.55 |
| 1:C:195:PHE:HE2 | 1:C:240:LEU:O | 1.89 | 0.54 |
| 1:D:195:PHE:HE2 | 1:D:240:LEU:O | 1.89 | 0.54 |
| 1:C:8:ALA:CB | 1:C:84:ASP:O | 2.55 | 0.54 |
| 1:B:8:ALA:CB | 1:B:84:ASP:O | 2.55 | 0.54 |
| 1:C:216:GLU:HB2 | 1:C:224:LYS:HB2 | 1.89 | 0.54 |
| 1:A:138:LEU:HD12 | 1:A:204:ASN:ND2 | 2.22 | 0.54 |
| 1:E:5:ILE:HA | 1:E:86:ILE:O | 2.07 | 0.54 |
| 1:D:225:LEU:O | 1:D:237:THR:HA | 2.06 | 0.54 |
| 1:C:1:MET:HG3 | 1:C:91:ASP:HB2 | 1.89 | 0.54 |
| 1:C:92:GLU:O | 1:C:93:GLU:HG2 | 2.05 | 0.54 |
| 1:F:138:LEU:HD12 | 1:F:204:ASN:ND2 | 2.22 | 0.54 |
| 1:A:1:MET:HG3 | 1:A:91:ASP:HB2 | 1.89 | 0.54 |
| 1:B:133:LEU:CG | 1:B:183:LEU:HD11 | 2.32 | 0.54 |
| 1:C:94:THR:O | 1:C:94:THR:HG22 | 2.08 | 0.54 |
| 1:B:20:VAL:HG13 | 1:B:202:ASP:CB | 2.37 | 0.54 |
| 1:C:136:THR:HB | 1:C:209:THR:CG2 | 2.37 | 0.54 |
| 1:B:149:SER:HB3 | 1:B:167:ALA:CB | 2.22 | 0.54 |
| 1:B:136:THR:HB | 1:B:209:THR:CG2 | 2.37 | 0.54 |
| 1:C:117:ARG:HG3 | 1:C:118:GLN:N | 2.21 | 0.54 |
| 1:A:196:SER:H | 1:A:240:LEU:CD2 | 2.21 | 0.54 |
| 1:C:146:ASP:HA | 1:C:197:LEU:HD12 | 1.87 | 0.54 |
| 1:D:153:ARG:HG2 | 1:D:194:LEU:HD22 | 1.90 | 0.54 |
| 1:B:133:LEU:CG | 1:B:183:LEU:CD1 | 2.80 | 0.54 |
| 1:D:94:THR:O | 1:D:94:THR:HG22 | 2.08 | 0.54 |
| 1:B:225:LEU:O | 1:B:237:THR:HA | 2.06 | 0.54 |
| 1:C:156:VAL:HG21 | 1:C:217:LEU:CG | 2.27 | 0.54 |
| 1:A:8:ALA:CB | 1:A:84:ASP:O | 2.55 | 0.54 |
| 1:B:5:ILE:HA | 1:B:86:ILE:O | 2.07 | 0.54 |
| 1:F:216:GLU:HB2 | 1:F:224:LYS:HB2 | 1.89 | 0.54 |
| 1:E:68:VAL:O | 1:E:70:LEU:N | 2.37 | 0.54 |
| 1:E:20:VAL:HG13 | 1:E:202:ASP:CB | 2.37 | 0.54 |
| 1:E:136:THR:HB | 1:E:209:THR:CG2 | 2.37 | 0.54 |
| 1:B:196:SER:H | 1:B:240:LEU:CD2 | 2.21 | 0.54 |
| 1:F:183:LEU:O | 1:F:185:SER:N | 2.41 | 0.54 |
| 1:F:195:PHE:HE2 | 1:F:240:LEU:O | 1.89 | 0.54 |
| 1:A:183:LEU:O | 1:A:185:SER:N | 2.41 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:127:LEU:HD22 | 1:F:218:GLY:HA3 | 1.88 | 0.54 |
| 1:D:136:THR:HB | 1:D:209:THR:CG2 | 2.37 | 0.54 |
| 1:E:117:ARG:HG3 | 1:E:118:GLN:N | 2.21 | 0.54 |
| 1:F:94:THR:HG22 | 1:F:94:THR:O | 2.08 | 0.54 |
| 1:F:196:SER:H | 1:F:240:LEU:CD2 | 2.21 | 0.54 |
| 1:F:200:LEU:HG | 1:F:240:LEU:HD13 | 1.88 | 0.54 |
| 1:E:200:LEU:HG | 1:E:240:LEU:HD13 | 1.88 | 0.54 |
| 1:B:183:LEU:O | 1:B:185:SER:N | 2.41 | 0.54 |
| 1:D:37:ARG:HB2 | 1:D:48:ASP:HA | 1.90 | 0.54 |
| 1:C:49:LEU:HD21 | 1:C:236:ILE:HG22 | 1.88 | 0.54 |
| 1:E:37:ARG:HB2 | 1:E:48:ASP:HA | 1.90 | 0.54 |
| 1:E:1:MET:HG3 | 1:E:91:ASP:HB2 | 1.89 | 0.54 |
| 1:C:138:LEU:HD12 | 1:C:204:ASN:ND2 | 2.22 | 0.54 |
| 1:C:183:LEU:O | 1:C:185:SER:N | 2.41 | 0.54 |
| 1:B:216:GLU:HB2 | 1:B:224:LYS:HB2 | 1.89 | 0.53 |
| 1:E:216:GLU:HB2 | 1:E:224:LYS:HB2 | 1.89 | 0.53 |
| 1:C:153:ARG:HG2 | 1:C:194:LEU:HD22 | 1.90 | 0.53 |
| 1:E:156:VAL:HG21 | 1:E:217:LEU:CG | 2.27 | 0.53 |
| 1:D:146:ASP:HA | 1:D:197:LEU:HD12 | 1.87 | 0.53 |
| 1:E:176:LEU:HD13 | 1:F:104:LEU:HB2 | 1.89 | 0.53 |
| 1:A:195:PHE:HE2 | 1:A:240:LEU:O | 1.89 | 0.53 |
| 1:A:37:ARG:HB2 | 1:A:48:ASP:HA | 1.90 | 0.53 |
| 1:A:146:ASP:HA | 1:A:197:LEU:HD12 | 1.87 | 0.53 |
| 1:B:146:ASP:HA | 1:B:197:LEU:HD12 | 1.87 | 0.53 |
| 1:E:11:LEU:HD21 | 1:E:77:ALA:HB1 | 1.91 | 0.53 |
| 1:B:37:ARG:HB2 | 1:B:48:ASP:HA | 1.90 | 0.53 |
| 1:B:6:VAL:CG2 | 1:B:56:PHE:HD2 | 2.14 | 0.53 |
| 1:E:231:GLU:HB2 | 1:E:233:MET:HE2 | 1.90 | 0.53 |
| 1:E:94:THR:O | 1:E:94:THR:HG22 | 2.08 | 0.53 |
| 1:E:153:ARG:HG2 | 1:E:194:LEU:HD22 | 1.90 | 0.53 |
| 1:E:183:LEU:O | 1:E:185:SER:N | 2.41 | 0.53 |
| 1:A:136:THR:HB | 1:A:209:THR:CG2 | 2.37 | 0.53 |
| 1:D:191:ALA:CB | 1:D:218:GLY:C | 2.66 | 0.53 |
| 1:A:11:LEU:HD21 | 1:A:77:ALA:HB1 | 1.91 | 0.53 |
| 1:A:94:THR:O | 1:A:94:THR:HG22 | 2.08 | 0.53 |
| 1:D:215:VAL:CG1 | 1:D:223:VAL:HG21 | 2.39 | 0.53 |
| 1:E:146:ASP:HA | 1:E:197:LEU:HD12 | 1.87 | 0.53 |
| 1:F:6:VAL:CG2 | 1:F:56:PHE:HD2 | 2.14 | 0.53 |
| 1:E:171:THR:HG21 | 1:F:72:ARG:NH1 | 2.13 | 0.53 |
| 1:F:222:PRO:CB | 1:F:239:MET:HG2 | 2.34 | 0.53 |
| 1:F:44:VAL:HG12 | 1:F:241:ALA:HB2 | 1.91 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:133:LEU:CG | 1:A:183:LEU:CD1 | 2.80 | 0.53 |
| 1:D:44:VAL:HG12 | 1:D:241:ALA:HB2 | 1.91 | 0.53 |
| 1:C:3:LYS:O | 1:C:59:TYR:CA | 2.57 | 0.53 |
| 1:D:183:LEU:O | 1:D:185:SER:N | 2.41 | 0.53 |
| 1:D:20:VAL:CG1 | 1:D:202:ASP:HB3 | 2.36 | 0.53 |
| 1:E:149:SER:HB3 | 1:E:167:ALA:CB | 2.22 | 0.53 |
| 1:B:153:ARG:HG2 | 1:B:194:LEU:HD22 | 1.90 | 0.53 |
| 1:D:196:SER:H | 1:D:240:LEU:CD2 | 2.21 | 0.53 |
| 1:E:44:VAL:HG12 | 1:E:241:ALA:CB | 2.39 | 0.53 |
| 1:B:94:THR:O | 1:B:94:THR:HG22 | 2.08 | 0.53 |
| 1:C:20:VAL:HG13 | 1:C:202:ASP:CB | 2.37 | 0.53 |
| 1:A:197:LEU:HD23 | 1:A:197:LEU:C | 2.29 | 0.53 |
| 1:F:11:LEU:HD21 | 1:F:77:ALA:HB1 | 1.91 | 0.53 |
| 1:D:194:LEU:CD2 | 1:D:245:GLN:HG3 | 2.30 | 0.53 |
| 1:D:133:LEU:CG | 1:D:183:LEU:CD1 | 2.80 | 0.53 |
| 1:B:11:LEU:HD21 | 1:B:77:ALA:HB1 | 1.91 | 0.53 |
| 1:F:1:MET:HG3 | 1:F:91:ASP:HB2 | 1.89 | 0.53 |
| 1:C:196:SER:H | 1:C:240:LEU:CD2 | 2.21 | 0.53 |
| 1:F:104:LEU:C | 1:F:104:LEU:HD13 | 2.30 | 0.53 |
| 1:E:133:LEU:CG | 1:E:183:LEU:HD11 | 2.32 | 0.53 |
| 1:C:149:SER:OG | 1:C:168:GLU:O | 2.27 | 0.52 |
| 1:B:194:LEU:O | 1:B:195:PHE:CG | 2.63 | 0.52 |
| 1:F:215:VAL:CG1 | 1:F:223:VAL:HG21 | 2.39 | 0.52 |
| 1:D:44:VAL:HG12 | 1:D:241:ALA:CB | 2.39 | 0.52 |
| 1:C:11:LEU:HD21 | 1:C:77:ALA:HB1 | 1.91 | 0.52 |
| 1:C:37:ARG:HB2 | 1:C:48:ASP:HA | 1.90 | 0.52 |
| 1:F:20:VAL:HG13 | 1:F:202:ASP:CB | 2.37 | 0.52 |
| 1:B:3:LYS:O | 1:B:59:TYR:CA | 2.57 | 0.52 |
| 1:A:149:SER:OG | 1:A:168:GLU:O | 2.27 | 0.52 |
| 1:B:215:VAL:CG1 | 1:B:223:VAL:HG21 | 2.39 | 0.52 |
| 1:C:131:ILE:CD1 | 1:C:217:LEU:HB2 | 2.40 | 0.52 |
| 1:E:131:ILE:CD1 | 1:E:217:LEU:HB2 | 2.40 | 0.52 |
| 1:E:196:SER:H | 1:E:240:LEU:CD2 | 2.21 | 0.52 |
| 1:B:149:SER:OG | 1:B:168:GLU:O | 2.27 | 0.52 |
| 1:A:194:LEU:O | 1:A:195:PHE:CG | 2.63 | 0.52 |
| 1:F:44:VAL:HG12 | 1:F:241:ALA:CB | 2.39 | 0.52 |
| 1:E:3:LYS:O | 1:E:59:TYR:CA | 2.57 | 0.52 |
| 1:F:131:ILE:CD1 | 1:F:217:LEU:HB2 | 2.40 | 0.52 |
| 1:F:3:LYS:O | 1:F:59:TYR:CA | 2.57 | 0.52 |
| 1:C:136:THR:OG1 | 1:C:209:THR:HG22 | 2.10 | 0.52 |
| 1:D:136:THR:OG1 | 1:D:209:THR:HG22 | 2.10 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:139:ASP:OD1 | 1:F:208:PRO:O | 2.28 | 0.52 |
| 1:F:37:ARG:HB2 | 1:F:48:ASP:HA | 1.90 | 0.52 |
| 1:C:44:VAL:HG12 | 1:C:241:ALA:CB | 2.39 | 0.52 |
| 1:F:136:THR:OG1 | 1:F:209:THR:HG22 | 2.10 | 0.52 |
| 1:C:194:LEU:O | 1:C:195:PHE:CG | 2.62 | 0.52 |
| 1:C:197:LEU:C | 1:C:197:LEU:HD23 | 2.29 | 0.52 |
| 1:B:136:THR:OG1 | 1:B:209:THR:HG22 | 2.10 | 0.52 |
| 1:A:139:ASP:OD1 | 1:A:208:PRO:O | 2.28 | 0.52 |
| 1:B:44:VAL:HG12 | 1:B:241:ALA:CB | 2.39 | 0.52 |
| 1:F:133:LEU:CG | 1:F:183:LEU:HD11 | 2.32 | 0.52 |
| 1:A:104:LEU:HD13 | 1:A:104:LEU:C | 2.30 | 0.52 |
| 1:E:194:LEU:O | 1:E:195:PHE:CG | 2.63 | 0.52 |
| 1:D:11:LEU:HD21 | 1:D:77:ALA:HB1 | 1.91 | 0.52 |
| 1:C:139:ASP:OD1 | 1:C:208:PRO:O | 2.28 | 0.52 |
| 1:D:139:ASP:OD1 | 1:D:208:PRO:O | 2.28 | 0.52 |
| 1:A:153:ARG:HG2 | 1:A:194:LEU:HD22 | 1.90 | 0.52 |
| 1:A:44:VAL:HG12 | 1:A:241:ALA:CB | 2.39 | 0.52 |
| 1:F:106:TYR:HE2 | 1:F:108:LEU:HB2 | 1.75 | 0.52 |
| 1:D:175:ASP:O | 1:E:104:LEU:HD22 | 2.09 | 0.52 |
| 1:E:104:LEU:HD13 | 1:E:104:LEU:C | 2.30 | 0.52 |
| 1:C:133:LEU:CD2 | 1:C:183:LEU:HD12 | 2.40 | 0.52 |
| 1:D:104:LEU:C | 1:D:104:LEU:HD13 | 2.30 | 0.52 |
| 1:F:197:LEU:HD23 | 1:F:197:LEU:C | 2.29 | 0.52 |
| 1:E:44:VAL:HG12 | 1:E:241:ALA:HB2 | 1.91 | 0.52 |
| 1:C:37:ARG:CG | 1:C:37:ARG:O | 2.49 | 0.52 |
| 1:C:20:VAL:CG1 | 1:C:202:ASP:HB3 | 2.36 | 0.52 |
| 1:D:3:LYS:O | 1:D:59:TYR:CA | 2.57 | 0.52 |
| 1:F:133:LEU:CD2 | 1:F:183:LEU:HD12 | 2.40 | 0.52 |
| 1:A:131:ILE:CD1 | 1:A:217:LEU:HB2 | 2.40 | 0.52 |
| 1:A:8:ALA:HB3 | 1:A:84:ASP:H | 1.75 | 0.52 |
| 1:D:194:LEU:O | 1:D:195:PHE:CG | 2.63 | 0.52 |
| 1:B:131:ILE:CD1 | 1:B:217:LEU:HB2 | 2.40 | 0.52 |
| 1:E:8:ALA:HB3 | 1:E:84:ASP:H | 1.75 | 0.52 |
| 1:D:95:ARG:O | 1:D:110:LEU:N | 2.43 | 0.52 |
| 1:C:66:ILE:HG21 | 1:C:110:LEU:HD13 | 1.93 | 0.52 |
| 1:C:133:LEU:CG | 1:C:183:LEU:HD11 | 2.32 | 0.52 |
| 1:B:139:ASP:OD1 | 1:B:208:PRO:O | 2.28 | 0.52 |
| 1:B:197:LEU:HD23 | 1:B:197:LEU:C | 2.29 | 0.51 |
| 1:B:222:PRO:CD | 1:B:242:PRO:CG | 2.64 | 0.51 |
| 1:D:8:ALA:HB3 | 1:D:84:ASP:H | 1.75 | 0.51 |
| 1:B:106:TYR:HE2 | 1:B:108:LEU:HB2 | 1.75 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:20:VAL:CG1 | 1:A:202:ASP:HB3 | 2.36 | 0.51 |
| 1:F:194:LEU:O | 1:F:195:PHE:CG | 2.62 | 0.51 |
| 1:E:95:ARG:O | 1:E:110:LEU:N | 2.43 | 0.51 |
| 1:A:106:TYR:HE2 | 1:A:108:LEU:HB2 | 1.75 | 0.51 |
| 1:D:222:PRO:CB | 1:D:239:MET:HG2 | 2.34 | 0.51 |
| 1:D:133:LEU:CD2 | 1:D:183:LEU:HD12 | 2.40 | 0.51 |
| 1:A:57:GLU:OE1 | 1:A:57:GLU:N | 2.44 | 0.51 |
| 1:F:20:VAL:CG1 | 1:F:202:ASP:HB3 | 2.36 | 0.51 |
| 1:B:133:LEU:CD2 | 1:B:183:LEU:HD12 | 2.40 | 0.51 |
| 1:C:57:GLU:OE1 | 1:C:57:GLU:N | 2.44 | 0.51 |
| 1:C:8:ALA:HB3 | 1:C:84:ASP:H | 1.75 | 0.51 |
| 1:F:8:ALA:HB3 | 1:F:84:ASP:H | 1.75 | 0.51 |
| 1:A:20:VAL:HG13 | 1:A:202:ASP:CB | 2.37 | 0.51 |
| 1:B:57:GLU:OE1 | 1:B:57:GLU:N | 2.44 | 0.51 |
| 1:E:139:ASP:OD1 | 1:E:208:PRO:O | 2.28 | 0.51 |
| 1:D:149:SER:OG | 1:D:168:GLU:O | 2.27 | 0.51 |
| 1:D:131:ILE:CD1 | 1:D:217:LEU:HB2 | 2.40 | 0.51 |
| 1:C:104:LEU:C | 1:C:104:LEU:HD13 | 2.30 | 0.51 |
| 1:C:215:VAL:CG1 | 1:C:223:VAL:HG21 | 2.39 | 0.51 |
| 1:E:215:VAL:CG1 | 1:E:223:VAL:HG21 | 2.39 | 0.51 |
| 1:F:161:GLU:HB3 | 1:F:188:ALA:CB | 2.41 | 0.51 |
| 1:E:133:LEU:CD2 | 1:E:183:LEU:HD12 | 2.40 | 0.51 |
| 1:A:3:LYS:O | 1:A:59:TYR:CA | 2.57 | 0.51 |
| 1:C:106:TYR:HE2 | 1:C:108:LEU:HB2 | 1.75 | 0.51 |
| 1:C:68:VAL:O | 1:C:70:LEU:N | 2.37 | 0.51 |
| 1:A:136:THR:OG1 | 1:A:209:THR:HG22 | 2.10 | 0.51 |
| 1:F:231:GLU:HB2 | 1:F:233:MET:HE2 | 1.91 | 0.51 |
| 1:D:161:GLU:HB3 | 1:D:188:ALA:CB | 2.41 | 0.51 |
| 1:A:44:VAL:HG12 | 1:A:241:ALA:HB2 | 1.91 | 0.51 |
| 1:B:44:VAL:HG12 | 1:B:241:ALA:HB2 | 1.91 | 0.51 |
| 1:D:170:ASP:C | 1:D:171:THR:HG22 | 2.31 | 0.51 |
| 1:C:95:ARG:O | 1:C:110:LEU:N | 2.43 | 0.51 |
| 1:A:29:LEU:HD12 | 1:A:29:LEU:N | 2.26 | 0.51 |
| 1:E:136:THR:OG1 | 1:E:209:THR:HG22 | 2.10 | 0.51 |
| 1:E:149:SER:OG | 1:E:168:GLU:O | 2.27 | 0.51 |
| 1:E:56:PHE:N | 1:E:56:PHE:CD1 | 2.79 | 0.51 |
| 1:B:8:ALA:HB3 | 1:B:84:ASP:H | 1.75 | 0.51 |
| 1:B:95:ARG:O | 1:B:110:LEU:N | 2.43 | 0.51 |
| 1:A:58:SER:C | 1:A:59:TYR:HD2 | 2.14 | 0.51 |
| 1:B:161:GLU:HB3 | 1:B:188:ALA:CB | 2.41 | 0.51 |
| 1:E:58:SER:C | 1:E:59:TYR:HD2 | 2.14 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:206:ALA:C | 1:C:207:ILE:HD12 | 2.32 | 0.51 |
| 1:B:104:LEU:C | 1:B:104:LEU:HD13 | 2.30 | 0.51 |
| 1:C:44:VAL:HG12 | 1:C:241:ALA:HB2 | 1.91 | 0.51 |
| 1:E:206:ALA:C | 1:E:207:ILE:HD12 | 2.32 | 0.51 |
| 1:A:66:ILE:HG21 | 1:A:110:LEU:HD13 | 1.93 | 0.51 |
| 1:D:197:LEU:HD23 | 1:D:197:LEU:C | 2.29 | 0.51 |
| 1:E:57:GLU:N | 1:E:57:GLU:OE1 | 2.44 | 0.51 |
| 1:D:29:LEU:HD12 | 1:D:29:LEU:N | 2.26 | 0.51 |
| 1:D:20:VAL:HG13 | 1:D:202:ASP:CB | 2.37 | 0.51 |
| 1:F:153:ARG:HG2 | 1:F:194:LEU:HD22 | 1.90 | 0.50 |
| 1:D:57:GLU:OE1 | 1:D:57:GLU:N | 2.44 | 0.50 |
| 1:F:58:SER:C | 1:F:59:TYR:HD2 | 2.14 | 0.50 |
| 1:E:66:ILE:HG21 | 1:E:110:LEU:HD13 | 1.93 | 0.50 |
| 1:D:106:TYR:HE2 | 1:D:108:LEU:HB2 | 1.75 | 0.50 |
| 1:D:66:ILE:HG21 | 1:D:110:LEU:HD13 | 1.93 | 0.50 |
| 1:C:108:LEU:HD23 | 1:C:109:ALA:O | 2.12 | 0.50 |
| 1:B:13:ASP:OD2 | 1:B:14:ALA:N | 2.45 | 0.50 |
| 1:F:108:LEU:HD23 | 1:F:109:ALA:O | 2.12 | 0.50 |
| 1:A:104:LEU:HD22 | 1:C:175:ASP:O | 2.11 | 0.50 |
| 1:E:161:GLU:HB3 | 1:E:188:ALA:CB | 2.41 | 0.50 |
| 1:A:95:ARG:O | 1:A:110:LEU:N | 2.43 | 0.50 |
| 1:A:107:THR:HG22 | 1:C:173:ASP:HB2 | 1.91 | 0.50 |
| 1:D:56:PHE:N | 1:D:56:PHE:CD1 | 2.79 | 0.50 |
| 1:F:56:PHE:N | 1:F:56:PHE:CD1 | 2.79 | 0.50 |
| 1:A:215:VAL:CG1 | 1:A:223:VAL:HG21 | 2.39 | 0.50 |
| 1:F:95:ARG:O | 1:F:110:LEU:N | 2.43 | 0.50 |
| 1:E:106:TYR:HE2 | 1:E:108:LEU:HB2 | 1.75 | 0.50 |
| 1:E:194:LEU:HD23 | 1:E:245:GLN:CG | 2.34 | 0.50 |
| 1:B:66:ILE:HG21 | 1:B:110:LEU:HD13 | 1.92 | 0.50 |
| 1:C:184:ILE:HD13 | 1:C:212:GLU:OE2 | 2.12 | 0.50 |
| 1:B:184:ILE:HD13 | 1:B:212:GLU:OE2 | 2.12 | 0.50 |
| 1:C:58:SER:C | 1:C:59:TYR:HD2 | 2.14 | 0.50 |
| 1:C:8:ALA:CB | 1:C:84:ASP:H | 2.25 | 0.50 |
| 1:B:29:LEU:N | 1:B:29:LEU:HD12 | 2.26 | 0.50 |
| 1:F:29:LEU:N | 1:F:29:LEU:HD12 | 2.26 | 0.50 |
| 1:D:13:ASP:OD2 | 1:D:14:ALA:N | 2.45 | 0.50 |
| 1:E:13:ASP:OD2 | 1:E:14:ALA:N | 2.45 | 0.50 |
| 1:A:133:LEU:CD2 | 1:A:183:LEU:HD12 | 2.40 | 0.50 |
| 1:A:206:ALA:C | 1:A:207:ILE:HD12 | 2.32 | 0.50 |
| 1:E:8:ALA:CB | 1:E:84:ASP:H | 2.25 | 0.50 |
| 1:E:153:ARG:CG | 1:E:194:LEU:HD21 | 2.42 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:184:ILE:HD13 | 1:D:212:GLU:OE2 | 2.12 | 0.50 |
| 1:A:173:ASP:HB2 | 1:B:107:THR:HG22 | 1.92 | 0.50 |
| 1:B:108:LEU:HD23 | 1:B:109:ALA:O | 2.12 | 0.50 |
| 1:B:56:PHE:CD1 | 1:B:56:PHE:N | 2.79 | 0.50 |
| 1:A:13:ASP:OD2 | 1:A:14:ALA:N | 2.45 | 0.50 |
| 1:F:153:ARG:CG | 1:F:194:LEU:HD21 | 2.42 | 0.50 |
| 1:D:194:LEU:HD23 | 1:D:245:GLN:CG | 2.34 | 0.50 |
| 1:F:184:ILE:HD13 | 1:F:212:GLU:OE2 | 2.12 | 0.50 |
| 1:A:184:ILE:HD13 | 1:A:212:GLU:OE2 | 2.12 | 0.50 |
| 1:A:153:ARG:CG | 1:A:194:LEU:HD21 | 2.42 | 0.50 |
| 1:D:108:LEU:HD23 | 1:D:109:ALA:O | 2.12 | 0.50 |
| 1:F:8:ALA:CB | 1:F:84:ASP:H | 2.25 | 0.50 |
| 1:C:29:LEU:N | 1:C:29:LEU:HD12 | 2.26 | 0.50 |
| 1:F:57:GLU:N | 1:F:57:GLU:OE1 | 2.44 | 0.50 |
| 1:D:10:THR:HA | 1:D:13:ASP:OD1 | 2.12 | 0.50 |
| 1:C:13:ASP:OD2 | 1:C:14:ALA:N | 2.45 | 0.50 |
| 1:F:13:ASP:OD2 | 1:F:14:ALA:N | 2.45 | 0.50 |
| 1:C:153:ARG:CG | 1:C:194:LEU:HD21 | 2.42 | 0.50 |
| 1:D:206:ALA:C | 1:D:207:ILE:HD12 | 2.32 | 0.50 |
| 1:F:191:ALA:CB | 1:F:218:GLY:C | 2.66 | 0.50 |
| 1:D:231:GLU:HB2 | 1:D:233:MET:HE2 | 1.94 | 0.50 |
| 1:B:10:THR:HA | 1:B:13:ASP:OD1 | 2.12 | 0.50 |
| 1:A:10:THR:O | 1:A:13:ASP:OD2 | 2.30 | 0.50 |
| 1:F:66:ILE:HG21 | 1:F:110:LEU:HD13 | 1.93 | 0.49 |
| 1:D:153:ARG:CG | 1:D:194:LEU:HD21 | 2.42 | 0.49 |
| 1:D:58:SER:C | 1:D:59:TYR:HD2 | 2.14 | 0.49 |
| 1:A:108:LEU:HD23 | 1:A:109:ALA:O | 2.12 | 0.49 |
| 1:E:10:THR:HA | 1:E:13:ASP:OD1 | 2.12 | 0.49 |
| 1:B:153:ARG:CG | 1:B:194:LEU:HD21 | 2.42 | 0.49 |
| 1:C:194:LEU:HD23 | 1:C:245:GLN:CG | 2.34 | 0.49 |
| 1:C:56:PHE:N | 1:C:56:PHE:CD1 | 2.79 | 0.49 |
| 1:B:8:ALA:CB | 1:B:84:ASP:H | 2.25 | 0.49 |
| 1:B:58:SER:C | 1:B:59:TYR:HD2 | 2.14 | 0.49 |
| 1:E:170:ASP:C | 1:E:171:THR:HG22 | 2.31 | 0.49 |
| 1:E:108:LEU:HD23 | 1:E:109:ALA:O | 2.12 | 0.49 |
| 1:F:206:ALA:C | 1:F:207:ILE:HD12 | 2.32 | 0.49 |
| 1:A:8:ALA:CB | 1:A:84:ASP:H | 2.25 | 0.49 |
| 1:C:170:ASP:C | 1:C:171:THR:HG22 | 2.31 | 0.49 |
| 1:E:29:LEU:N | 1:E:29:LEU:HD12 | 2.26 | 0.49 |
| 1:B:10:THR:O | 1:B:13:ASP:OD2 | 2.30 | 0.49 |
| 1:F:149:SER:OG | 1:F:168:GLU:O | 2.27 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:194:LEU:HD23 | 1:F:245:GLN:CG | 2.34 | 0.49 |
| 1:C:56:PHE:HE1 | 1:C:59:TYR:CZ | 2.31 | 0.49 |
| 1:E:56:PHE:HE1 | 1:E:59:TYR:CZ | 2.31 | 0.49 |
| 1:B:56:PHE:HE1 | 1:B:59:TYR:CZ | 2.31 | 0.49 |
| 1:A:10:THR:HA | 1:A:13:ASP:OD1 | 2.12 | 0.49 |
| 1:A:194:LEU:HD23 | 1:A:245:GLN:CG | 2.34 | 0.49 |
| 1:D:8:ALA:CB | 1:D:84:ASP:H | 2.25 | 0.49 |
| 1:C:162:THR:HG22 | 1:C:163:PHE:N | 2.28 | 0.49 |
| 1:E:68:VAL:HG11 | 1:E:73:LEU:HD12 | 1.95 | 0.49 |
| 1:D:142:ILE:HA | 1:D:152:ILE:HD11 | 1.95 | 0.49 |
| 1:C:68:VAL:HG11 | 1:C:73:LEU:HD12 | 1.95 | 0.49 |
| 1:D:56:PHE:HE1 | 1:D:59:TYR:CZ | 2.31 | 0.49 |
| 1:C:231:GLU:HB2 | 1:C:233:MET:HE3 | 1.92 | 0.49 |
| 1:E:10:THR:O | 1:E:13:ASP:OD2 | 2.30 | 0.49 |
| 1:E:184:ILE:HD13 | 1:E:212:GLU:OE2 | 2.12 | 0.49 |
| 1:B:195:PHE:HD2 | 1:B:240:LEU:CD2 | 2.26 | 0.49 |
| 1:C:195:PHE:HD2 | 1:C:240:LEU:CD2 | 2.26 | 0.49 |
| 1:D:68:VAL:HG11 | 1:D:73:LEU:HD12 | 1.95 | 0.49 |
| 1:A:231:GLU:HB2 | 1:A:233:MET:HE3 | 1.95 | 0.49 |
| 1:C:10:THR:O | 1:C:13:ASP:OD2 | 2.30 | 0.49 |
| 1:F:68:VAL:HG11 | 1:F:73:LEU:HD12 | 1.95 | 0.49 |
| 1:F:195:PHE:HD2 | 1:F:240:LEU:CD2 | 2.26 | 0.49 |
| 1:F:194:LEU:HB3 | 1:F:243:ARG:HB2 | 1.95 | 0.49 |
| 1:E:142:ILE:HA | 1:E:152:ILE:HD11 | 1.95 | 0.49 |
| 1:F:157:ASP:CA | 1:F:160:GLU:O | 2.61 | 0.49 |
| 1:B:206:ALA:C | 1:B:207:ILE:HD12 | 2.32 | 0.49 |
| 1:D:10:THR:O | 1:D:13:ASP:OD2 | 2.30 | 0.49 |
| 1:C:10:THR:HA | 1:C:13:ASP:OD1 | 2.12 | 0.49 |
| 1:F:10:THR:HA | 1:F:13:ASP:OD1 | 2.12 | 0.49 |
| 1:A:194:LEU:HB3 | 1:A:243:ARG:HB2 | 1.95 | 0.48 |
| 1:B:142:ILE:HA | 1:B:152:ILE:HD11 | 1.95 | 0.48 |
| 1:A:56:PHE:HE1 | 1:A:59:TYR:CZ | 2.31 | 0.48 |
| 1:F:10:THR:O | 1:F:13:ASP:OD2 | 2.30 | 0.48 |
| 1:B:194:LEU:HB3 | 1:B:243:ARG:HB2 | 1.95 | 0.48 |
| 1:A:161:GLU:HB3 | 1:A:188:ALA:CB | 2.41 | 0.48 |
| 1:E:162:THR:HG22 | 1:E:163:PHE:N | 2.28 | 0.48 |
| 1:D:157:ASP:CA | 1:D:160:GLU:O | 2.61 | 0.48 |
| 1:C:194:LEU:HB3 | 1:C:243:ARG:HB2 | 1.95 | 0.48 |
| 1:A:68:VAL:HG11 | 1:A:73:LEU:HD12 | 1.95 | 0.48 |
| 1:C:5:ILE:HD13 | 1:D:184:ILE:O | 2.13 | 0.48 |
| 1:C:107:THR:CG2 | 1:C:107:THR:O | 2.61 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:157:ASP:CA | 1:E:160:GLU:O | 2.61 | 0.48 |
| 1:C:161:GLU:HB3 | 1:C:188:ALA:CB | 2.41 | 0.48 |
| 1:C:142:ILE:HA | 1:C:152:ILE:HD11 | 1.95 | 0.48 |
| 1:D:107:THR:O | 1:D:107:THR:CG2 | 2.61 | 0.48 |
| 1:B:170:ASP:C | 1:B:171:THR:HG22 | 2.31 | 0.48 |
| 1:A:170:ASP:C | 1:A:171:THR:HG22 | 2.31 | 0.48 |
| 1:A:142:ILE:HA | 1:A:152:ILE:HD11 | 1.95 | 0.48 |
| 1:A:195:PHE:HD2 | 1:A:240:LEU:CD2 | 2.26 | 0.48 |
| 1:C:157:ASP:CA | 1:C:160:GLU:O | 2.61 | 0.48 |
| 1:F:107:THR:CG2 | 1:F:107:THR:O | 2.61 | 0.48 |
| 1:F:142:ILE:HA | 1:F:152:ILE:HD11 | 1.95 | 0.48 |
| 1:D:195:PHE:HD2 | 1:D:240:LEU:CD2 | 2.26 | 0.48 |
| 1:B:162:THR:HG22 | 1:B:163:PHE:N | 2.28 | 0.48 |
| 1:A:20:VAL:HG12 | 1:A:21:LEU:HD23 | 1.96 | 0.48 |
| 1:A:56:PHE:CD1 | 1:A:56:PHE:N | 2.79 | 0.48 |
| 1:D:56:PHE:CD1 | 1:D:59:TYR:CD2 | 3.02 | 0.48 |
| 1:D:104:LEU:HD22 | 1:F:175:ASP:O | 2.12 | 0.48 |
| 1:C:56:PHE:CD1 | 1:C:59:TYR:CD2 | 3.02 | 0.48 |
| 1:F:170:ASP:C | 1:F:171:THR:HG22 | 2.31 | 0.48 |
| 1:F:162:THR:HG22 | 1:F:163:PHE:N | 2.28 | 0.48 |
| 1:D:20:VAL:HG12 | 1:D:21:LEU:HD23 | 1.95 | 0.48 |
| 1:B:175:ASP:O | 1:C:104:LEU:CD2 | 2.62 | 0.48 |
| 1:A:162:THR:HG22 | 1:A:163:PHE:N | 2.28 | 0.48 |
| 1:E:156:VAL:CG1 | 1:E:191:ALA:O | 2.62 | 0.48 |
| 1:E:56:PHE:CD1 | 1:E:59:TYR:CD2 | 3.02 | 0.48 |
| 1:F:56:PHE:HE1 | 1:F:59:TYR:CZ | 2.31 | 0.48 |
| 1:A:152:ILE:HD13 | 1:A:165:ILE:HG21 | 1.96 | 0.48 |
| 1:F:152:ILE:HD13 | 1:F:165:ILE:HG21 | 1.96 | 0.48 |
| 1:D:195:PHE:CE2 | 1:D:242:PRO:CD | 2.73 | 0.48 |
| 1:E:195:PHE:CE2 | 1:E:242:PRO:CD | 2.73 | 0.48 |
| 1:B:47:VAL:HB | 1:B:238:TYR:CE2 | 2.49 | 0.48 |
| 1:C:47:VAL:HB | 1:C:238:TYR:CE2 | 2.49 | 0.48 |
| 1:C:20:VAL:HG12 | 1:C:21:LEU:HD23 | 1.96 | 0.48 |
| 1:F:56:PHE:CD1 | 1:F:59:TYR:CD2 | 3.02 | 0.48 |
| 1:C:149:SER:HB3 | 1:C:167:ALA:CB | 2.22 | 0.48 |
| 1:C:156:VAL:CG1 | 1:C:191:ALA:O | 2.62 | 0.48 |
| 1:E:97:LEU:HB2 | 1:E:110:LEU:HD21 | 1.96 | 0.48 |
| 1:D:152:ILE:HD13 | 1:D:165:ILE:HG21 | 1.96 | 0.48 |
| 1:F:156:VAL:CG1 | 1:F:191:ALA:O | 2.62 | 0.48 |
| 1:F:47:VAL:HB | 1:F:238:TYR:CE2 | 2.49 | 0.48 |
| 1:B:3:LYS:O | 1:B:59:TYR:HB3 | 2.14 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:44:VAL:CG1 | 1:B:241:ALA:HB2 | 2.44 | 0.47 |
| 1:A:72:ARG:NH1 | 1:C:171:THR:HG21 | 2.13 | 0.47 |
| 1:D:194:LEU:HB3 | 1:D:243:ARG:HB2 | 1.95 | 0.47 |
| 1:B:56:PHE:CD1 | 1:B:59:TYR:CD2 | 3.02 | 0.47 |
| 1:F:3:LYS:O | 1:F:59:TYR:HB3 | 2.14 | 0.47 |
| 1:C:151:HIS:CB | 1:C:195:PHE:O | 2.62 | 0.47 |
| 1:C:44:VAL:CG1 | 1:C:241:ALA:HB2 | 2.44 | 0.47 |
| 1:D:186:ILE:CG2 | 1:D:187:GLU:N | 2.77 | 0.47 |
| 1:D:97:LEU:HB2 | 1:D:110:LEU:HD21 | 1.96 | 0.47 |
| 1:D:47:VAL:HB | 1:D:238:TYR:CE2 | 2.49 | 0.47 |
| 1:B:152:ILE:HD13 | 1:B:165:ILE:HG21 | 1.96 | 0.47 |
| 1:B:151:HIS:CB | 1:B:195:PHE:O | 2.62 | 0.47 |
| 1:A:133:LEU:CG | 1:A:183:LEU:HD11 | 2.32 | 0.47 |
| 1:D:151:HIS:CB | 1:D:195:PHE:O | 2.62 | 0.47 |
| 1:E:195:PHE:HD2 | 1:E:240:LEU:CD2 | 2.26 | 0.47 |
| 1:E:151:HIS:CB | 1:E:195:PHE:O | 2.62 | 0.47 |
| 1:B:68:VAL:HG11 | 1:B:73:LEU:HD12 | 1.95 | 0.47 |
| 1:E:65:VAL:HG22 | 1:E:113:PRO:CG | 2.44 | 0.47 |
| 1:D:44:VAL:CG1 | 1:D:241:ALA:HB2 | 2.44 | 0.47 |
| 1:B:157:ASP:CA | 1:B:160:GLU:O | 2.61 | 0.47 |
| 1:E:186:ILE:CG2 | 1:E:187:GLU:N | 2.78 | 0.47 |
| 1:A:5:ILE:O | 1:A:56:PHE:HA | 2.15 | 0.47 |
| 1:E:20:VAL:HG12 | 1:E:21:LEU:HD23 | 1.95 | 0.47 |
| 1:D:162:THR:HG22 | 1:D:163:PHE:N | 2.28 | 0.47 |
| 1:A:44:VAL:CG1 | 1:A:241:ALA:HB2 | 2.44 | 0.47 |
| 1:F:240:LEU:HD23 | 1:F:241:ALA:N | 2.30 | 0.47 |
| 1:A:65:VAL:HG22 | 1:A:113:PRO:CG | 2.45 | 0.47 |
| 1:E:152:ILE:HD13 | 1:E:165:ILE:HG21 | 1.96 | 0.47 |
| 1:E:175:ASP:O | 1:F:104:LEU:HD22 | 2.14 | 0.47 |
| 1:C:97:LEU:HB2 | 1:C:110:LEU:HD21 | 1.96 | 0.47 |
| 1:B:194:LEU:HD23 | 1:B:245:GLN:CG | 2.34 | 0.47 |
| 1:F:151:HIS:CB | 1:F:195:PHE:O | 2.62 | 0.47 |
| 1:E:194:LEU:HB3 | 1:E:243:ARG:HB2 | 1.95 | 0.47 |
| 1:E:5:ILE:O | 1:E:56:PHE:HA | 2.15 | 0.47 |
| 1:B:173:ASP:HB2 | 1:C:107:THR:HG23 | 1.90 | 0.47 |
| 1:C:133:LEU:O | 1:C:213:VAL:N | 2.29 | 0.47 |
| 1:E:47:VAL:HB | 1:E:238:TYR:CE2 | 2.49 | 0.47 |
| 1:A:56:PHE:CD1 | 1:A:59:TYR:CD2 | 3.02 | 0.47 |
| 1:D:5:ILE:O | 1:D:56:PHE:HA | 2.15 | 0.47 |
| 1:A:151:HIS:CB | 1:A:195:PHE:O | 2.62 | 0.47 |
| 1:B:146:ASP:C | 1:B:147:MET:HG3 | 2.35 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:133:LEU:HD23 | 1:F:133:LEU:HA | 1.74 | 0.47 |
| 1:F:65:VAL:HG22 | 1:F:113:PRO:CG | 2.45 | 0.47 |
| 1:C:146:ASP:C | 1:C:147:MET:HG3 | 2.35 | 0.47 |
| 1:F:44:VAL:CG1 | 1:F:241:ALA:HB2 | 2.44 | 0.47 |
| 1:A:157:ASP:CA | 1:A:160:GLU:O | 2.61 | 0.47 |
| 1:A:97:LEU:HB2 | 1:A:110:LEU:HD21 | 1.96 | 0.47 |
| 1:B:186:ILE:CG2 | 1:B:187:GLU:N | 2.78 | 0.47 |
| 1:D:65:VAL:HG22 | 1:D:113:PRO:CG | 2.44 | 0.47 |
| 1:C:65:VAL:HG22 | 1:C:113:PRO:CG | 2.45 | 0.47 |
| 1:B:97:LEU:HB2 | 1:B:110:LEU:HD21 | 1.96 | 0.47 |
| 1:A:47:VAL:HB | 1:A:238:TYR:CE2 | 2.49 | 0.47 |
| 1:A:3:LYS:O | 1:A:59:TYR:HB3 | 2.14 | 0.47 |
| 1:D:3:LYS:O | 1:D:59:TYR:HB3 | 2.14 | 0.47 |
| 1:B:20:VAL:HG12 | 1:B:21:LEU:HD23 | 1.96 | 0.47 |
| 1:F:4:ALA:HB1 | 1:F:56:PHE:CD2 | 2.50 | 0.47 |
| 1:A:240:LEU:HD23 | 1:A:241:ALA:N | 2.30 | 0.47 |
| 1:D:240:LEU:HD23 | 1:D:241:ALA:N | 2.30 | 0.47 |
| 1:E:4:ALA:HB1 | 1:E:56:PHE:CD2 | 2.50 | 0.47 |
| 1:F:20:VAL:HG12 | 1:F:21:LEU:HD23 | 1.96 | 0.47 |
| 1:B:4:ALA:HB1 | 1:B:56:PHE:CD2 | 2.50 | 0.47 |
| 1:B:195:PHE:CE2 | 1:B:242:PRO:CD | 2.73 | 0.47 |
| 1:B:240:LEU:HD23 | 1:B:241:ALA:N | 2.30 | 0.47 |
| 1:E:44:VAL:CG1 | 1:E:241:ALA:HB2 | 2.44 | 0.47 |
| 1:C:3:LYS:O | 1:C:59:TYR:HB3 | 2.14 | 0.47 |
| 1:E:3:LYS:O | 1:E:59:TYR:HB3 | 2.14 | 0.47 |
| 1:B:65:VAL:HG22 | 1:B:113:PRO:CG | 2.44 | 0.47 |
| 1:C:4:ALA:HB1 | 1:C:56:PHE:CD2 | 2.50 | 0.47 |
| 1:C:5:ILE:O | 1:C:56:PHE:HA | 2.15 | 0.47 |
| 1:F:8:ALA:HB3 | 1:F:82:ALA:CA | 2.45 | 0.47 |
| 1:A:4:ALA:HB1 | 1:A:56:PHE:CD2 | 2.50 | 0.47 |
| 1:F:5:ILE:O | 1:F:56:PHE:HA | 2.15 | 0.47 |
| 1:D:156:VAL:HA | 1:D:162:THR:O | 2.16 | 0.46 |
| 1:A:175:ASP:O | 1:B:104:LEU:HD22 | 2.14 | 0.46 |
| 1:C:152:ILE:HD13 | 1:C:165:ILE:HG21 | 1.96 | 0.46 |
| 1:C:8:ALA:HB3 | 1:C:82:ALA:CA | 2.45 | 0.46 |
| 1:F:158:GLY:O | 1:F:159:ALA:CB | 2.63 | 0.46 |
| 1:C:240:LEU:HD23 | 1:C:241:ALA:N | 2.30 | 0.46 |
| 1:E:107:THR:O | 1:E:107:THR:CG2 | 2.61 | 0.46 |
| 1:D:146:ASP:C | 1:D:147:MET:HG3 | 2.35 | 0.46 |
| 1:D:133:LEU:CG | 1:D:183:LEU:HD11 | 2.32 | 0.46 |
| 1:F:156:VAL:HA | 1:F:162:THR:O | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:146:ASP:C | 1:F:147:MET:HG3 | 2.35 | 0.46 |
| 1:A:186:ILE:CG2 | 1:A:187:GLU:N | 2.78 | 0.46 |
| 1:C:5:ILE:HB | 1:C:57:GLU:OE1 | 2.15 | 0.46 |
| 1:B:172:ASP:OD1 | 1:C:108:LEU:HG | 2.15 | 0.46 |
| 1:B:5:ILE:O | 1:B:56:PHE:HA | 2.15 | 0.46 |
| 1:D:4:ALA:HB1 | 1:D:56:PHE:CD2 | 2.50 | 0.46 |
| 1:A:146:ASP:C | 1:A:147:MET:HG3 | 2.35 | 0.46 |
| 1:F:97:LEU:HB2 | 1:F:110:LEU:HD21 | 1.96 | 0.46 |
| 1:F:186:ILE:CG2 | 1:F:187:GLU:N | 2.78 | 0.46 |
| 1:A:173:ASP:HB2 | 1:B:107:THR:HG23 | 1.93 | 0.46 |
| 1:B:73:LEU:O | 1:B:76:VAL:HG12 | 2.16 | 0.46 |
| 1:E:133:LEU:HD23 | 1:E:133:LEU:HA | 1.74 | 0.46 |
| 1:B:5:ILE:HB | 1:B:57:GLU:OE1 | 2.15 | 0.46 |
| 1:C:131:ILE:HD13 | 1:C:217:LEU:HD23 | 1.98 | 0.46 |
| 1:E:156:VAL:HA | 1:E:162:THR:O | 2.16 | 0.46 |
| 1:E:146:ASP:C | 1:E:147:MET:HG3 | 2.35 | 0.46 |
| 1:C:47:VAL:HG13 | 1:C:47:VAL:O | 2.16 | 0.46 |
| 1:B:107:THR:O | 1:B:107:THR:CG2 | 2.61 | 0.46 |
| 1:A:149:SER:HB3 | 1:A:167:ALA:CB | 2.22 | 0.46 |
| 1:C:195:PHE:CE2 | 1:C:242:PRO:CD | 2.73 | 0.46 |
| 1:A:156:VAL:CG1 | 1:A:191:ALA:O | 2.62 | 0.46 |
| 1:E:5:ILE:HB | 1:E:57:GLU:OE1 | 2.15 | 0.46 |
| 1:C:8:ALA:HB2 | 1:C:84:ASP:HB2 | 1.98 | 0.46 |
| 1:C:186:ILE:CG2 | 1:C:187:GLU:N | 2.78 | 0.46 |
| 1:D:47:VAL:O | 1:D:47:VAL:HG13 | 2.16 | 0.46 |
| 1:F:47:VAL:O | 1:F:47:VAL:HG13 | 2.16 | 0.46 |
| 1:F:5:ILE:HB | 1:F:57:GLU:OE1 | 2.15 | 0.46 |
| 1:A:133:LEU:CG | 1:A:183:LEU:HD12 | 2.45 | 0.46 |
| 1:B:156:VAL:CG1 | 1:B:191:ALA:O | 2.62 | 0.46 |
| 1:B:8:ALA:HB2 | 1:B:84:ASP:HB2 | 1.98 | 0.46 |
| 1:D:5:ILE:HB | 1:D:57:GLU:OE1 | 2.16 | 0.46 |
| 1:B:65:VAL:HG22 | 1:B:113:PRO:HG2 | 1.98 | 0.46 |
| 1:A:47:VAL:HG13 | 1:A:47:VAL:O | 2.16 | 0.46 |
| 1:D:8:ALA:HB3 | 1:D:82:ALA:CA | 2.45 | 0.46 |
| 1:A:8:ALA:HB2 | 1:A:84:ASP:HB2 | 1.98 | 0.46 |
| 1:E:131:ILE:HG22 | 1:E:132:VAL:N | 2.31 | 0.46 |
| 1:A:107:THR:O | 1:A:107:THR:CG2 | 2.61 | 0.46 |
| 1:B:156:VAL:HA | 1:B:162:THR:O | 2.16 | 0.46 |
| 1:D:133:LEU:HA | 1:D:133:LEU:HD23 | 1.74 | 0.46 |
| 1:C:133:LEU:CG | 1:C:183:LEU:HD12 | 2.45 | 0.46 |
| 1:B:29:LEU:HB3 | 1:B:34:LEU:HD22 | 1.98 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:18:VAL:HB | 1:B:22:VAL:HG22 | 1.98 | 0.46 |
| 1:F:133:LEU:CG | 1:F:183:LEU:HD12 | 2.45 | 0.46 |
| 1:D:133:LEU:CG | 1:D:183:LEU:HD12 | 2.45 | 0.46 |
| 1:F:131:ILE:HG22 | 1:F:132:VAL:N | 2.31 | 0.46 |
| 1:B:8:ALA:HB3 | 1:B:82:ALA:CA | 2.45 | 0.46 |
| 1:A:5:ILE:HB | 1:A:57:GLU:OE1 | 2.15 | 0.46 |
| 1:A:18:VAL:HB | 1:A:22:VAL:HG22 | 1.98 | 0.46 |
| 1:D:131:ILE:HD13 | 1:D:217:LEU:HD23 | 1.98 | 0.45 |
| 1:C:131:ILE:HG22 | 1:C:132:VAL:N | 2.31 | 0.45 |
| 1:C:156:VAL:HA | 1:C:162:THR:O | 2.16 | 0.45 |
| 1:F:138:LEU:O | 1:F:138:LEU:HD13 | 2.17 | 0.45 |
| 1:A:131:ILE:HG22 | 1:A:132:VAL:N | 2.31 | 0.45 |
| 1:A:8:ALA:HB3 | 1:A:82:ALA:CA | 2.45 | 0.45 |
| 1:D:176:LEU:HD13 | 1:E:104:LEU:HD23 | 1.97 | 0.45 |
| 1:B:131:ILE:HG22 | 1:B:132:VAL:N | 2.31 | 0.45 |
| 1:B:47:VAL:HG13 | 1:B:47:VAL:O | 2.16 | 0.45 |
| 1:C:65:VAL:HG22 | 1:C:113:PRO:HG2 | 1.98 | 0.45 |
| 1:F:131:ILE:HD13 | 1:F:217:LEU:HD23 | 1.98 | 0.45 |
| 1:E:73:LEU:O | 1:E:76:VAL:HG12 | 2.16 | 0.45 |
| 1:A:180:PRO:O | 1:A:183:LEU:CB | 2.65 | 0.45 |
| 1:A:69:ASN:HB2 | 1:A:108:LEU:HD21 | 1.99 | 0.45 |
| 1:B:131:ILE:HD13 | 1:B:217:LEU:HD23 | 1.98 | 0.45 |
| 1:B:173:ASP:HB2 | 1:C:107:THR:HG22 | 1.92 | 0.45 |
| 1:C:180:PRO:O | 1:C:183:LEU:CB | 2.65 | 0.45 |
| 1:E:133:LEU:CG | 1:E:183:LEU:HD12 | 2.45 | 0.45 |
| 1:F:29:LEU:HB3 | 1:F:34:LEU:HD22 | 1.98 | 0.45 |
| 1:E:18:VAL:HB | 1:E:22:VAL:HG22 | 1.98 | 0.45 |
| 1:F:73:LEU:O | 1:F:76:VAL:HG12 | 2.16 | 0.45 |
| 1:E:131:ILE:HD13 | 1:E:217:LEU:HD23 | 1.98 | 0.45 |
| 1:E:47:VAL:HG13 | 1:E:47:VAL:O | 2.16 | 0.45 |
| 1:C:18:VAL:HB | 1:C:22:VAL:HG22 | 1.98 | 0.45 |
| 1:D:240:LEU:CD2 | 1:D:241:ALA:O | 2.62 | 0.45 |
| 1:D:65:VAL:HG22 | 1:D:113:PRO:HG2 | 1.98 | 0.45 |
| 1:D:138:LEU:O | 1:D:138:LEU:HD13 | 2.17 | 0.45 |
| 1:E:180:PRO:O | 1:E:183:LEU:CB | 2.65 | 0.45 |
| 1:A:156:VAL:HA | 1:A:162:THR:O | 2.16 | 0.45 |
| 1:D:73:LEU:O | 1:D:76:VAL:HG12 | 2.16 | 0.45 |
| 1:F:8:ALA:HB2 | 1:F:84:ASP:HB2 | 1.98 | 0.45 |
| 1:A:29:LEU:HB3 | 1:A:34:LEU:HD22 | 1.98 | 0.45 |
| 1:F:65:VAL:HG22 | 1:F:113:PRO:HG2 | 1.98 | 0.45 |
| 1:B:158:GLY:O | 1:B:159:ALA:CB | 2.63 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:180:PRO:O | 1:B:183:LEU:CB | 2.65 | 0.45 |
| 1:D:49:LEU:CD2 | 1:D:236:ILE:HG22 | 2.47 | 0.45 |
| 1:C:69:ASN:HB2 | 1:C:108:LEU:HD21 | 1.99 | 0.45 |
| 1:C:73:LEU:O | 1:C:76:VAL:HG12 | 2.16 | 0.45 |
| 1:B:138:LEU:O | 1:B:138:LEU:HD13 | 2.17 | 0.45 |
| 1:E:29:LEU:HB3 | 1:E:34:LEU:HD22 | 1.98 | 0.45 |
| 1:D:155:ARG:O | 1:D:163:PHE:HA | 2.17 | 0.45 |
| 1:B:176:LEU:HD13 | 1:C:104:LEU:HD23 | 1.98 | 0.45 |
| 1:E:155:ARG:O | 1:E:163:PHE:HA | 2.17 | 0.45 |
| 1:E:240:LEU:HD23 | 1:E:241:ALA:N | 2.30 | 0.45 |
| 1:D:180:PRO:O | 1:D:183:LEU:CB | 2.65 | 0.45 |
| 1:C:29:LEU:HB3 | 1:C:34:LEU:HD22 | 1.98 | 0.45 |
| 1:F:95:ARG:C | 1:F:110:LEU:H | 2.20 | 0.45 |
| 1:C:240:LEU:O | 1:C:242:PRO:HD3 | 2.17 | 0.45 |
| 1:A:108:LEU:HG | 1:C:172:ASP:OD1 | 2.17 | 0.45 |
| 1:A:107:THR:HG23 | 1:C:173:ASP:HB2 | 1.95 | 0.45 |
| 1:C:106:TYR:CE2 | 1:C:108:LEU:HB2 | 2.52 | 0.45 |
| 1:B:26:LYS:HA | 1:B:67:GLY:HA2 | 1.99 | 0.45 |
| 1:F:180:PRO:O | 1:F:183:LEU:CB | 2.65 | 0.45 |
| 1:D:8:ALA:HB2 | 1:D:84:ASP:HB2 | 1.98 | 0.45 |
| 1:D:173:ASP:HB2 | 1:E:107:THR:HG23 | 1.93 | 0.45 |
| 1:E:138:LEU:HD13 | 1:E:138:LEU:O | 2.17 | 0.45 |
| 1:E:69:ASN:HB2 | 1:E:108:LEU:HD21 | 1.98 | 0.45 |
| 1:E:199:TYR:O | 1:E:203:MET:HG3 | 2.17 | 0.45 |
| 1:C:49:LEU:CD2 | 1:C:236:ILE:HG22 | 2.47 | 0.45 |
| 1:B:240:LEU:O | 1:B:242:PRO:HD3 | 2.17 | 0.45 |
| 1:A:155:ARG:O | 1:A:163:PHE:HA | 2.17 | 0.45 |
| 1:A:49:LEU:CD2 | 1:A:236:ILE:HG22 | 2.47 | 0.45 |
| 1:A:26:LYS:HA | 1:A:67:GLY:HA2 | 1.99 | 0.45 |
| 1:D:133:LEU:O | 1:D:213:VAL:N | 2.29 | 0.45 |
| 1:C:26:LYS:HA | 1:C:67:GLY:HA2 | 1.99 | 0.45 |
| 1:F:155:ARG:O | 1:F:163:PHE:HA | 2.17 | 0.45 |
| 1:D:156:VAL:CG1 | 1:D:191:ALA:O | 2.62 | 0.44 |
| 1:C:151:HIS:HB3 | 1:C:195:PHE:O | 2.18 | 0.44 |
| 1:C:199:TYR:O | 1:C:203:MET:HG3 | 2.17 | 0.44 |
| 1:F:240:LEU:O | 1:F:242:PRO:HD3 | 2.17 | 0.44 |
| 1:A:131:ILE:HG12 | 1:A:163:PHE:CD1 | 2.52 | 0.44 |
| 1:E:65:VAL:HG22 | 1:E:113:PRO:HG2 | 1.98 | 0.44 |
| 1:A:95:ARG:C | 1:A:110:LEU:H | 2.20 | 0.44 |
| 1:B:155:ARG:O | 1:B:163:PHE:HA | 2.17 | 0.44 |
| 1:E:197:LEU:C | 1:E:197:LEU:HD23 | 2.30 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:66:ILE:CD1 | 1:D:90:LEU:HD13 | 2.47 | 0.44 |
| 1:B:49:LEU:CD2 | 1:B:236:ILE:HG22 | 2.47 | 0.44 |
| 1:D:131:ILE:HG22 | 1:D:132:VAL:N | 2.31 | 0.44 |
| 1:F:106:TYR:CE2 | 1:F:108:LEU:HB2 | 2.52 | 0.44 |
| 1:A:66:ILE:CD1 | 1:A:90:LEU:HD13 | 2.47 | 0.44 |
| 1:D:106:TYR:CE2 | 1:D:108:LEU:HB2 | 2.52 | 0.44 |
| 1:B:66:ILE:CD1 | 1:B:90:LEU:HD13 | 2.47 | 0.44 |
| 1:F:18:VAL:HB | 1:F:22:VAL:HG22 | 1.98 | 0.44 |
| 1:D:18:VAL:HB | 1:D:22:VAL:HG22 | 1.98 | 0.44 |
| 1:F:26:LYS:HA | 1:F:67:GLY:HA2 | 1.99 | 0.44 |
| 1:F:66:ILE:CD1 | 1:F:90:LEU:HD13 | 2.48 | 0.44 |
| 1:A:158:GLY:O | 1:A:159:ALA:CB | 2.63 | 0.44 |
| 1:A:73:LEU:O | 1:A:76:VAL:HG12 | 2.16 | 0.44 |
| 1:D:240:LEU:O | 1:D:242:PRO:HD3 | 2.17 | 0.44 |
| 1:E:8:ALA:HB2 | 1:E:84:ASP:HB2 | 1.98 | 0.44 |
| 1:B:179:PRO:HG2 | 1:D:179:PRO:CG | 2.47 | 0.44 |
| 1:C:138:LEU:HD13 | 1:C:138:LEU:O | 2.17 | 0.44 |
| 1:C:95:ARG:C | 1:C:110:LEU:H | 2.20 | 0.44 |
| 1:D:131:ILE:HG12 | 1:D:163:PHE:CD1 | 2.52 | 0.44 |
| 1:A:199:TYR:O | 1:A:203:MET:HG3 | 2.17 | 0.44 |
| 1:E:106:TYR:CE2 | 1:E:108:LEU:HB2 | 2.52 | 0.44 |
| 1:E:158:GLY:O | 1:E:159:ALA:CB | 2.64 | 0.44 |
| 1:A:138:LEU:HD13 | 1:A:138:LEU:O | 2.17 | 0.44 |
| 1:D:69:ASN:HB2 | 1:D:108:LEU:HD21 | 1.99 | 0.44 |
| 1:B:95:ARG:C | 1:B:110:LEU:H | 2.20 | 0.44 |
| 1:D:29:LEU:HB3 | 1:D:34:LEU:HD22 | 1.98 | 0.44 |
| 1:B:151:HIS:HB3 | 1:B:195:PHE:O | 2.18 | 0.44 |
| 1:C:155:ARG:O | 1:C:163:PHE:HA | 2.17 | 0.44 |
| 1:E:66:ILE:CD1 | 1:E:90:LEU:HD13 | 2.48 | 0.44 |
| 1:E:131:ILE:HG12 | 1:E:163:PHE:CD1 | 2.52 | 0.44 |
| 1:A:65:VAL:HG22 | 1:A:113:PRO:HG2 | 1.98 | 0.44 |
| 1:D:95:ARG:C | 1:D:110:LEU:H | 2.20 | 0.44 |
| 1:D:2:PHE:CD1 | 1:D:90:LEU:HD12 | 2.53 | 0.44 |
| 1:C:207:ILE:N | 1:C:207:ILE:CD1 | 2.81 | 0.44 |
| 1:F:69:ASN:HB2 | 1:F:108:LEU:HD21 | 1.99 | 0.44 |
| 1:F:151:HIS:HB3 | 1:F:195:PHE:O | 2.18 | 0.44 |
| 1:D:151:HIS:HB3 | 1:D:195:PHE:O | 2.18 | 0.44 |
| 1:E:240:LEU:O | 1:E:242:PRO:HD3 | 2.17 | 0.44 |
| 1:C:2:PHE:CD1 | 1:C:90:LEU:HD12 | 2.53 | 0.44 |
| 1:B:69:ASN:HB2 | 1:B:108:LEU:HD21 | 1.98 | 0.44 |
| 1:B:199:TYR:O | 1:B:203:MET:HG3 | 2.17 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:49:LEU:CD2 | 1:F:236:ILE:HG22 | 2.47 | 0.44 |
| 1:A:131:ILE:HD13 | 1:A:217:LEU:HD23 | 1.98 | 0.44 |
| 1:E:95:ARG:C | 1:E:110:LEU:H | 2.20 | 0.44 |
| 1:E:8:ALA:HB3 | 1:E:82:ALA:CA | 2.45 | 0.44 |
| 1:D:155:ARG:HB3 | 1:D:164:HIS:HB2 | 2.00 | 0.44 |
| 1:A:240:LEU:O | 1:A:242:PRO:HD3 | 2.17 | 0.44 |
| 1:A:133:LEU:O | 1:A:213:VAL:N | 2.28 | 0.44 |
| 1:E:150:ASP:O | 1:E:197:LEU:HB3 | 2.18 | 0.44 |
| 1:C:66:ILE:CD1 | 1:C:90:LEU:HD13 | 2.47 | 0.44 |
| 1:A:173:ASP:HB2 | 1:B:107:THR:HG21 | 1.93 | 0.44 |
| 1:B:207:ILE:N | 1:B:207:ILE:CD1 | 2.81 | 0.44 |
| 1:D:157:ASP:CB | 1:D:160:GLU:O | 2.66 | 0.44 |
| 1:C:150:ASP:O | 1:C:197:LEU:HB3 | 2.18 | 0.44 |
| 1:F:195:PHE:CE2 | 1:F:242:PRO:CD | 2.73 | 0.44 |
| 1:E:207:ILE:CD1 | 1:E:207:ILE:N | 2.81 | 0.44 |
| 1:B:131:ILE:HG12 | 1:B:163:PHE:CD1 | 2.52 | 0.44 |
| 1:D:26:LYS:HA | 1:D:67:GLY:HA2 | 1.99 | 0.44 |
| 1:F:29:LEU:HG | 1:F:34:LEU:HB3 | 2.00 | 0.44 |
| 1:A:240:LEU:CD2 | 1:A:241:ALA:O | 2.62 | 0.43 |
| 1:C:155:ARG:HB3 | 1:C:164:HIS:HB2 | 2.00 | 0.43 |
| 1:F:35:SER:HB2 | 1:F:49:LEU:O | 2.18 | 0.43 |
| 1:A:155:ARG:HB3 | 1:A:164:HIS:HB2 | 2.00 | 0.43 |
| 1:D:173:ASP:HB2 | 1:E:107:THR:HG21 | 1.96 | 0.43 |
| 1:A:207:ILE:HG21 | 1:A:227:TYR:OH | 2.18 | 0.43 |
| 1:A:2:PHE:CD1 | 1:A:90:LEU:HD12 | 2.53 | 0.43 |
| 1:D:199:TYR:O | 1:D:203:MET:HG3 | 2.17 | 0.43 |
| 1:B:106:TYR:CE2 | 1:B:108:LEU:HB2 | 2.52 | 0.43 |
| 1:A:195:PHE:CE2 | 1:A:242:PRO:CD | 2.73 | 0.43 |
| 1:C:131:ILE:HG12 | 1:C:163:PHE:CD1 | 2.52 | 0.43 |
| 1:C:157:ASP:CB | 1:C:160:GLU:O | 2.66 | 0.43 |
| 1:F:73:LEU:HD23 | 1:F:76:VAL:HG13 | 2.00 | 0.43 |
| 1:F:150:ASP:O | 1:F:197:LEU:HB3 | 2.18 | 0.43 |
| 1:F:199:TYR:O | 1:F:203:MET:HG3 | 2.17 | 0.43 |
| 1:E:207:ILE:HG21 | 1:E:227:TYR:OH | 2.18 | 0.43 |
| 1:D:150:ASP:O | 1:D:197:LEU:HB3 | 2.18 | 0.43 |
| 1:B:157:ASP:CB | 1:B:160:GLU:O | 2.66 | 0.43 |
| 1:C:73:LEU:HD23 | 1:C:76:VAL:HG13 | 2.00 | 0.43 |
| 1:F:131:ILE:HG12 | 1:F:163:PHE:CD1 | 2.52 | 0.43 |
| 1:A:172:ASP:OD1 | 1:B:108:LEU:HG | 2.18 | 0.43 |
| 1:C:122:ILE:O | 1:C:123:PRO:C | 2.56 | 0.43 |
| 1:A:198:ASP:C | 1:A:200:LEU:H | 2.22 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:82:ALA:O | 1:C:84:ASP:N | 2.51 | 0.43 |
| 1:C:207:ILE:HG21 | 1:C:227:TYR:OH | 2.19 | 0.43 |
| 1:B:35:SER:HB2 | 1:B:49:LEU:O | 2.18 | 0.43 |
| 1:A:150:ASP:O | 1:A:197:LEU:HB3 | 2.18 | 0.43 |
| 1:E:49:LEU:CD2 | 1:E:236:ILE:HG22 | 2.47 | 0.43 |
| 1:A:235:THR:HG22 | 1:A:236:ILE:N | 2.34 | 0.43 |
| 1:D:207:ILE:HG21 | 1:D:227:TYR:OH | 2.18 | 0.43 |
| 1:D:107:THR:HG22 | 1:F:173:ASP:HB2 | 1.98 | 0.43 |
| 1:B:82:ALA:O | 1:B:84:ASP:N | 2.51 | 0.43 |
| 1:D:20:VAL:HG12 | 1:D:21:LEU:CD2 | 2.49 | 0.43 |
| 1:E:20:VAL:HG12 | 1:E:21:LEU:CD2 | 2.49 | 0.43 |
| 1:A:176:LEU:HD13 | 1:B:104:LEU:HD23 | 2.00 | 0.43 |
| 1:B:184:ILE:O | 1:E:5:ILE:HD13 | 2.18 | 0.43 |
| 1:F:155:ARG:HB3 | 1:F:164:HIS:HB2 | 2.00 | 0.43 |
| 1:F:157:ASP:CB | 1:F:160:GLU:O | 2.66 | 0.43 |
| 1:B:2:PHE:CD1 | 1:B:90:LEU:HD12 | 2.53 | 0.43 |
| 1:F:20:VAL:HG12 | 1:F:21:LEU:CD2 | 2.49 | 0.43 |
| 1:F:235:THR:HG22 | 1:F:236:ILE:N | 2.34 | 0.43 |
| 1:F:145:ALA:O | 1:F:197:LEU:HD13 | 2.19 | 0.43 |
| 1:D:171:THR:HG21 | 1:E:72:ARG:NH1 | 2.19 | 0.43 |
| 1:E:2:PHE:CD1 | 1:E:90:LEU:HD12 | 2.53 | 0.43 |
| 1:B:155:ARG:HB3 | 1:B:164:HIS:HB2 | 2.00 | 0.43 |
| 1:B:133:LEU:HD23 | 1:B:133:LEU:HA | 1.74 | 0.43 |
| 1:F:82:ALA:O | 1:F:84:ASP:N | 2.51 | 0.43 |
| 1:B:27:ILE:HD12 | 1:B:68:VAL:HG21 | 2.01 | 0.43 |
| 1:B:73:LEU:HD23 | 1:B:76:VAL:HG13 | 2.00 | 0.43 |
| 1:C:20:VAL:HG12 | 1:C:21:LEU:CD2 | 2.49 | 0.43 |
| 1:E:122:ILE:O | 1:E:123:PRO:C | 2.56 | 0.43 |
| 1:C:145:ALA:O | 1:C:197:LEU:HD13 | 2.19 | 0.43 |
| 1:C:240:LEU:CD2 | 1:C:241:ALA:O | 2.62 | 0.43 |
| 1:F:198:ASP:C | 1:F:200:LEU:H | 2.22 | 0.43 |
| 1:E:82:ALA:O | 1:E:84:ASP:N | 2.51 | 0.43 |
| 1:D:73:LEU:CA | 1:D:76:VAL:HG12 | 2.49 | 0.43 |
| 1:E:56:PHE:CD1 | 1:E:59:TYR:CE2 | 3.07 | 0.43 |
| 1:B:56:PHE:CD1 | 1:B:59:TYR:CE2 | 3.07 | 0.43 |
| 1:F:56:PHE:CD1 | 1:F:59:TYR:CE2 | 3.07 | 0.43 |
| 1:A:151:HIS:HB3 | 1:A:195:PHE:O | 2.18 | 0.43 |
| 1:B:145:ALA:O | 1:B:197:LEU:HD13 | 2.19 | 0.43 |
| 1:F:73:LEU:CA | 1:F:76:VAL:HG12 | 2.49 | 0.43 |
| 1:E:235:THR:HG22 | 1:E:236:ILE:N | 2.34 | 0.43 |
| 1:E:73:LEU:HD23 | 1:E:76:VAL:HG13 | 2.00 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:151:HIS:HB3 | 1:E:195:PHE:O | 2.18 | 0.43 |
| 1:C:56:PHE:CD1 | 1:C:59:TYR:CE2 | 3.07 | 0.43 |
| 1:D:27:ILE:HD12 | 1:D:68:VAL:HG21 | 2.01 | 0.43 |
| 1:A:20:VAL:HG12 | 1:A:21:LEU:CD2 | 2.49 | 0.43 |
| 1:B:150:ASP:O | 1:B:197:LEU:HB3 | 2.18 | 0.43 |
| 1:F:207:ILE:HG21 | 1:F:227:TYR:OH | 2.18 | 0.43 |
| 1:F:27:ILE:HG23 | 1:F:36:ILE:HD11 | 2.01 | 0.43 |
| 1:F:2:PHE:CD1 | 1:F:90:LEU:HD12 | 2.53 | 0.43 |
| 1:C:198:ASP:C | 1:C:200:LEU:H | 2.22 | 0.43 |
| 1:E:70:LEU:HD22 | 1:E:70:LEU:O | 2.19 | 0.43 |
| 1:D:73:LEU:HD23 | 1:D:76:VAL:HG13 | 2.00 | 0.43 |
| 1:B:171:THR:HG21 | 1:C:72:ARG:NH1 | 2.13 | 0.43 |
| 1:C:35:SER:HB2 | 1:C:49:LEU:O | 2.19 | 0.43 |
| 1:A:171:THR:HG21 | 1:B:72:ARG:NH1 | 2.16 | 0.43 |
| 1:B:235:THR:HG22 | 1:B:236:ILE:N | 2.34 | 0.43 |
| 1:E:157:ASP:CB | 1:E:160:GLU:O | 2.66 | 0.43 |
| 1:F:133:LEU:O | 1:F:213:VAL:N | 2.28 | 0.43 |
| 1:E:131:ILE:HD12 | 1:E:131:ILE:N | 2.34 | 0.43 |
| 1:A:27:ILE:HD12 | 1:A:68:VAL:HG21 | 2.01 | 0.43 |
| 1:A:73:LEU:HD23 | 1:A:76:VAL:HG13 | 2.00 | 0.43 |
| 1:A:109:ALA:HB3 | 1:C:171:THR:OG1 | 2.19 | 0.43 |
| 1:D:145:ALA:O | 1:D:197:LEU:HD13 | 2.19 | 0.43 |
| 1:D:35:SER:HB2 | 1:D:49:LEU:O | 2.18 | 0.43 |
| 1:D:27:ILE:HG23 | 1:D:36:ILE:HD11 | 2.01 | 0.43 |
| 1:E:5:ILE:HD12 | 1:E:57:GLU:HB2 | 2.01 | 0.43 |
| 1:A:171:THR:OG1 | 1:B:109:ALA:HB3 | 2.19 | 0.43 |
| 1:E:26:LYS:HA | 1:E:67:GLY:HA2 | 1.99 | 0.42 |
| 1:B:131:ILE:HD12 | 1:B:131:ILE:N | 2.34 | 0.42 |
| 1:C:70:LEU:O | 1:C:70:LEU:HD22 | 2.19 | 0.42 |
| 1:D:5:ILE:HD12 | 1:D:57:GLU:HB2 | 2.01 | 0.42 |
| 1:B:20:VAL:HG12 | 1:B:21:LEU:CD2 | 2.49 | 0.42 |
| 1:E:35:SER:HB2 | 1:E:49:LEU:O | 2.18 | 0.42 |
| 1:E:27:ILE:HD12 | 1:E:68:VAL:HG21 | 2.01 | 0.42 |
| 1:A:35:SER:HB2 | 1:A:49:LEU:O | 2.19 | 0.42 |
| 1:C:27:ILE:HD12 | 1:C:68:VAL:HG21 | 2.01 | 0.42 |
| 1:B:207:ILE:HG21 | 1:B:227:TYR:OH | 2.18 | 0.42 |
| 1:A:106:TYR:CE2 | 1:A:108:LEU:HB2 | 2.52 | 0.42 |
| 1:D:207:ILE:CD1 | 1:D:207:ILE:N | 2.81 | 0.42 |
| 1:F:82:ALA:C | 1:F:84:ASP:H | 2.23 | 0.42 |
| 1:D:131:ILE:N | 1:D:131:ILE:HD12 | 2.34 | 0.42 |
| 1:A:145:ALA:O | 1:A:197:LEU:HD13 | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:239:MET:HB3 | 1:A:239:MET:HE2 | 1.96 | 0.42 |
| 1:C:131:ILE:HD12 | 1:C:131:ILE:N | 2.34 | 0.42 |
| 1:F:27:ILE:HD12 | 1:F:68:VAL:HG21 | 2.01 | 0.42 |
| 1:A:17:SER:OG | 1:A:236:ILE:HG21 | 2.20 | 0.42 |
| 1:D:235:THR:HG22 | 1:D:236:ILE:N | 2.34 | 0.42 |
| 1:C:82:ALA:C | 1:C:84:ASP:H | 2.23 | 0.42 |
| 1:C:17:SER:OG | 1:C:236:ILE:HG21 | 2.20 | 0.42 |
| 1:F:131:ILE:HD12 | 1:F:131:ILE:N | 2.34 | 0.42 |
| 1:C:43:ASN:HD22 | 1:C:43:ASN:N | 2.18 | 0.42 |
| 1:E:27:ILE:HG23 | 1:E:36:ILE:HD11 | 2.01 | 0.42 |
| 1:C:27:ILE:HG23 | 1:C:36:ILE:HD11 | 2.01 | 0.42 |
| 1:A:29:LEU:HG | 1:A:34:LEU:HB3 | 2.00 | 0.42 |
| 1:B:198:ASP:C | 1:B:200:LEU:H | 2.22 | 0.42 |
| 1:A:157:ASP:CB | 1:A:160:GLU:O | 2.66 | 0.42 |
| 1:A:82:ALA:O | 1:A:84:ASP:N | 2.51 | 0.42 |
| 1:B:133:LEU:CG | 1:B:183:LEU:HD12 | 2.45 | 0.42 |
| 1:B:27:ILE:HG23 | 1:B:36:ILE:HD11 | 2.01 | 0.42 |
| 1:C:29:LEU:HG | 1:C:34:LEU:HB3 | 2.00 | 0.42 |
| 1:D:29:LEU:HG | 1:D:34:LEU:HB3 | 2.00 | 0.42 |
| 1:A:73:LEU:CA | 1:A:76:VAL:HG12 | 2.49 | 0.42 |
| 1:E:82:ALA:C | 1:E:84:ASP:H | 2.23 | 0.42 |
| 1:B:70:LEU:HD22 | 1:B:70:LEU:O | 2.19 | 0.42 |
| 1:B:29:LEU:HG | 1:B:34:LEU:HB3 | 2.00 | 0.42 |
| 1:A:56:PHE:CD1 | 1:A:59:TYR:CE2 | 3.07 | 0.42 |
| 1:D:56:PHE:CD1 | 1:D:59:TYR:CE2 | 3.07 | 0.42 |
| 1:F:5:ILE:HD12 | 1:F:57:GLU:HB2 | 2.01 | 0.42 |
| 1:A:122:ILE:O | 1:A:123:PRO:C | 2.56 | 0.42 |
| 1:D:82:ALA:O | 1:D:84:ASP:N | 2.51 | 0.42 |
| 1:E:17:SER:OG | 1:E:236:ILE:HG21 | 2.20 | 0.42 |
| 1:E:25:CYS:O | 1:E:67:GLY:CA | 2.66 | 0.42 |
| 1:E:73:LEU:CA | 1:E:76:VAL:HG12 | 2.49 | 0.42 |
| 1:E:155:ARG:HB3 | 1:E:164:HIS:HB2 | 2.00 | 0.42 |
| 1:D:122:ILE:O | 1:D:123:PRO:C | 2.56 | 0.42 |
| 1:C:49:LEU:HD23 | 1:C:235:THR:O | 2.20 | 0.42 |
| 1:C:25:CYS:O | 1:C:67:GLY:CA | 2.66 | 0.42 |
| 1:C:73:LEU:CA | 1:C:76:VAL:HG12 | 2.49 | 0.42 |
| 1:E:29:LEU:HG | 1:E:34:LEU:HB3 | 2.00 | 0.42 |
| 1:E:172:ASP:OD1 | 1:F:108:LEU:HG | 2.19 | 0.42 |
| 1:F:17:SER:OG | 1:F:236:ILE:HG21 | 2.20 | 0.42 |
| 1:A:131:ILE:N | 1:A:131:ILE:HD12 | 2.34 | 0.42 |
| 1:D:198:ASP:C | 1:D:200:LEU:H | 2.22 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:70:LEU:O | 1:D:70:LEU:HD22 | 2.19 | 0.42 |
| 1:D:20:VAL:CG2 | 1:D:202:ASP:O | 2.66 | 0.42 |
| 1:B:122:ILE:O | 1:B:123:PRO:C | 2.56 | 0.42 |
| 1:E:173:ASP:HB2 | 1:F:107:THR:HG22 | 1.95 | 0.42 |
| 1:F:49:LEU:HD23 | 1:F:235:THR:O | 2.20 | 0.42 |
| 1:C:5:ILE:CA | 1:C:86:ILE:O | 2.68 | 0.42 |
| 1:C:235:THR:HG22 | 1:C:236:ILE:N | 2.34 | 0.42 |
| 1:B:73:LEU:CA | 1:B:76:VAL:HG12 | 2.49 | 0.42 |
| 1:F:47:VAL:HB | 1:F:238:TYR:CD2 | 2.55 | 0.42 |
| 1:B:43:ASN:N | 1:B:43:ASN:HD22 | 2.18 | 0.42 |
| 1:A:246:SER:O | 1:A:247:ASP:HB2 | 2.20 | 0.42 |
| 1:B:240:LEU:CD2 | 1:B:241:ALA:O | 2.62 | 0.41 |
| 1:C:158:GLY:O | 1:C:159:ALA:CB | 2.63 | 0.41 |
| 1:D:82:ALA:C | 1:D:84:ASP:H | 2.23 | 0.41 |
| 1:E:240:LEU:CD2 | 1:E:241:ALA:O | 2.62 | 0.41 |
| 1:B:49:LEU:HD23 | 1:B:235:THR:O | 2.20 | 0.41 |
| 1:E:47:VAL:HB | 1:E:238:TYR:CD2 | 2.55 | 0.41 |
| 1:F:5:ILE:CA | 1:F:86:ILE:O | 2.68 | 0.41 |
| 1:E:145:ALA:O | 1:E:197:LEU:HD13 | 2.19 | 0.41 |
| 1:C:86:ILE:HG21 | 1:C:99:ILE:HD11 | 2.02 | 0.41 |
| 1:D:17:SER:OG | 1:D:236:ILE:HG21 | 2.20 | 0.41 |
| 1:D:49:LEU:HD23 | 1:D:235:THR:O | 2.20 | 0.41 |
| 1:E:5:ILE:CA | 1:E:86:ILE:O | 2.68 | 0.41 |
| 1:B:32:GLU:O | 1:B:33:SER:OG | 2.35 | 0.41 |
| 1:A:5:ILE:HD12 | 1:A:57:GLU:HB2 | 2.01 | 0.41 |
| 1:C:246:SER:O | 1:C:247:ASP:HB2 | 2.20 | 0.41 |
| 1:A:27:ILE:HG23 | 1:A:36:ILE:HD11 | 2.01 | 0.41 |
| 1:A:70:LEU:HD22 | 1:A:70:LEU:O | 2.19 | 0.41 |
| 1:D:175:ASP:O | 1:E:104:LEU:CD2 | 2.68 | 0.41 |
| 1:D:123:PRO:HG3 | 1:D:239:MET:HE1 | 2.02 | 0.41 |
| 1:E:198:ASP:C | 1:E:200:LEU:H | 2.22 | 0.41 |
| 1:D:47:VAL:HB | 1:D:238:TYR:CD2 | 2.55 | 0.41 |
| 1:A:34:LEU:HD23 | 1:A:34:LEU:N | 2.35 | 0.41 |
| 1:A:86:ILE:HG21 | 1:A:99:ILE:HD11 | 2.02 | 0.41 |
| 1:D:158:GLY:O | 1:D:159:ALA:CB | 2.63 | 0.41 |
| 1:A:174:VAL:CG2 | 1:B:104:LEU:HD21 | 2.47 | 0.41 |
| 1:E:49:LEU:HD23 | 1:E:235:THR:O | 2.20 | 0.41 |
| 1:B:17:SER:OG | 1:B:236:ILE:HG21 | 2.20 | 0.41 |
| 1:A:214:THR:HG1 | 1:A:226:HIS:HB2 | 1.82 | 0.41 |
| 1:D:34:LEU:HD23 | 1:D:34:LEU:N | 2.35 | 0.41 |
| 1:F:240:LEU:CD2 | 1:F:241:ALA:O | 2.63 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:5:ILE:HD12 | 1:C:57:GLU:HB2 | 2.01 | 0.41 |
| 1:B:179:PRO:CG | 1:D:179:PRO:HG2 | 2.48 | 0.41 |
| 1:C:32:GLU:O | 1:C:33:SER:OG | 2.35 | 0.41 |
| 1:E:43:ASN:N | 1:E:43:ASN:HD22 | 2.18 | 0.41 |
| 1:F:246:SER:O | 1:F:247:ASP:HB2 | 2.20 | 0.41 |
| 1:F:36:ILE:HG22 | 1:F:37:ARG:N | 2.36 | 0.41 |
| 1:E:131:ILE:HD11 | 1:E:156:VAL:HG21 | 2.03 | 0.41 |
| 1:B:76:VAL:HG13 | 1:B:77:ALA:N | 2.36 | 0.41 |
| 1:B:209:THR:O | 1:B:210:ASP:HB2 | 2.21 | 0.41 |
| 1:D:209:THR:O | 1:D:210:ASP:HB2 | 2.21 | 0.41 |
| 1:F:70:LEU:O | 1:F:70:LEU:HD22 | 2.19 | 0.41 |
| 1:E:2:PHE:HA | 1:E:60:GLU:O | 2.21 | 0.41 |
| 1:A:76:VAL:HG13 | 1:A:77:ALA:N | 2.36 | 0.41 |
| 1:D:25:CYS:O | 1:D:67:GLY:CA | 2.66 | 0.41 |
| 1:B:82:ALA:C | 1:B:84:ASP:H | 2.23 | 0.41 |
| 1:D:176:LEU:N | 1:D:176:LEU:HD22 | 2.36 | 0.41 |
| 1:D:36:ILE:HG22 | 1:D:37:ARG:N | 2.36 | 0.41 |
| 1:D:37:ARG:O | 1:D:37:ARG:CG | 2.49 | 0.41 |
| 1:C:47:VAL:HB | 1:C:238:TYR:CD2 | 2.55 | 0.41 |
| 1:D:86:ILE:HG21 | 1:D:99:ILE:HD11 | 2.02 | 0.41 |
| 1:E:246:SER:O | 1:E:247:ASP:HB2 | 2.20 | 0.41 |
| 1:A:123:PRO:HG3 | 1:A:239:MET:HE1 | 2.03 | 0.41 |
| 1:F:2:PHE:HA | 1:F:60:GLU:O | 2.21 | 0.41 |
| 1:F:176:LEU:HD22 | 1:F:176:LEU:N | 2.36 | 0.41 |
| 1:F:221:PHE:C | 1:F:242:PRO:HG3 | 2.42 | 0.41 |
| 1:A:159:ALA:O | 1:A:160:GLU:HB2 | 2.21 | 0.41 |
| 1:A:131:ILE:HD11 | 1:A:156:VAL:HG21 | 2.03 | 0.41 |
| 1:A:82:ALA:C | 1:A:84:ASP:H | 2.23 | 0.41 |
| 1:A:49:LEU:HD23 | 1:A:235:THR:O | 2.20 | 0.41 |
| 1:D:199:TYR:HB2 | 1:D:240:LEU:HD11 | 2.03 | 0.41 |
| 1:B:159:ALA:O | 1:B:160:GLU:HB2 | 2.21 | 0.41 |
| 1:E:176:LEU:N | 1:E:176:LEU:HD22 | 2.36 | 0.41 |
| 1:C:76:VAL:HG13 | 1:C:77:ALA:N | 2.36 | 0.41 |
| 1:B:36:ILE:HG22 | 1:B:37:ARG:N | 2.36 | 0.41 |
| 1:E:180:PRO:O | 1:E:183:LEU:HB2 | 2.21 | 0.41 |
| 1:A:5:ILE:CA | 1:A:86:ILE:O | 2.68 | 0.41 |
| 1:F:34:LEU:N | 1:F:34:LEU:HD23 | 2.35 | 0.41 |
| 1:E:209:THR:O | 1:E:210:ASP:HB2 | 2.21 | 0.41 |
| 1:D:246:SER:O | 1:D:247:ASP:HB2 | 2.20 | 0.41 |
| 1:F:69:ASN:CG | 1:F:108:LEU:HD21 | 2.42 | 0.41 |
| 1:A:180:PRO:O | 1:A:183:LEU:HB2 | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:107:THR:HG21 | 1:C:173:ASP:HB2 | 1.96 | 0.41 |
| 1:D:69:ASN:CG | 1:D:108:LEU:HD21 | 2.42 | 0.41 |
| 1:B:69:ASN:CG | 1:B:108:LEU:HD21 | 2.42 | 0.41 |
| 1:A:47:VAL:HB | 1:A:238:TYR:CD2 | 2.55 | 0.41 |
| 1:B:7:SER:HA | 1:B:85:LEU:HD23 | 2.04 | 0.41 |
| 1:F:209:THR:O | 1:F:210:ASP:HB2 | 2.21 | 0.41 |
| 1:A:199:TYR:HB2 | 1:A:240:LEU:HD11 | 2.03 | 0.40 |
| 1:B:239:MET:HB3 | 1:B:239:MET:HE2 | 1.96 | 0.40 |
| 1:A:104:LEU:CD2 | 1:C:175:ASP:O | 2.69 | 0.40 |
| 1:D:104:LEU:CD2 | 1:F:175:ASP:O | 2.69 | 0.40 |
| 1:A:2:PHE:HA | 1:A:60:GLU:O | 2.21 | 0.40 |
| 1:C:7:SER:HA | 1:C:85:LEU:HD23 | 2.04 | 0.40 |
| 1:C:2:PHE:HA | 1:C:60:GLU:O | 2.21 | 0.40 |
| 1:E:34:LEU:HD23 | 1:E:34:LEU:N | 2.35 | 0.40 |
| 1:B:5:ILE:HD12 | 1:B:57:GLU:HB2 | 2.01 | 0.40 |
| 1:D:5:ILE:CA | 1:D:86:ILE:O | 2.68 | 0.40 |
| 1:A:43:ASN:HD22 | 1:A:43:ASN:N | 2.18 | 0.40 |
| 1:E:43:ASN:HD21 | 1:E:117:ARG:HH22 | 1.69 | 0.40 |
| 1:F:43:ASN:HD21 | 1:F:117:ARG:HH22 | 1.69 | 0.40 |
| 1:F:43:ASN:N | 1:F:43:ASN:HD22 | 2.18 | 0.40 |
| 1:D:117:ARG:CG | 1:D:118:GLN:N | 2.84 | 0.40 |
| 1:A:176:LEU:N | 1:A:176:LEU:HD22 | 2.36 | 0.40 |
| 1:B:176:LEU:N | 1:B:176:LEU:HD22 | 2.36 | 0.40 |
| 1:F:76:VAL:HG13 | 1:F:77:ALA:N | 2.36 | 0.40 |
| 1:C:145:ALA:C | 1:C:197:LEU:HD12 | 2.42 | 0.40 |
| 1:E:69:ASN:CG | 1:E:108:LEU:HD21 | 2.42 | 0.40 |
| 1:A:36:ILE:HG22 | 1:A:37:ARG:N | 2.36 | 0.40 |
| 1:A:73:LEU:C | 1:A:76:VAL:HG12 | 2.42 | 0.40 |
| 1:E:195:PHE:HD2 | 1:E:240:LEU:HD23 | 1.86 | 0.40 |
| 1:D:76:VAL:HG13 | 1:D:77:ALA:N | 2.36 | 0.40 |
| 1:C:69:ASN:CG | 1:C:108:LEU:HD21 | 2.42 | 0.40 |
| 1:B:34:LEU:HD23 | 1:B:34:LEU:N | 2.35 | 0.40 |
| 1:B:145:ALA:C | 1:B:197:LEU:HD12 | 2.42 | 0.40 |
| 1:B:195:PHE:HD2 | 1:B:240:LEU:HD23 | 1.86 | 0.40 |
| 1:C:176:LEU:HD22 | 1:C:176:LEU:N | 2.36 | 0.40 |
| 1:C:199:TYR:HB2 | 1:C:240:LEU:HD11 | 2.03 | 0.40 |
| 1:A:69:ASN:CG | 1:A:108:LEU:HD21 | 2.42 | 0.40 |
| 1:D:221:PHE:C | 1:D:242:PRO:HG3 | 2.42 | 0.40 |
| 1:E:7:SER:HA | 1:E:85:LEU:HD23 | 2.04 | 0.40 |
| 1:F:159:ALA:O | 1:F:160:GLU:HB2 | 2.21 | 0.40 |
| 1:D:43:ASN:HD21 | 1:D:117:ARG:HH22 | 1.69 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:15:LEU:N | 1:D:15:LEU:HD23 | 2.37 | 0.40 |
| 1:B:246:SER:O | 1:B:247:ASP:HB2 | 2.20 | 0.40 |
| 1:F:1:MET:O | 1:F:60:GLU:O | 2.40 | 0.40 |
| 1:A:131:ILE:HD13 | 1:A:163:PHE:HE1 | 1.87 | 0.40 |
| 1:D:172:ASP:OD1 | 1:E:108:LEU:HG | 2.22 | 0.40 |
| 1:B:131:ILE:HD13 | 1:B:163:PHE:HE1 | 1.87 | 0.40 |
| 1:E:86:ILE:HG21 | 1:E:99:ILE:HD11 | 2.02 | 0.40 |
| 1:B:47:VAL:HB | 1:B:238:TYR:CD2 | 2.55 | 0.40 |
| 1:C:34:LEU:HD23 | 1:C:34:LEU:N | 2.35 | 0.40 |
| 1:C:209:THR:O | 1:C:210:ASP:HB2 | 2.21 | 0.40 |
| 1:B:1:MET:O | 1:B:60:GLU:O | 2.40 | 0.40 |
| 1:C:46:MET:HE2 | 1:C:46:MET:HB3 | 1.97 | 0.40 |
| 1:B:15:LEU:HD23 | 1:B:15:LEU:N | 2.37 | 0.40 |
| 1:A:221:PHE:C | 1:A:242:PRO:HG3 | 2.42 | 0.40 |
| 1:B:199:TYR:HB2 | 1:B:240:LEU:HD11 | 2.03 | 0.40 |
| 1:C:159:ALA:O | 1:C:160:GLU:HB2 | 2.21 | 0.40 |
| 1:A:1:MET:O | 1:A:60:GLU:O | 2.40 | 0.40 |
| 1:D:195:PHE:HD2 | 1:D:240:LEU:HD23 | 1.86 | 0.40 |
| 1:E:221:PHE:C | 1:E:242:PRO:HG3 | 2.42 | 0.40 |
| 1:C:58:SER:C | 1:C:59:TYR:CD2 | 2.94 | 0.40 |
| 1:D:2:PHE:HA | 1:D:60:GLU:O | 2.21 | 0.40 |
| 1:B:25:CYS:O | 1:B:67:GLY:CA | 2.66 | 0.40 |
| 1:D:32:GLU:O | 1:D:33:SER:OG | 2.35 | 0.40 |
| 1:F:32:GLU:O | 1:F:33:SER:OG | 2.35 | 0.40 |
| 1:B:86:ILE:HG21 | 1:B:99:ILE:HD11 | 2.02 | 0.40 |
| 1:F:86:ILE:HG21 | 1:F:99:ILE:HD11 | 2.02 | 0.40 |
| 1:A:43:ASN:HD21 | 1:A:117:ARG:HH22 | 1.69 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1 | A | 245/247 (99%) | 206 (84%) | 30 (12%) | 9 (4%) | 4 | 29 |
| 1 | B | 245/247 (99%) | 206 (84%) | 30 (12%) | 9 (4%) | 4 | 29 |
| 1 | C | 245/247 (99%) | 206 (84%) | 30 (12%) | 9 (4%) | 4 | 29 |
| 1 | D | 245/247 (99%) | 206 (84%) | 30 (12%) | 9 (4%) | 4 | 29 |
| 1 | E | 245/247 (99%) | 206 (84%) | 30 (12%) | 9 (4%) | 4 | 29 |
| 1 | F | 245/247 (99%) | 206 (84%) | 30 (12%) | 9 (4%) | 4 | 29 |
| All | All | 1470/1482 (99%) | 1236 (84%) | 180 (12%) | 54 (4%) | 4 | 29 |

All (54) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 184 | ILE |
| 1 | A | 208 | PRO |
| 1 | B | 184 | ILE |
| 1 | B | 208 | PRO |
| 1 | C | 184 | ILE |
| 1 | C | 208 | PRO |
| 1 | D | 184 | ILE |
| 1 | D | 208 | PRO |
| 1 | E | 184 | ILE |
| 1 | E | 208 | PRO |
| 1 | F | 184 | ILE |
| 1 | F | 208 | PRO |
| 1 | A | 83 | GLY |
| 1 | A | 160 | GLU |
| 1 | A | 180 | PRO |
| 1 | B | 83 | GLY |
| 1 | B | 160 | GLU |
| 1 | B | 180 | PRO |
| 1 | C | 83 | GLY |
| 1 | C | 160 | GLU |
| 1 | C | 180 | PRO |
| 1 | D | 83 | GLY |
| 1 | D | 160 | GLU |
| 1 | D | 180 | PRO |
| 1 | E | 83 | GLY |
| 1 | E | 160 | GLU |
| 1 | E | 180 | PRO |
| 1 | F | 83 | GLY |
| 1 | F | 160 | GLU |
| 1 | F | 180 | PRO |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 37 | ARG |
| 1 | A | 159 | ALA |
| 1 | B | 37 | ARG |
| 1 | B | 159 | ALA |
| 1 | C | 37 | ARG |
| 1 | C | 159 | ALA |
| 1 | D | 37 | ARG |
| 1 | D | 159 | ALA |
| 1 | E | 37 | ARG |
| 1 | F | 37 | ARG |
| 1 | F | 159 | ALA |
| 1 | E | 159 | ALA |
| 1 | A | 181 | ALA |
| 1 | B | 181 | ALA |
| 1 | C | 181 | ALA |
| 1 | D | 181 | ALA |
| 1 | E | 181 | ALA |
| 1 | F | 181 | ALA |
| 1 | A | 242 | PRO |
| 1 | B | 242 | PRO |
| 1 | C | 242 | PRO |
| 1 | D | 242 | PRO |
| 1 | E | 242 | PRO |
| 1 | F | 242 | PRO |

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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | A | 203/203 (100%) | 159 (78%) | 44 (22%) | 1 | 6 |
| 1 | B | 203/203 (100%) | 159 (78%) | 44 (22%) | 1 | 6 |
| 1 | C | 203/203 (100%) | 159 (78%) | 44 (22%) | 1 | 6 |
| 1 | D | 203/203 (100%) | 159 (78%) | 44 (22%) | 1 | 6 |
| 1 | E | 203/203 (100%) | 159 (78%) | 44 (22%) | 1 | 6 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|-----------|-----------|-------------|---|
| 1 | F | 203/203 (100%) | 159 (78%) | 44 (22%) | 1 | 6 |
| All | All | 1218/1218 (100%) | 954 (78%) | 264 (22%) | 1 | 6 |

All (264) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 3 | LYS |
| 1 | A | 5 | ILE |
| 1 | A | 21 | LEU |
| 1 | A | 23 | ASP |
| 1 | A | 34 | LEU |
| 1 | A | 37 | ARG |
| 1 | A | 41 | PRO |
| 1 | A | 44 | VAL |
| 1 | A | 56 | PHE |
| 1 | A | 59 | TYR |
| 1 | A | 65 | VAL |
| 1 | A | 70 | LEU |
| 1 | A | 73 | LEU |
| 1 | A | 75 | GLU |
| 1 | A | 90 | LEU |
| 1 | A | 91 | ASP |
| 1 | A | 95 | ARG |
| 1 | A | 104 | LEU |
| 1 | A | 114 | ASP |
| 1 | A | 120 | PRO |
| 1 | A | 121 | ASP |
| 1 | A | 125 | LEU |
| 1 | A | 133 | LEU |
| 1 | A | 138 | LEU |
| 1 | A | 147 | MET |
| 1 | A | 149 | SER |
| 1 | A | 151 | HIS |
| 1 | A | 157 | ASP |
| 1 | A | 161 | GLU |
| 1 | A | 170 | ASP |
| 1 | A | 171 | THR |
| 1 | A | 176 | LEU |
| 1 | A | 180 | PRO |
| 1 | A | 185 | SER |
| 1 | A | 187 | GLU |
| 1 | A | 197 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 208 | PRO |
| 1 | A | 217 | LEU |
| 1 | A | 219 | GLU |
| 1 | A | 222 | PRO |
| 1 | A | 233 | MET |
| 1 | A | 239 | MET |
| 1 | A | 242 | PRO |
| 1 | A | 247 | ASP |
| 1 | B | 3 | LYS |
| 1 | B | 5 | ILE |
| 1 | B | 21 | LEU |
| 1 | B | 23 | ASP |
| 1 | B | 34 | LEU |
| 1 | B | 37 | ARG |
| 1 | B | 41 | PRO |
| 1 | B | 44 | VAL |
| 1 | B | 56 | PHE |
| 1 | B | 59 | TYR |
| 1 | B | 65 | VAL |
| 1 | B | 70 | LEU |
| 1 | B | 73 | LEU |
| 1 | B | 75 | GLU |
| 1 | B | 90 | LEU |
| 1 | B | 91 | ASP |
| 1 | B | 95 | ARG |
| 1 | B | 104 | LEU |
| 1 | B | 114 | ASP |
| 1 | B | 120 | PRO |
| 1 | B | 121 | ASP |
| 1 | B | 125 | LEU |
| 1 | B | 133 | LEU |
| 1 | B | 138 | LEU |
| 1 | B | 147 | MET |
| 1 | B | 149 | SER |
| 1 | B | 151 | HIS |
| 1 | B | 157 | ASP |
| 1 | B | 161 | GLU |
| 1 | B | 170 | ASP |
| 1 | B | 171 | THR |
| 1 | B | 176 | LEU |
| 1 | B | 180 | PRO |
| 1 | B | 185 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 187 | GLU |
| 1 | B | 197 | LEU |
| 1 | B | 208 | PRO |
| 1 | B | 217 | LEU |
| 1 | B | 219 | GLU |
| 1 | B | 222 | PRO |
| 1 | B | 233 | MET |
| 1 | B | 239 | MET |
| 1 | B | 242 | PRO |
| 1 | B | 247 | ASP |
| 1 | C | 3 | LYS |
| 1 | C | 5 | ILE |
| 1 | C | 21 | LEU |
| 1 | C | 23 | ASP |
| 1 | C | 34 | LEU |
| 1 | C | 37 | ARG |
| 1 | C | 41 | PRO |
| 1 | C | 44 | VAL |
| 1 | C | 56 | PHE |
| 1 | C | 59 | TYR |
| 1 | C | 65 | VAL |
| 1 | C | 70 | LEU |
| 1 | C | 73 | LEU |
| 1 | C | 75 | GLU |
| 1 | C | 90 | LEU |
| 1 | C | 91 | ASP |
| 1 | C | 95 | ARG |
| 1 | C | 104 | LEU |
| 1 | C | 114 | ASP |
| 1 | C | 120 | PRO |
| 1 | C | 121 | ASP |
| 1 | C | 125 | LEU |
| 1 | C | 133 | LEU |
| 1 | C | 138 | LEU |
| 1 | C | 147 | MET |
| 1 | C | 149 | SER |
| 1 | C | 151 | HIS |
| 1 | C | 157 | ASP |
| 1 | C | 161 | GLU |
| 1 | C | 170 | ASP |
| 1 | C | 171 | THR |
| 1 | C | 176 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 180 | PRO |
| 1 | C | 185 | SER |
| 1 | C | 187 | GLU |
| 1 | C | 197 | LEU |
| 1 | C | 208 | PRO |
| 1 | C | 217 | LEU |
| 1 | C | 219 | GLU |
| 1 | C | 222 | PRO |
| 1 | C | 233 | MET |
| 1 | C | 239 | MET |
| 1 | C | 242 | PRO |
| 1 | C | 247 | ASP |
| 1 | D | 3 | LYS |
| 1 | D | 5 | ILE |
| 1 | D | 21 | LEU |
| 1 | D | 23 | ASP |
| 1 | D | 34 | LEU |
| 1 | D | 37 | ARG |
| 1 | D | 41 | PRO |
| 1 | D | 44 | VAL |
| 1 | D | 56 | PHE |
| 1 | D | 59 | TYR |
| 1 | D | 65 | VAL |
| 1 | D | 70 | LEU |
| 1 | D | 73 | LEU |
| 1 | D | 75 | GLU |
| 1 | D | 90 | LEU |
| 1 | D | 91 | ASP |
| 1 | D | 95 | ARG |
| 1 | D | 104 | LEU |
| 1 | D | 114 | ASP |
| 1 | D | 120 | PRO |
| 1 | D | 121 | ASP |
| 1 | D | 125 | LEU |
| 1 | D | 133 | LEU |
| 1 | D | 138 | LEU |
| 1 | D | 147 | MET |
| 1 | D | 149 | SER |
| 1 | D | 151 | HIS |
| 1 | D | 157 | ASP |
| 1 | D | 161 | GLU |
| 1 | D | 170 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 171 | THR |
| 1 | D | 176 | LEU |
| 1 | D | 180 | PRO |
| 1 | D | 185 | SER |
| 1 | D | 187 | GLU |
| 1 | D | 197 | LEU |
| 1 | D | 208 | PRO |
| 1 | D | 217 | LEU |
| 1 | D | 219 | GLU |
| 1 | D | 222 | PRO |
| 1 | D | 233 | MET |
| 1 | D | 239 | MET |
| 1 | D | 242 | PRO |
| 1 | D | 247 | ASP |
| 1 | E | 3 | LYS |
| 1 | E | 5 | ILE |
| 1 | E | 21 | LEU |
| 1 | E | 23 | ASP |
| 1 | E | 34 | LEU |
| 1 | E | 37 | ARG |
| 1 | E | 41 | PRO |
| 1 | E | 44 | VAL |
| 1 | E | 56 | PHE |
| 1 | E | 59 | TYR |
| 1 | E | 65 | VAL |
| 1 | E | 70 | LEU |
| 1 | E | 73 | LEU |
| 1 | E | 75 | GLU |
| 1 | E | 90 | LEU |
| 1 | E | 91 | ASP |
| 1 | E | 95 | ARG |
| 1 | E | 104 | LEU |
| 1 | E | 114 | ASP |
| 1 | E | 120 | PRO |
| 1 | E | 121 | ASP |
| 1 | E | 125 | LEU |
| 1 | E | 133 | LEU |
| 1 | E | 138 | LEU |
| 1 | E | 147 | MET |
| 1 | E | 149 | SER |
| 1 | E | 151 | HIS |
| 1 | E | 157 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 161 | GLU |
| 1 | E | 170 | ASP |
| 1 | E | 171 | THR |
| 1 | E | 176 | LEU |
| 1 | E | 180 | PRO |
| 1 | E | 185 | SER |
| 1 | E | 187 | GLU |
| 1 | E | 197 | LEU |
| 1 | E | 208 | PRO |
| 1 | E | 217 | LEU |
| 1 | E | 219 | GLU |
| 1 | E | 222 | PRO |
| 1 | E | 233 | MET |
| 1 | E | 239 | MET |
| 1 | E | 242 | PRO |
| 1 | E | 247 | ASP |
| 1 | F | 3 | LYS |
| 1 | F | 5 | ILE |
| 1 | F | 21 | LEU |
| 1 | F | 23 | ASP |
| 1 | F | 34 | LEU |
| 1 | F | 37 | ARG |
| 1 | F | 41 | PRO |
| 1 | F | 44 | VAL |
| 1 | F | 56 | PHE |
| 1 | F | 59 | TYR |
| 1 | F | 65 | VAL |
| 1 | F | 70 | LEU |
| 1 | F | 73 | LEU |
| 1 | F | 75 | GLU |
| 1 | F | 90 | LEU |
| 1 | F | 91 | ASP |
| 1 | F | 95 | ARG |
| 1 | F | 104 | LEU |
| 1 | F | 114 | ASP |
| 1 | F | 120 | PRO |
| 1 | F | 121 | ASP |
| 1 | F | 125 | LEU |
| 1 | F | 133 | LEU |
| 1 | F | 138 | LEU |
| 1 | F | 147 | MET |
| 1 | F | 149 | SER |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 151 | HIS |
| 1 | F | 157 | ASP |
| 1 | F | 161 | GLU |
| 1 | F | 170 | ASP |
| 1 | F | 171 | THR |
| 1 | F | 176 | LEU |
| 1 | F | 180 | PRO |
| 1 | F | 185 | SER |
| 1 | F | 187 | GLU |
| 1 | F | 197 | LEU |
| 1 | F | 208 | PRO |
| 1 | F | 217 | LEU |
| 1 | F | 219 | GLU |
| 1 | F | 222 | PRO |
| 1 | F | 233 | MET |
| 1 | F | 239 | MET |
| 1 | F | 242 | PRO |
| 1 | F | 247 | ASP |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 43 | ASN |
| 1 | B | 43 | ASN |
| 1 | C | 43 | ASN |
| 1 | C | 87 | HIS |
| 1 | D | 43 | ASN |
| 1 | E | 43 | ASN |
| 1 | E | 87 | HIS |
| 1 | F | 43 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 1 | A | 247/247 (100%) | -0.20 | 10 (4%) 42 27 | 93, 138, 172, 203 | 0 |
| 1 | B | 247/247 (100%) | -0.13 | 10 (4%) 42 27 | 95, 139, 172, 204 | 0 |
| 1 | C | 247/247 (100%) | -0.20 | 8 (3%) 51 36 | 94, 139, 172, 203 | 0 |
| 1 | D | 247/247 (100%) | -0.19 | 12 (4%) 33 20 | 94, 138, 173, 204 | 0 |
| 1 | E | 247/247 (100%) | -0.20 | 7 (2%) 56 42 | 95, 139, 172, 203 | 0 |
| 1 | F | 247/247 (100%) | -0.21 | 6 (2%) 62 47 | 94, 139, 172, 205 | 0 |
| All | All | 1482/1482 (100%) | -0.19 | 53 (3%) 46 31 | 93, 139, 175, 205 | 0 |

All (53) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 246 | SER | 5.8 |
| 1 | F | 244 | ILE | 5.8 |
| 1 | D | 244 | ILE | 5.5 |
| 1 | F | 243 | ARG | 5.2 |
| 1 | D | 245 | GLN | 5.1 |
| 1 | E | 244 | ILE | 4.9 |
| 1 | A | 244 | ILE | 4.9 |
| 1 | B | 245 | GLN | 4.7 |
| 1 | B | 244 | ILE | 4.6 |
| 1 | A | 245 | GLN | 4.5 |
| 1 | C | 243 | ARG | 4.4 |
| 1 | A | 148 | VAL | 4.3 |
| 1 | A | 246 | SER | 4.3 |
| 1 | F | 246 | SER | 4.3 |
| 1 | C | 148 | VAL | 4.1 |
| 1 | B | 94 | THR | 4.0 |
| 1 | B | 243 | ARG | 3.9 |
| 1 | C | 245 | GLN | 3.9 |
| 1 | D | 243 | ARG | 3.9 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 220 | GLU | 3.8 |
| 1 | E | 246 | SER | 3.7 |
| 1 | F | 245 | GLN | 3.7 |
| 1 | D | 246 | SER | 3.6 |
| 1 | A | 220 | GLU | 3.3 |
| 1 | C | 244 | ILE | 3.3 |
| 1 | F | 220 | GLU | 3.3 |
| 1 | A | 159 | ALA | 3.3 |
| 1 | A | 243 | ARG | 3.3 |
| 1 | C | 15 | LEU | 3.3 |
| 1 | E | 245 | GLN | 3.1 |
| 1 | D | 94 | THR | 3.0 |
| 1 | E | 243 | ARG | 3.0 |
| 1 | E | 219 | GLU | 3.0 |
| 1 | D | 15 | LEU | 2.9 |
| 1 | D | 131 | ILE | 2.9 |
| 1 | A | 15 | LEU | 2.8 |
| 1 | B | 220 | GLU | 2.6 |
| 1 | C | 93 | GLU | 2.6 |
| 1 | E | 189 | GLY | 2.6 |
| 1 | D | 111 | ILE | 2.6 |
| 1 | C | 246 | SER | 2.6 |
| 1 | E | 15 | LEU | 2.5 |
| 1 | B | 26 | LYS | 2.5 |
| 1 | B | 132 | VAL | 2.5 |
| 1 | C | 94 | THR | 2.4 |
| 1 | D | 148 | VAL | 2.4 |
| 1 | B | 22 | VAL | 2.3 |
| 1 | B | 236 | ILE | 2.3 |
| 1 | F | 153 | ARG | 2.2 |
| 1 | A | 236 | ILE | 2.2 |
| 1 | D | 110 | LEU | 2.1 |
| 1 | D | 184 | ILE | 2.0 |
| 1 | A | 189 | GLY | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.