



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:50 pm GMT

PDB ID : 1AON
Title : CRYSTAL STRUCTURE OF THE ASYMMETRIC CHAPERONIN COM-
PLEX GROEL/GROES/(ADP)7
Authors : Xu, Z.; Horwich, A.L.; Sigler, P.B.
Deposited on : 1997-07-08
Resolution : 3.00 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:

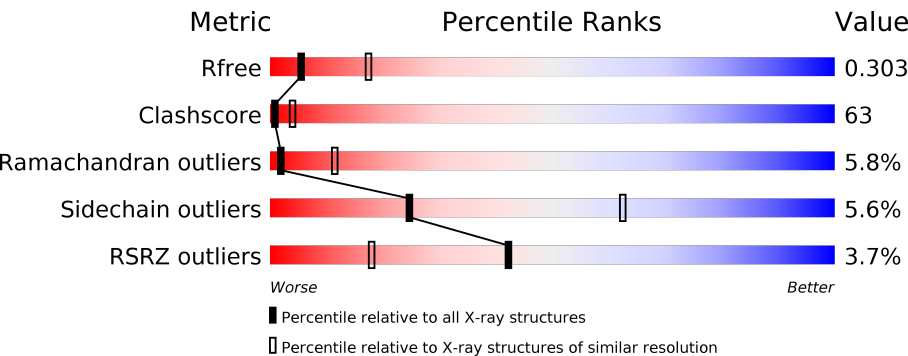
| | | |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.2 (RC1), CSD as538be (2017) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | trunk28620 |
| Percentile statistics | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac | : | 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) | : | trunk28620 |

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 100719 | 1692 (3.00-3.00) |
| Clashscore | 112137 | 2037 (3.00-3.00) |
| Ramachandran outliers | 110173 | 1973 (3.00-3.00) |
| Sidechain outliers | 110143 | 1976 (3.00-3.00) |
| RSRZ outliers | 101464 | 1716 (3.00-3.00) |

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 | 547 | |
| 1 | B | 547 | |
| 1 | C | 547 | |
| 1 | D | 547 | |
| 1 | E | 547 | |
| 1 | F | 547 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | G | 547 | |
| 1 | H | 547 | |
| 1 | I | 547 | |
| 1 | J | 547 | |
| 1 | K | 547 | |
| 1 | L | 547 | |
| 1 | M | 547 | |
| 1 | N | 547 | |
| 2 | O | 97 | |
| 2 | P | 97 | |
| 2 | Q | 97 | |
| 2 | R | 97 | |
| 2 | S | 97 | |
| 2 | T | 97 | |
| 2 | U | 97 | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4 | ADP | A | 1 | - | - | - | X |
| 4 | ADP | B | 1 | - | - | - | X |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 58870 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 GROEL.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3808 | 2368 | 653 | 767 | 20 | | | |
| 1 | B | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3808 | 2368 | 653 | 767 | 20 | | | |
| 1 | C | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3808 | 2368 | 653 | 767 | 20 | | | |
| 1 | D | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3808 | 2368 | 653 | 767 | 20 | | | |
| 1 | E | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3808 | 2368 | 653 | 767 | 20 | | | |
| 1 | F | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3808 | 2368 | 653 | 767 | 20 | | | |
| 1 | G | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3808 | 2368 | 653 | 767 | 20 | | | |
| 1 | H | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3849 | 2394 | 662 | 773 | 20 | | | |
| 1 | I | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3849 | 2394 | 662 | 773 | 20 | | | |
| 1 | J | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3849 | 2394 | 662 | 773 | 20 | | | |
| 1 | K | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3849 | 2394 | 662 | 773 | 20 | | | |
| 1 | L | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3849 | 2394 | 662 | 773 | 20 | | | |
| 1 | M | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3849 | 2394 | 662 | 773 | 20 | | | |
| 1 | N | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3849 | 2394 | 662 | 773 | 20 | | | |

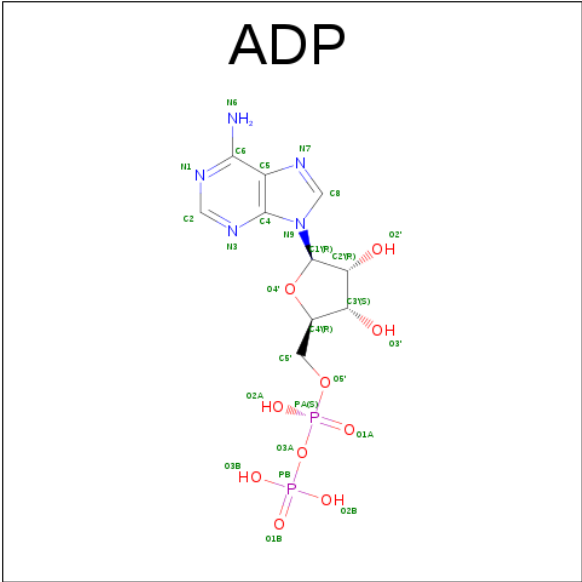
- Molecule 2 is a protein called GROEL/GROES COMPLEX.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | O | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 725 | 452 | 127 | 145 | 1 | | | |
| 2 | P | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 725 | 452 | 127 | 145 | 1 | | | |
| 2 | Q | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 725 | 452 | 127 | 145 | 1 | | | |
| 2 | R | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 725 | 452 | 127 | 145 | 1 | | | |
| 2 | S | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 725 | 452 | 127 | 145 | 1 | | | |
| 2 | T | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 725 | 452 | 127 | 145 | 1 | | | |
| 2 | U | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 725 | 452 | 127 | 145 | 1 | | | |

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

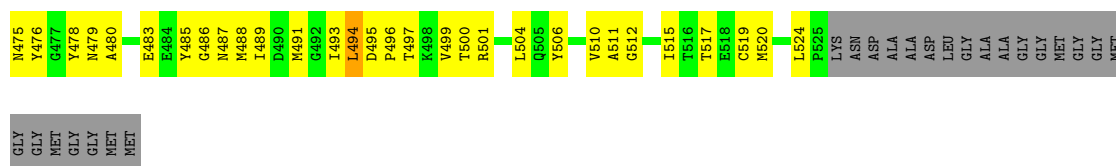
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | G | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | D | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | E | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | C | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | A | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | F | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

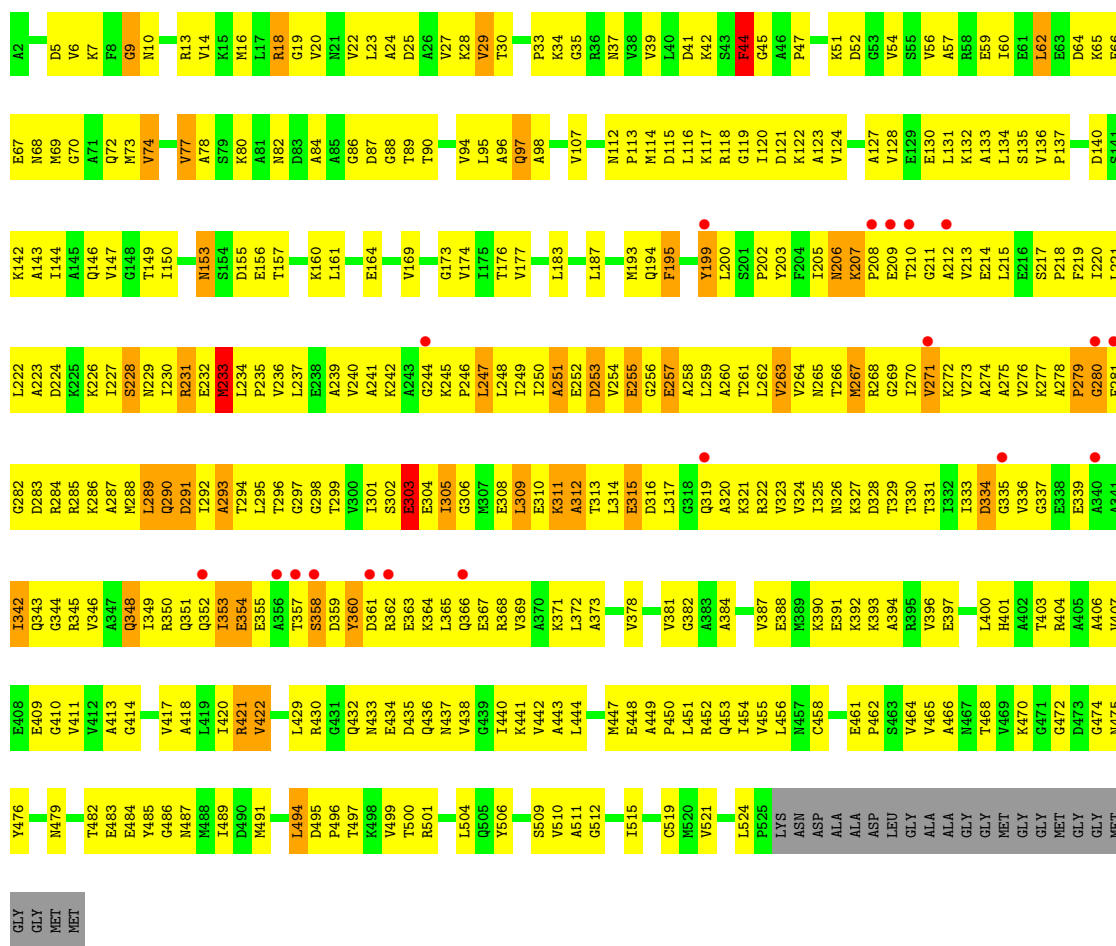


| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 4 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 4 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 4 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 4 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 4 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 4 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 4 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |

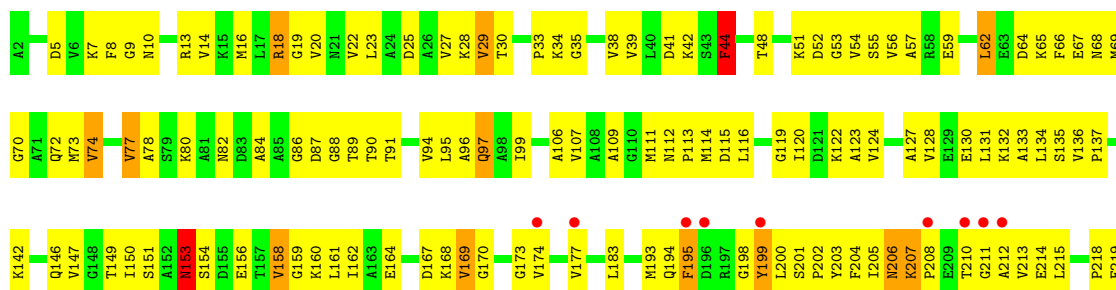


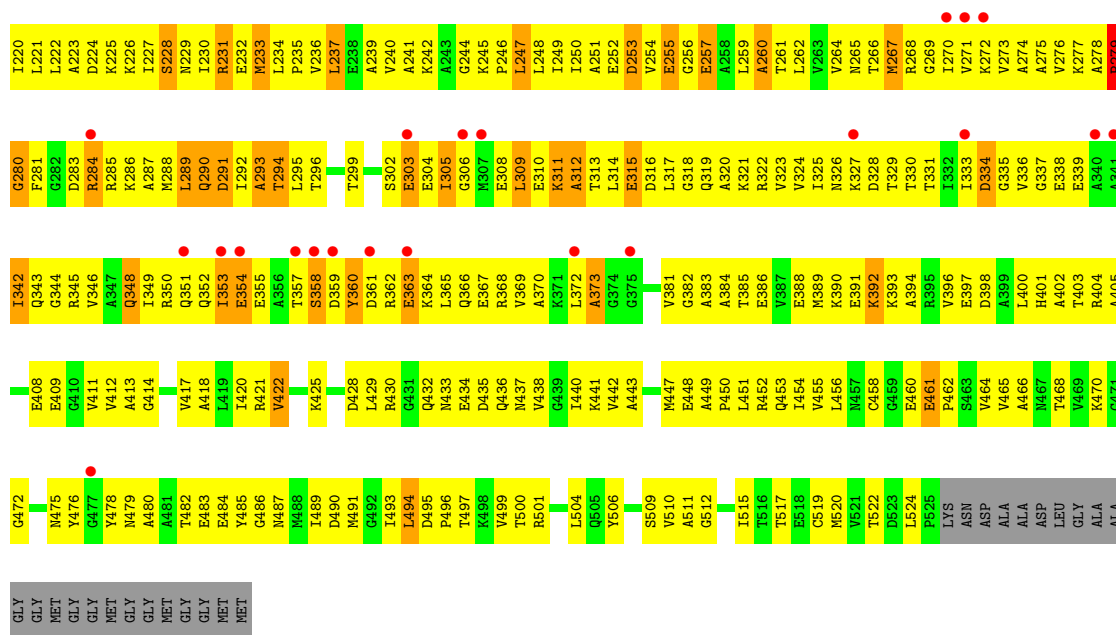


• Molecule 1: GROEL



• Molecule 1: GROEL





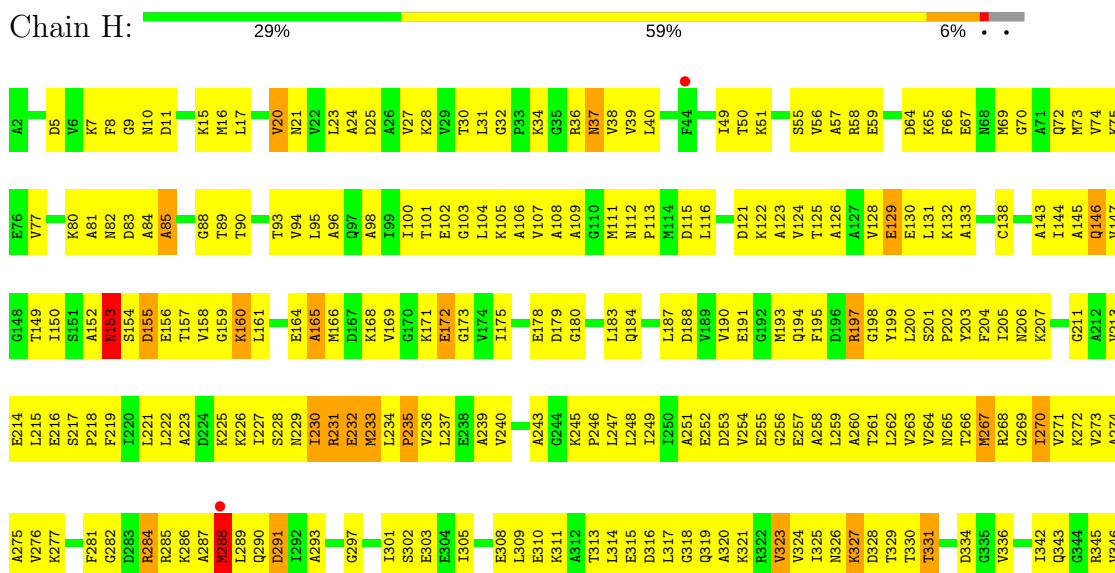
• Molecule 1: GROEL

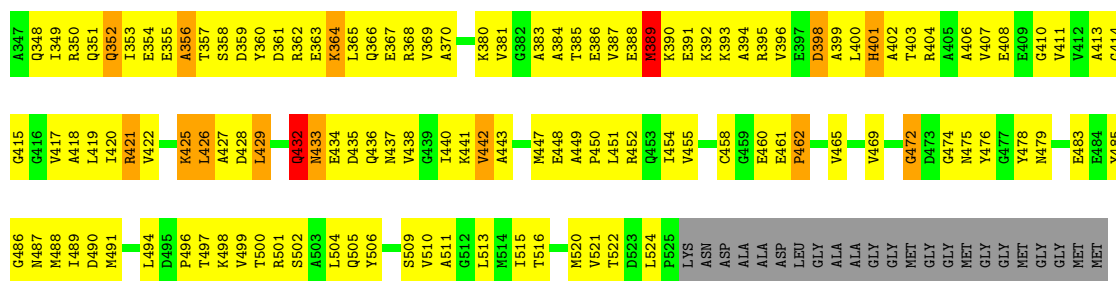


- Molecule 1: GROEL



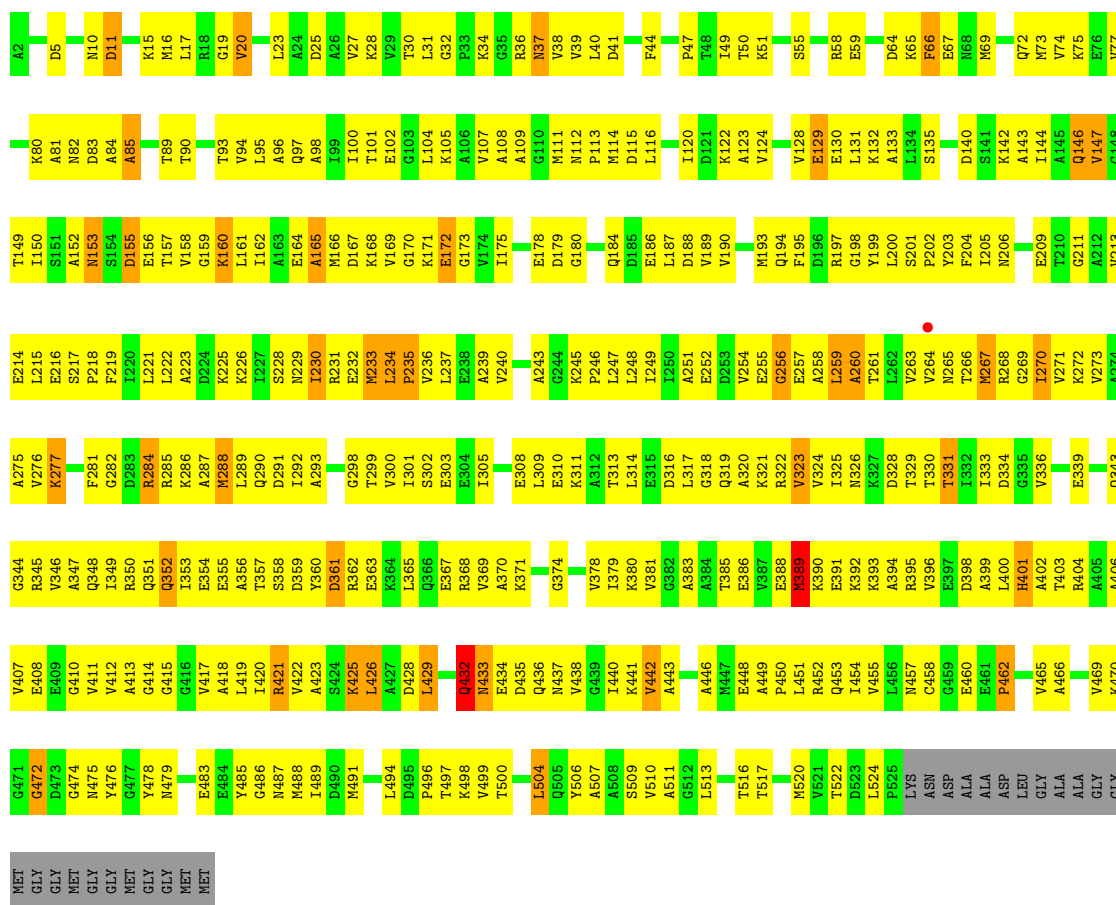
- Molecule 1: GROEL





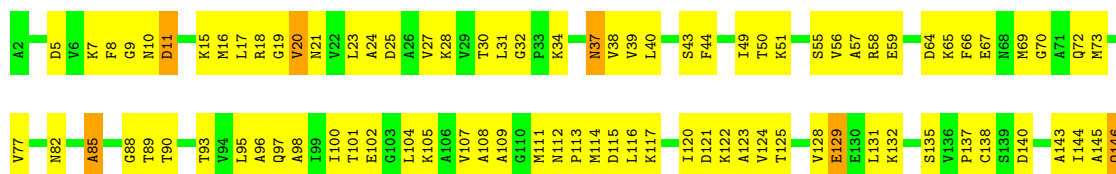
• Molecule 1: GROEL

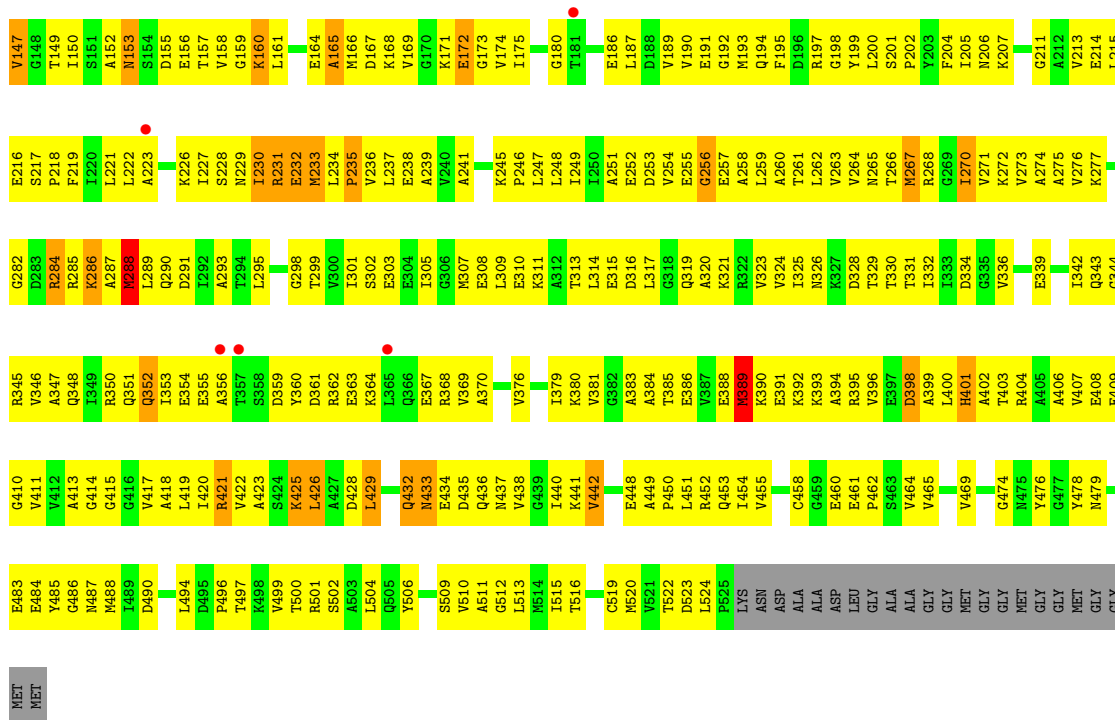
Chain I: 30% 58% 7% .



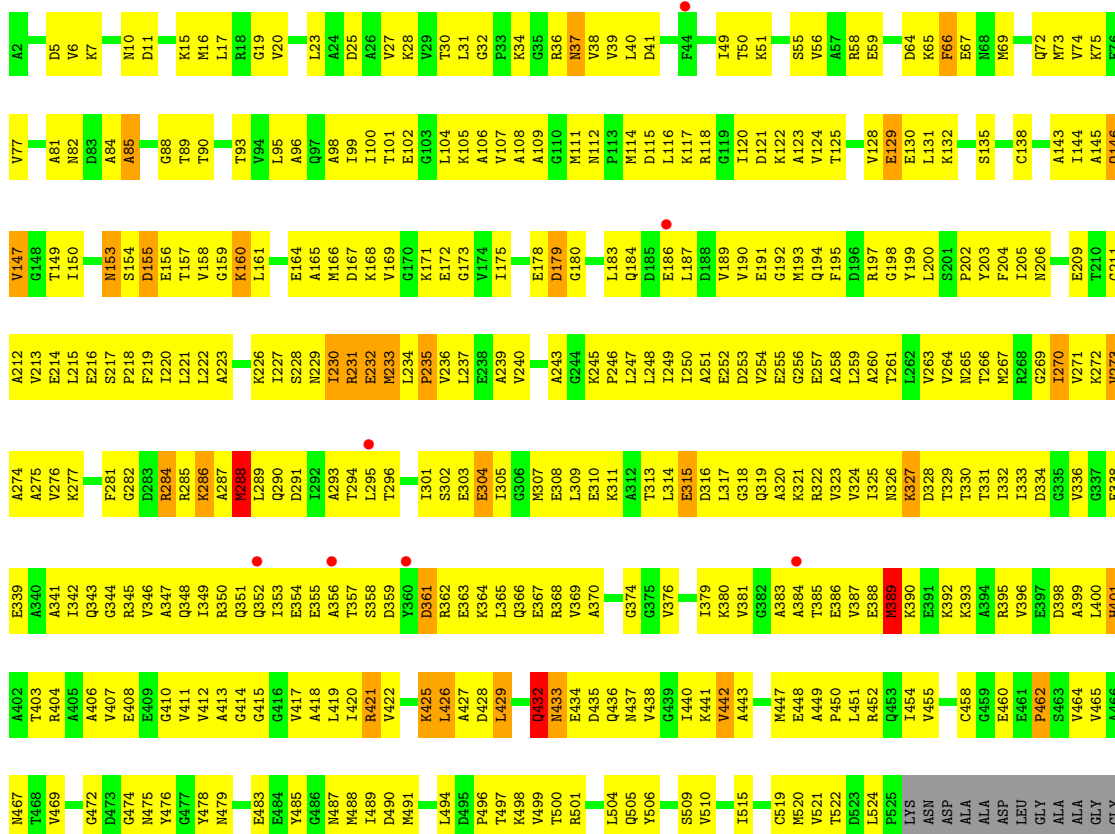
• Molecule 1: GROEL

Chain J: 31% 59% 6% .





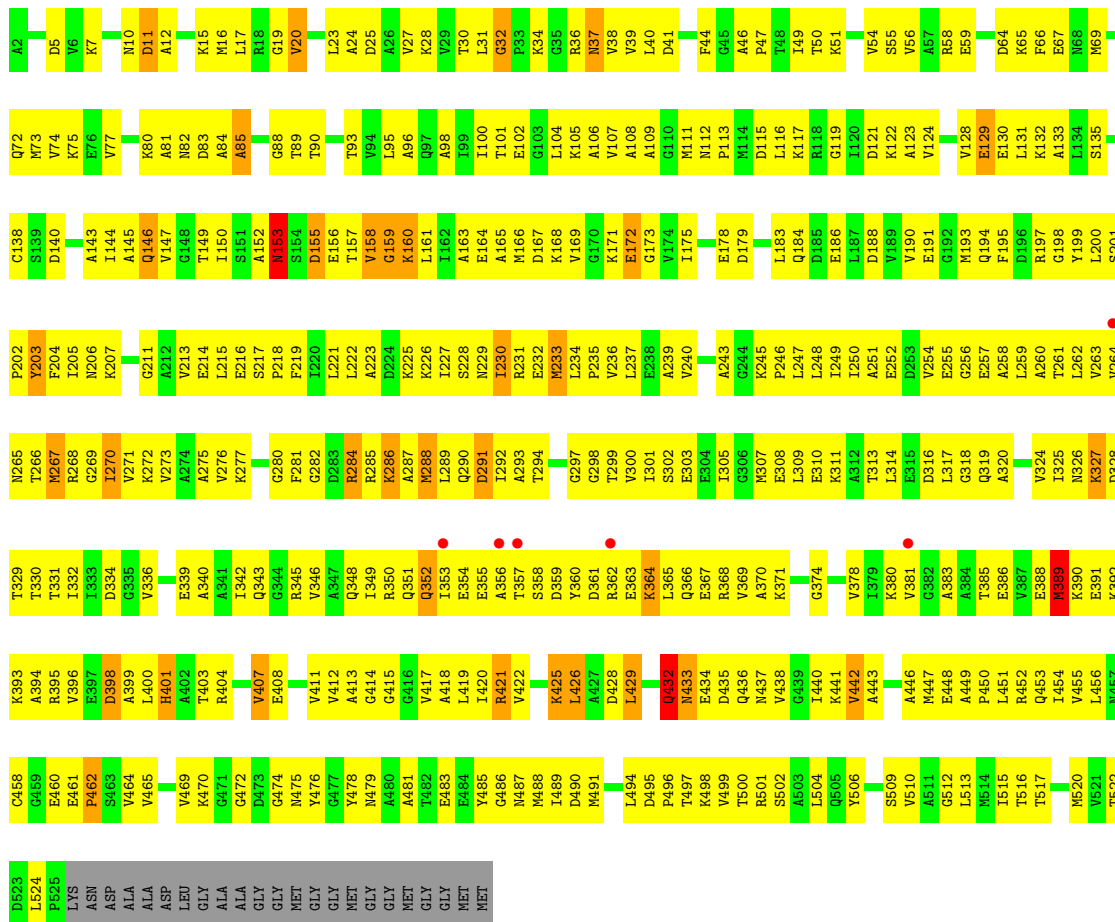
- Molecule 1: GROEL



MET
GLY
GLY
MET
GLY
GLY
MET
GLY
MET
MET

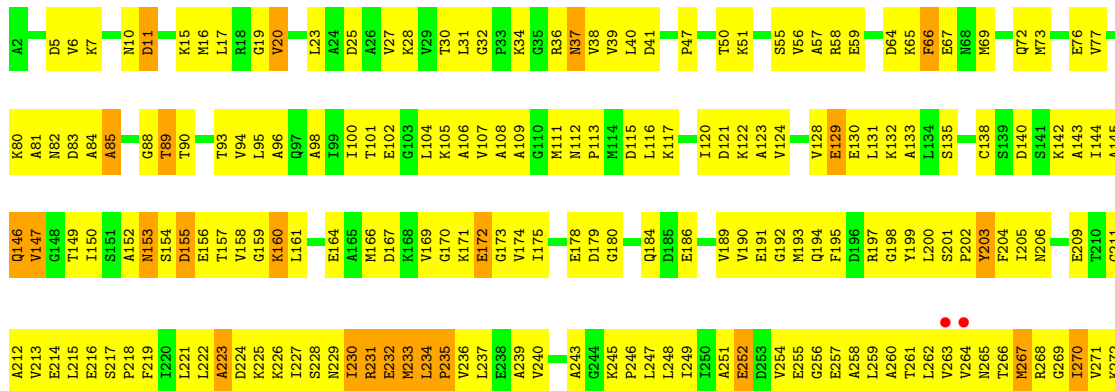
• Molecule 1: GROEL

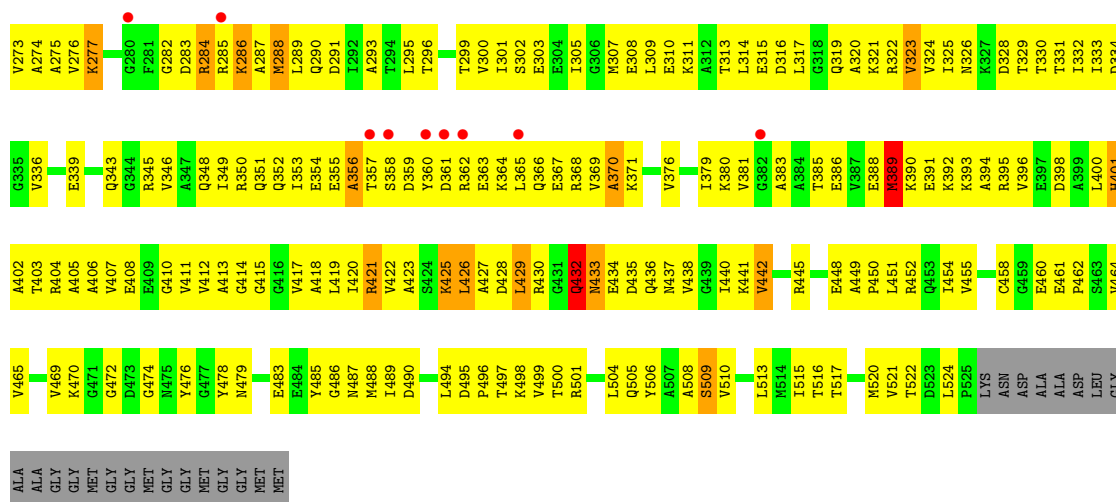
Chain L:  27% 62% 6%



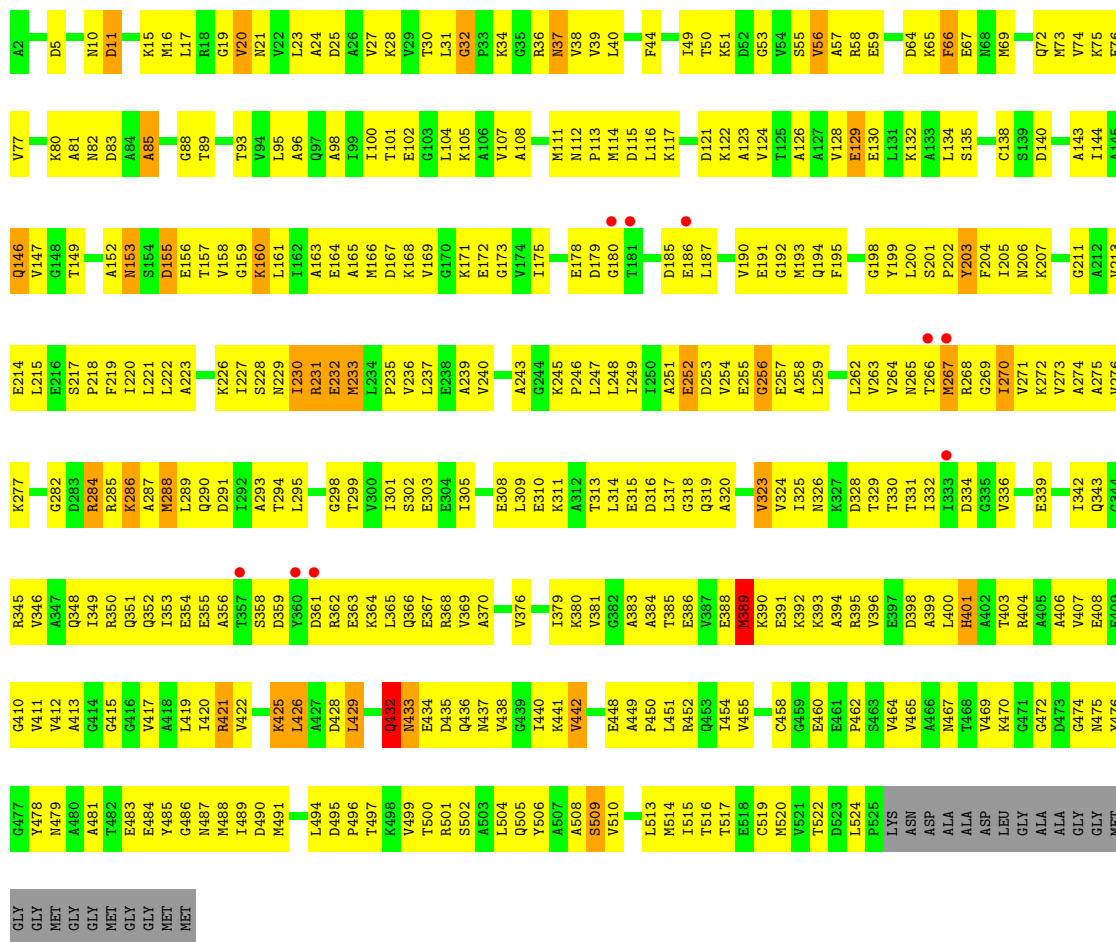
• Molecule 1: GROEL

Chain M:  28% 61% 7%



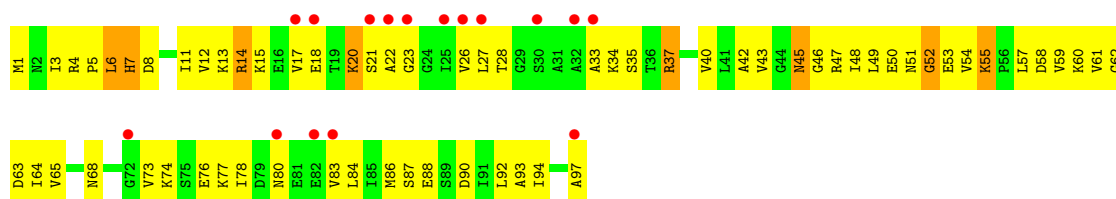


• Molecule 1: GROEL

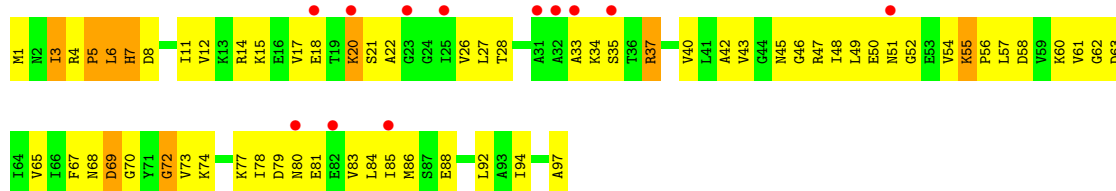


• Molecule 2: GROEL/GROES COMPLEX

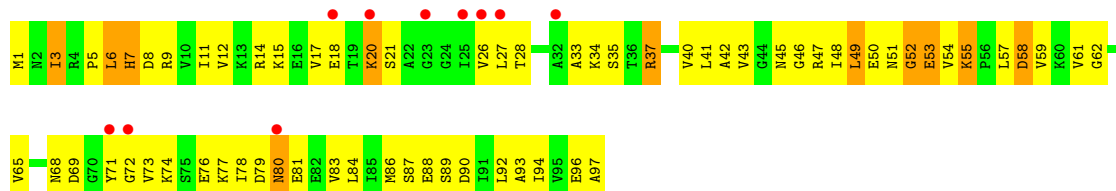




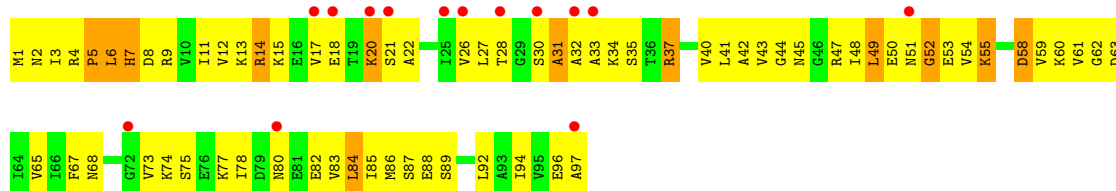
• Molecule 2: GROEL/GROES COMPLEX



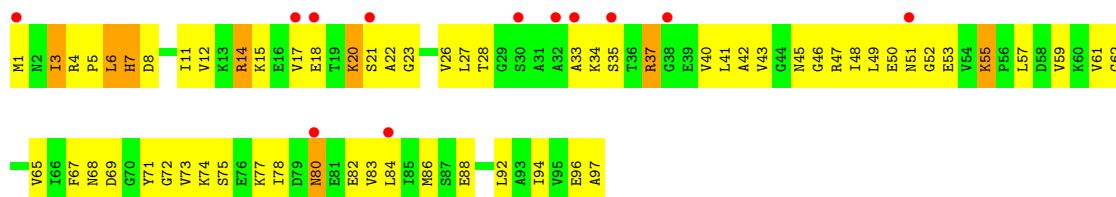
• Molecule 2: GROEL/GROES COMPLEX



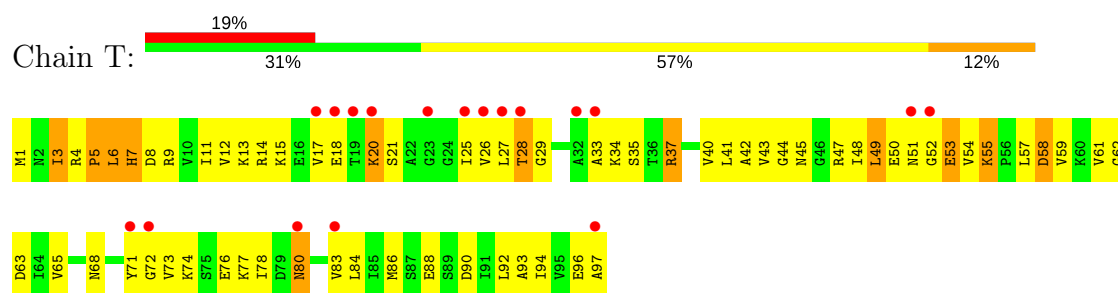
• Molecule 2: GROEL/GROES COMPLEX



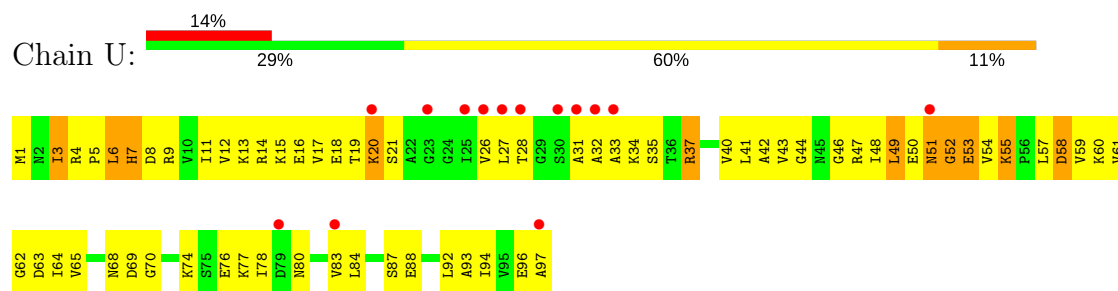
• Molecule 2: GROEL/GROES COMPLEX



• Molecule 2: GROEL/GROES COMPLEX



• Molecule 2: GROEL/GROES COMPLEX



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 255.26Å 265.25Å 184.40Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 3.00 40.07 – 2.99 | Depositor EDS |
| % Data completeness (in resolution range) | 79.7 (40.00-3.00) 96.7 (40.07-2.99) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.12 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.25 (at 3.01Å) | Xtriage |
| Refinement program | X-PLOR | Depositor |
| R, R_{free} | 0.248 , 0.291 0.266 , 0.303 | Depositor DCC |
| R_{free} test set | 12040 reflections (4.98%) | DCC |
| Wilson B-factor (Å ²) | 50.3 | Xtriage |
| Anisotropy | 0.614 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.31 , 70.3 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$ | Xtriage |
| Estimated twinning fraction | 0.003 for k,h,-l | Xtriage |
| F_o, F_c correlation | 0.89 | EDS |
| Total number of atoms | 58870 | wwPDB-VP |
| Average B, all atoms (Å ²) | 61.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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 | 0.52 | 0/3835 | 0.76 | 0/5186 |
| 1 | B | 0.52 | 0/3835 | 0.75 | 0/5186 |
| 1 | C | 0.52 | 0/3835 | 0.74 | 0/5186 |
| 1 | D | 0.53 | 0/3835 | 0.74 | 0/5186 |
| 1 | E | 0.52 | 0/3835 | 0.76 | 0/5186 |
| 1 | F | 0.52 | 0/3835 | 0.75 | 0/5186 |
| 1 | G | 0.52 | 0/3835 | 0.75 | 0/5186 |
| 1 | H | 0.48 | 0/3877 | 0.73 | 0/5236 |
| 1 | I | 0.49 | 0/3877 | 0.71 | 0/5236 |
| 1 | J | 0.47 | 0/3877 | 0.72 | 0/5236 |
| 1 | K | 0.47 | 0/3877 | 0.72 | 0/5236 |
| 1 | L | 0.46 | 0/3877 | 0.72 | 0/5236 |
| 1 | M | 0.47 | 0/3877 | 0.71 | 0/5236 |
| 1 | N | 0.48 | 0/3877 | 0.73 | 0/5236 |
| 2 | O | 0.39 | 0/729 | 0.68 | 0/980 |
| 2 | P | 0.36 | 0/729 | 0.68 | 0/980 |
| 2 | Q | 0.37 | 0/729 | 0.69 | 0/980 |
| 2 | R | 0.40 | 0/729 | 0.69 | 0/980 |
| 2 | S | 0.37 | 0/729 | 0.69 | 0/980 |
| 2 | T | 0.39 | 0/729 | 0.69 | 0/980 |
| 2 | U | 0.36 | 0/729 | 0.68 | 0/980 |
| All | All | 0.49 | 0/59087 | 0.73 | 0/79814 |

There are no bond length outliers.

There are no bond angle outliers.

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 | 3808 | 0 | 3890 | 563 | 1 |
| 1 | B | 3808 | 0 | 3890 | 513 | 0 |
| 1 | C | 3808 | 0 | 3890 | 525 | 0 |
| 1 | D | 3808 | 0 | 3890 | 527 | 0 |
| 1 | E | 3808 | 0 | 3890 | 537 | 0 |
| 1 | F | 3808 | 0 | 3890 | 556 | 0 |
| 1 | G | 3808 | 0 | 3890 | 535 | 0 |
| 1 | H | 3849 | 0 | 3965 | 479 | 0 |
| 1 | I | 3849 | 0 | 3965 | 439 | 0 |
| 1 | J | 3849 | 0 | 3965 | 444 | 1 |
| 1 | K | 3849 | 0 | 3965 | 479 | 0 |
| 1 | L | 3849 | 0 | 3965 | 504 | 0 |
| 1 | M | 3849 | 0 | 3965 | 486 | 0 |
| 1 | N | 3849 | 0 | 3965 | 435 | 0 |
| 2 | O | 725 | 0 | 755 | 119 | 0 |
| 2 | P | 725 | 0 | 755 | 98 | 0 |
| 2 | Q | 725 | 0 | 755 | 106 | 0 |
| 2 | R | 725 | 0 | 755 | 104 | 0 |
| 2 | S | 725 | 0 | 755 | 98 | 0 |
| 2 | T | 725 | 0 | 755 | 112 | 0 |
| 2 | U | 725 | 0 | 755 | 101 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | E | 1 | 0 | 0 | 0 | 0 |
| 3 | F | 1 | 0 | 0 | 0 | 0 |
| 3 | G | 1 | 0 | 0 | 0 | 0 |
| 4 | A | 27 | 0 | 12 | 2 | 0 |
| 4 | B | 27 | 0 | 12 | 5 | 0 |
| 4 | C | 27 | 0 | 12 | 5 | 0 |
| 4 | D | 27 | 0 | 12 | 1 | 0 |
| 4 | E | 27 | 0 | 12 | 1 | 0 |
| 4 | F | 27 | 0 | 12 | 6 | 0 |
| 4 | G | 27 | 0 | 12 | 2 | 0 |
| All | All | 58870 | 0 | 60354 | 7568 | 1 |

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 63.

All (7568) 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:G:233:MET:HA | 1:G:310:GLU:HG3 | 1.20 | 1.19 |
| 1:F:322:ARG:HB3 | 1:F:333:ILE:HD12 | 1.24 | 1.18 |
| 1:B:228:SER:HA | 1:B:255:GLU:HB2 | 1.27 | 1.13 |
| 1:D:214:GLU:HB3 | 1:D:322:ARG:HD3 | 1.30 | 1.13 |
| 2:O:55:LYS:H | 2:O:55:LYS:HE2 | 1.15 | 1.12 |
| 1:B:214:GLU:HB3 | 1:B:322:ARG:HD3 | 1.32 | 1.12 |
| 1:H:230:ILE:HG13 | 1:H:258:ALA:HA | 1.32 | 1.11 |
| 1:G:18:ARG:HH11 | 1:G:18:ARG:HB3 | 1.15 | 1.10 |
| 1:A:233:MET:HA | 1:A:310:GLU:HG3 | 1.31 | 1.10 |
| 2:U:55:LYS:H | 2:U:55:LYS:HE2 | 1.11 | 1.10 |
| 1:D:305:ILE:HG22 | 1:D:306:GLY:H | 1.10 | 1.09 |
| 1:L:232:GLU:HB3 | 1:L:309:LEU:HB2 | 1.25 | 1.09 |
| 1:F:233:MET:HA | 1:F:310:GLU:HG3 | 1.33 | 1.09 |
| 1:H:308:GLU:HB3 | 1:H:311:LYS:HD3 | 1.35 | 1.09 |
| 1:A:228:SER:HA | 1:A:255:GLU:HB2 | 1.29 | 1.08 |
| 1:B:18:ARG:HB3 | 1:B:18:ARG:HH11 | 1.14 | 1.08 |
| 1:C:18:ARG:HB3 | 1:C:18:ARG:HH11 | 1.02 | 1.08 |
| 1:F:228:SER:HA | 1:F:255:GLU:HB2 | 1.32 | 1.08 |
| 1:C:233:MET:HA | 1:C:310:GLU:HG3 | 1.29 | 1.07 |
| 1:C:322:ARG:HB3 | 1:C:333:ILE:HD12 | 1.37 | 1.07 |
| 1:G:214:GLU:HB3 | 1:G:322:ARG:HD3 | 1.34 | 1.07 |
| 1:B:233:MET:HA | 1:B:310:GLU:HG3 | 1.30 | 1.07 |
| 1:K:359:ASP:HA | 1:K:362:ARG:HH12 | 1.17 | 1.07 |
| 2:Q:55:LYS:HE2 | 2:Q:55:LYS:H | 1.14 | 1.06 |
| 1:E:296:THR:HG22 | 1:E:335:GLY:HA3 | 1.35 | 1.06 |
| 1:E:18:ARG:HH11 | 1:E:18:ARG:HB3 | 1.16 | 1.05 |
| 1:F:296:THR:HG22 | 1:F:335:GLY:HA3 | 1.39 | 1.05 |
| 1:D:18:ARG:HB3 | 1:D:18:ARG:HH11 | 1.14 | 1.05 |
| 1:E:228:SER:HA | 1:E:255:GLU:HB2 | 1.33 | 1.05 |
| 1:L:230:ILE:HG13 | 1:L:258:ALA:HA | 1.39 | 1.05 |
| 1:A:18:ARG:HH11 | 1:A:18:ARG:HB3 | 1.18 | 1.04 |
| 1:G:322:ARG:HB3 | 1:G:333:ILE:HD12 | 1.37 | 1.04 |
| 1:H:232:GLU:HB3 | 1:H:309:LEU:HB2 | 1.38 | 1.04 |
| 1:E:322:ARG:HB3 | 1:E:333:ILE:HD12 | 1.39 | 1.04 |
| 1:F:18:ARG:HH11 | 1:F:18:ARG:HB3 | 1.19 | 1.04 |
| 1:N:230:ILE:H | 1:N:230:ILE:HD12 | 1.17 | 1.04 |
| 1:J:230:ILE:HG13 | 1:J:258:ALA:HA | 1.37 | 1.03 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:356:ALA:HB1 | 1:J:362:ARG:HE | 1.24 | 1.03 |
| 1:D:322:ARG:HB3 | 1:D:333:ILE:HD12 | 1.40 | 1.03 |
| 1:K:223:ALA:HB3 | 1:K:251:ALA:HB2 | 1.40 | 1.02 |
| 1:I:308:GLU:HB3 | 1:I:311:LYS:HD3 | 1.38 | 1.02 |
| 1:N:223:ALA:HB3 | 1:N:251:ALA:HB2 | 1.40 | 1.02 |
| 1:M:239:ALA:HB1 | 1:M:314:LEU:HD11 | 1.36 | 1.02 |
| 1:L:359:ASP:HA | 1:L:362:ARG:HH12 | 1.23 | 1.02 |
| 1:H:230:ILE:HD12 | 1:H:230:ILE:H | 1.21 | 1.01 |
| 1:L:314:LEU:HD12 | 1:L:314:LEU:H | 1.25 | 1.01 |
| 1:D:233:MET:HA | 1:D:310:GLU:HG3 | 1.42 | 1.01 |
| 1:B:322:ARG:HB3 | 1:B:333:ILE:HD12 | 1.40 | 1.01 |
| 1:G:305:ILE:HG22 | 1:G:306:GLY:H | 1.26 | 1.01 |
| 1:I:230:ILE:H | 1:I:230:ILE:HD12 | 1.17 | 1.01 |
| 1:G:239:ALA:HB1 | 1:G:314:LEU:HD23 | 1.43 | 1.01 |
| 1:C:228:SER:HA | 1:C:255:GLU:HB2 | 1.41 | 1.00 |
| 1:J:314:LEU:H | 1:J:314:LEU:HD12 | 1.21 | 1.00 |
| 1:J:239:ALA:HB1 | 1:J:314:LEU:HD11 | 1.44 | 1.00 |
| 1:M:230:ILE:H | 1:M:230:ILE:HD12 | 1.20 | 1.00 |
| 1:H:223:ALA:HB3 | 1:H:251:ALA:HB2 | 1.43 | 1.00 |
| 1:E:214:GLU:HB3 | 1:E:322:ARG:HD3 | 1.44 | 1.00 |
| 1:G:33:PRO:HA | 1:G:153:ASN:HD21 | 1.27 | 1.00 |
| 1:I:232:GLU:HB3 | 1:I:309:LEU:HB2 | 1.44 | 1.00 |
| 1:N:65:LYS:O | 1:N:66:PHE:HB2 | 1.61 | 1.00 |
| 1:J:230:ILE:HD12 | 1:J:230:ILE:H | 1.27 | 0.99 |
| 1:F:214:GLU:HB3 | 1:F:322:ARG:HD3 | 1.42 | 0.99 |
| 1:K:230:ILE:H | 1:K:230:ILE:HD12 | 1.27 | 0.99 |
| 1:A:265:ASN:HA | 1:A:270:ILE:HD12 | 1.40 | 0.99 |
| 1:L:16:MET:O | 1:L:20:VAL:HG12 | 1.60 | 0.99 |
| 2:Q:47:ARG:HD3 | 2:Q:49:LEU:HD12 | 1.42 | 0.99 |
| 1:A:322:ARG:HB3 | 1:A:333:ILE:HD12 | 1.43 | 0.99 |
| 1:I:359:ASP:HA | 1:I:362:ARG:HH12 | 1.28 | 0.98 |
| 1:B:33:PRO:HA | 1:B:153:ASN:HD21 | 1.28 | 0.98 |
| 1:E:207:LYS:HB3 | 1:E:208:PRO:HD3 | 1.43 | 0.98 |
| 1:G:228:SER:HA | 1:G:255:GLU:HB2 | 1.45 | 0.98 |
| 1:M:235:PRO:HG3 | 1:M:310:GLU:HA | 1.44 | 0.98 |
| 1:I:314:LEU:HD12 | 1:I:314:LEU:H | 1.26 | 0.98 |
| 1:N:426:LEU:H | 1:N:426:LEU:HD23 | 1.28 | 0.98 |
| 2:U:47:ARG:HD3 | 2:U:49:LEU:HD12 | 1.40 | 0.98 |
| 1:K:166:MET:HE2 | 1:K:171:LYS:HA | 1.46 | 0.98 |
| 1:K:232:GLU:HB3 | 1:K:309:LEU:HB2 | 1.43 | 0.98 |
| 1:K:308:GLU:HB3 | 1:K:311:LYS:HD3 | 1.44 | 0.98 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:17:VAL:HG21 | 2:R:34:LYS:HD2 | 1.46 | 0.98 |
| 1:L:149:THR:HG23 | 1:L:159:GLY:HA3 | 1.46 | 0.97 |
| 1:L:308:GLU:HG2 | 1:L:309:LEU:H | 1.28 | 0.97 |
| 1:E:273:VAL:HG12 | 1:E:274:ALA:H | 1.29 | 0.97 |
| 1:K:314:LEU:H | 1:K:314:LEU:HD12 | 1.25 | 0.97 |
| 2:U:55:LYS:H | 2:U:55:LYS:CE | 1.75 | 0.97 |
| 1:B:199:TYR:HA | 1:B:276:VAL:HG12 | 1.46 | 0.97 |
| 1:H:314:LEU:H | 1:H:314:LEU:HD12 | 1.28 | 0.97 |
| 1:I:314:LEU:HA | 1:I:317:LEU:HD13 | 1.45 | 0.97 |
| 1:M:249:ILE:HB | 1:M:275:ALA:HB2 | 1.45 | 0.97 |
| 1:B:322:ARG:HG2 | 1:B:323:VAL:H | 1.27 | 0.97 |
| 1:L:308:GLU:HB3 | 1:L:311:LYS:HD3 | 1.43 | 0.96 |
| 1:M:249:ILE:HB | 1:M:275:ALA:CB | 1.95 | 0.96 |
| 1:F:33:PRO:HA | 1:F:153:ASN:HD21 | 1.30 | 0.96 |
| 1:M:232:GLU:HB3 | 1:M:309:LEU:HB2 | 1.48 | 0.96 |
| 1:D:207:LYS:HB3 | 1:D:208:PRO:HD3 | 1.42 | 0.96 |
| 1:G:291:ASP:HB3 | 1:G:345:ARG:HH21 | 1.30 | 0.96 |
| 2:Q:55:LYS:H | 2:Q:55:LYS:CE | 1.78 | 0.96 |
| 1:N:239:ALA:HB1 | 1:N:314:LEU:HD11 | 1.47 | 0.96 |
| 1:H:381:VAL:HG21 | 1:H:393:LYS:HA | 1.48 | 0.95 |
| 2:R:55:LYS:HE2 | 2:R:55:LYS:H | 1.30 | 0.95 |
| 1:C:245:LYS:HE2 | 1:C:245:LYS:HA | 1.49 | 0.95 |
| 1:J:426:LEU:HD23 | 1:J:426:LEU:H | 1.30 | 0.95 |
| 1:C:18:ARG:HB3 | 1:C:18:ARG:NH1 | 1.79 | 0.95 |
| 1:C:207:LYS:HB3 | 1:C:208:PRO:HD3 | 1.46 | 0.95 |
| 1:A:207:LYS:HB3 | 1:A:208:PRO:HD3 | 1.47 | 0.95 |
| 2:O:17:VAL:HG21 | 2:O:34:LYS:HD2 | 1.48 | 0.95 |
| 1:B:452:ARG:HB2 | 1:B:462:PRO:HB3 | 1.49 | 0.95 |
| 1:K:426:LEU:H | 1:K:426:LEU:HD23 | 1.30 | 0.95 |
| 1:F:322:ARG:HG2 | 1:F:323:VAL:H | 1.29 | 0.95 |
| 1:M:308:GLU:HB3 | 1:M:311:LYS:HD3 | 1.48 | 0.95 |
| 1:M:426:LEU:H | 1:M:426:LEU:HD23 | 1.30 | 0.95 |
| 1:B:245:LYS:HA | 1:B:245:LYS:HE2 | 1.47 | 0.95 |
| 1:A:346:VAL:HG12 | 1:A:350:ARG:HH22 | 1.29 | 0.95 |
| 1:J:232:GLU:HB3 | 1:J:309:LEU:HB2 | 1.46 | 0.95 |
| 1:N:230:ILE:HG13 | 1:N:258:ALA:HA | 1.47 | 0.94 |
| 1:J:69:MET:HE1 | 1:J:522:THR:HB | 1.49 | 0.94 |
| 1:I:230:ILE:HG13 | 1:I:258:ALA:HA | 1.47 | 0.94 |
| 1:M:449:ALA:HB3 | 1:M:450:PRO:HD3 | 1.49 | 0.94 |
| 1:J:308:GLU:HB3 | 1:J:311:LYS:HD3 | 1.48 | 0.94 |
| 1:L:239:ALA:HB1 | 1:L:314:LEU:HD11 | 1.47 | 0.94 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:256:GLY:HA2 | 1:L:259:LEU:HB3 | 1.49 | 0.94 |
| 1:L:223:ALA:HB3 | 1:L:251:ALA:HB2 | 1.47 | 0.94 |
| 2:S:78:ILE:HD13 | 2:S:83:VAL:HG21 | 1.51 | 0.93 |
| 1:F:452:ARG:HB2 | 1:F:462:PRO:HB3 | 1.49 | 0.93 |
| 1:H:433:ASN:HB3 | 1:H:436:GLN:HG3 | 1.50 | 0.93 |
| 1:J:69:MET:CE | 1:J:522:THR:HB | 1.99 | 0.93 |
| 1:L:249:ILE:HB | 1:L:275:ALA:HB2 | 1.51 | 0.93 |
| 2:P:65:VAL:HG12 | 2:P:94:ILE:HG12 | 1.50 | 0.93 |
| 1:D:228:SER:HA | 1:D:255:GLU:HB2 | 1.50 | 0.93 |
| 1:D:277:LYS:HD3 | 1:D:285:ARG:HH22 | 1.31 | 0.93 |
| 1:I:65:LYS:O | 1:I:66:PHE:HB2 | 1.65 | 0.93 |
| 1:L:426:LEU:HD23 | 1:L:426:LEU:H | 1.33 | 0.93 |
| 1:D:411:VAL:HG12 | 1:D:496:PRO:HA | 1.51 | 0.93 |
| 1:F:207:LYS:HB3 | 1:F:208:PRO:HD3 | 1.50 | 0.93 |
| 1:A:237:LEU:HD22 | 2:O:26:VAL:HG22 | 1.50 | 0.93 |
| 1:E:346:VAL:HG12 | 1:E:350:ARG:HH22 | 1.31 | 0.93 |
| 1:A:245:LYS:HE2 | 1:A:245:LYS:HA | 1.50 | 0.92 |
| 1:I:449:ALA:HB3 | 1:I:450:PRO:HD3 | 1.49 | 0.92 |
| 1:F:360:TYR:O | 1:F:364:LYS:HE2 | 1.69 | 0.92 |
| 1:I:249:ILE:HB | 1:I:275:ALA:CB | 1.99 | 0.92 |
| 1:J:65:LYS:O | 1:J:66:PHE:HB2 | 1.68 | 0.92 |
| 1:N:356:ALA:HB1 | 1:N:362:ARG:HE | 1.34 | 0.92 |
| 1:G:199:TYR:HA | 1:G:276:VAL:HG12 | 1.50 | 0.92 |
| 1:I:249:ILE:HB | 1:I:275:ALA:HB2 | 1.51 | 0.92 |
| 1:M:65:LYS:O | 1:M:66:PHE:HB2 | 1.67 | 0.92 |
| 1:M:230:ILE:HG13 | 1:M:258:ALA:HA | 1.50 | 0.92 |
| 1:G:322:ARG:HG2 | 1:G:323:VAL:H | 1.31 | 0.92 |
| 1:A:305:ILE:HG22 | 1:A:306:GLY:H | 1.35 | 0.92 |
| 1:C:305:ILE:HG22 | 1:C:306:GLY:H | 1.34 | 0.92 |
| 1:D:452:ARG:HB2 | 1:D:462:PRO:HB3 | 1.51 | 0.92 |
| 1:I:426:LEU:H | 1:I:426:LEU:HD23 | 1.35 | 0.92 |
| 2:O:55:LYS:H | 2:O:55:LYS:CE | 1.83 | 0.92 |
| 2:T:55:LYS:H | 2:T:55:LYS:CE | 1.82 | 0.92 |
| 1:J:308:GLU:HG2 | 1:J:309:LEU:H | 1.34 | 0.91 |
| 1:I:16:MET:O | 1:I:20:VAL:HG12 | 1.70 | 0.91 |
| 1:C:452:ARG:HB2 | 1:C:462:PRO:HB3 | 1.51 | 0.91 |
| 1:D:74:VAL:O | 1:D:77:VAL:HG13 | 1.71 | 0.91 |
| 1:I:359:ASP:HA | 1:I:362:ARG:NH1 | 1.85 | 0.91 |
| 1:L:235:PRO:HG3 | 1:L:310:GLU:HA | 1.50 | 0.91 |
| 1:M:166:MET:HE2 | 1:M:171:LYS:HA | 1.49 | 0.91 |
| 1:E:322:ARG:HG2 | 1:E:323:VAL:H | 1.34 | 0.91 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:487:ASN:O | 1:G:491:MET:HG3 | 1.69 | 0.91 |
| 1:K:143:ALA:O | 1:K:146:GLN:HB3 | 1.71 | 0.91 |
| 1:K:239:ALA:HB1 | 1:K:314:LEU:HD11 | 1.52 | 0.91 |
| 2:R:14:ARG:HD3 | 2:R:35:SER:HB3 | 1.53 | 0.91 |
| 1:A:223:ALA:HB3 | 1:A:251:ALA:HB2 | 1.53 | 0.91 |
| 1:I:239:ALA:HB1 | 1:I:314:LEU:HD11 | 1.53 | 0.91 |
| 1:I:69:MET:CE | 1:I:522:THR:HB | 2.01 | 0.91 |
| 1:D:245:LYS:HA | 1:D:245:LYS:HE2 | 1.53 | 0.91 |
| 1:M:314:LEU:H | 1:M:314:LEU:HD12 | 1.35 | 0.91 |
| 2:U:65:VAL:HG12 | 2:U:94:ILE:HG12 | 1.51 | 0.91 |
| 1:K:230:ILE:HG13 | 1:K:258:ALA:HA | 1.50 | 0.90 |
| 1:B:207:LYS:HB3 | 1:B:208:PRO:HD3 | 1.51 | 0.90 |
| 1:C:265:ASN:HA | 1:C:270:ILE:HD12 | 1.53 | 0.90 |
| 1:M:308:GLU:HG2 | 1:M:309:LEU:H | 1.32 | 0.90 |
| 2:O:47:ARG:HD3 | 2:O:49:LEU:HD12 | 1.51 | 0.90 |
| 1:D:350:ARG:HD3 | 1:D:353:ILE:HD12 | 1.53 | 0.90 |
| 1:M:359:ASP:HA | 1:M:362:ARG:HH12 | 1.37 | 0.90 |
| 1:N:381:VAL:HG21 | 1:N:393:LYS:HA | 1.53 | 0.90 |
| 1:N:286:LYS:HA | 1:N:286:LYS:HE2 | 1.51 | 0.90 |
| 1:B:305:ILE:HG22 | 1:B:306:GLY:H | 1.36 | 0.90 |
| 1:C:273:VAL:HG12 | 1:C:274:ALA:H | 1.37 | 0.90 |
| 1:L:157:THR:O | 1:L:160:LYS:HB3 | 1.70 | 0.90 |
| 1:D:215:LEU:HB3 | 1:D:246:PRO:HB2 | 1.54 | 0.90 |
| 1:H:308:GLU:HG2 | 1:H:309:LEU:H | 1.37 | 0.90 |
| 1:I:284:ARG:HB2 | 1:I:284:ARG:HH11 | 1.36 | 0.89 |
| 1:K:65:LYS:O | 1:K:66:PHE:HB2 | 1.71 | 0.89 |
| 1:L:284:ARG:HH11 | 1:L:284:ARG:HB2 | 1.36 | 0.89 |
| 1:F:314:LEU:HD12 | 1:F:315:GLU:N | 1.86 | 0.89 |
| 1:H:449:ALA:HB3 | 1:H:450:PRO:HD3 | 1.53 | 0.89 |
| 1:G:256:GLY:HA2 | 1:G:259:LEU:HB2 | 1.54 | 0.89 |
| 1:J:449:ALA:HB3 | 1:J:450:PRO:HD3 | 1.54 | 0.89 |
| 1:H:65:LYS:O | 1:H:66:PHE:HB2 | 1.70 | 0.89 |
| 1:H:436:GLN:O | 1:H:440:ILE:HG13 | 1.72 | 0.89 |
| 1:C:487:ASN:O | 1:C:491:MET:HG3 | 1.73 | 0.89 |
| 1:G:349:ILE:HA | 1:G:352:GLN:NE2 | 1.87 | 0.89 |
| 1:F:245:LYS:HA | 1:F:245:LYS:HE2 | 1.54 | 0.89 |
| 1:G:207:LYS:HB3 | 1:G:208:PRO:HD3 | 1.52 | 0.89 |
| 1:B:18:ARG:HB3 | 1:B:18:ARG:NH1 | 1.86 | 0.89 |
| 2:T:55:LYS:HE2 | 2:T:55:LYS:H | 1.36 | 0.89 |
| 1:L:69:MET:CE | 1:L:522:THR:HB | 2.03 | 0.88 |
| 1:H:239:ALA:HB1 | 1:H:314:LEU:HD11 | 1.56 | 0.88 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:308:GLU:HG2 | 1:I:309:LEU:H | 1.36 | 0.88 |
| 1:M:143:ALA:O | 1:M:146:GLN:HB3 | 1.72 | 0.88 |
| 1:M:381:VAL:HG21 | 1:M:393:LYS:HA | 1.53 | 0.88 |
| 1:E:215:LEU:O | 1:E:218:PRO:HD3 | 1.73 | 0.88 |
| 1:E:349:ILE:HA | 1:E:352:GLN:NE2 | 1.88 | 0.88 |
| 1:M:149:THR:HG23 | 1:M:159:GLY:HA3 | 1.53 | 0.88 |
| 1:A:411:VAL:HG12 | 1:A:496:PRO:HA | 1.56 | 0.88 |
| 1:B:296:THR:HG22 | 1:B:335:GLY:HA3 | 1.56 | 0.88 |
| 1:G:414:GLY:O | 1:G:417:VAL:HG12 | 1.72 | 0.88 |
| 2:P:47:ARG:HD3 | 2:P:49:LEU:HD12 | 1.55 | 0.88 |
| 1:C:64:ASP:HB3 | 1:C:67:GLU:HB2 | 1.55 | 0.88 |
| 1:J:433:ASN:HB3 | 1:J:436:GLN:HG3 | 1.54 | 0.88 |
| 1:N:69:MET:HE1 | 1:N:522:THR:HB | 1.56 | 0.88 |
| 2:R:55:LYS:H | 2:R:55:LYS:CE | 1.87 | 0.87 |
| 2:U:78:ILE:HD13 | 2:U:83:VAL:HG21 | 1.56 | 0.87 |
| 1:J:254:VAL:HG12 | 1:J:259:LEU:HB2 | 1.56 | 0.87 |
| 1:L:381:VAL:HG21 | 1:L:393:LYS:HA | 1.53 | 0.87 |
| 1:L:85:ALA:HB1 | 1:L:499:VAL:HG12 | 1.56 | 0.87 |
| 1:H:143:ALA:O | 1:H:146:GLN:HB3 | 1.73 | 0.87 |
| 1:J:215:LEU:HB3 | 1:J:218:PRO:HG2 | 1.54 | 0.87 |
| 1:G:411:VAL:HG12 | 1:G:496:PRO:HA | 1.56 | 0.87 |
| 1:N:308:GLU:HG2 | 1:N:309:LEU:H | 1.39 | 0.87 |
| 1:E:18:ARG:NH1 | 1:E:18:ARG:HB3 | 1.89 | 0.87 |
| 1:N:232:GLU:HB3 | 1:N:309:LEU:HB2 | 1.56 | 0.87 |
| 1:J:249:ILE:HB | 1:J:275:ALA:CB | 2.05 | 0.87 |
| 1:M:16:MET:O | 1:M:20:VAL:HG12 | 1.74 | 0.87 |
| 1:N:359:ASP:HA | 1:N:362:ARG:HH12 | 1.39 | 0.87 |
| 1:D:18:ARG:HB3 | 1:D:18:ARG:NH1 | 1.90 | 0.87 |
| 1:K:433:ASN:HB3 | 1:K:436:GLN:HG3 | 1.56 | 0.87 |
| 2:O:78:ILE:HD13 | 2:O:83:VAL:HG21 | 1.57 | 0.87 |
| 1:A:360:TYR:HA | 1:A:363:GLU:OE1 | 1.75 | 0.87 |
| 1:I:235:PRO:HG3 | 1:I:310:GLU:HA | 1.55 | 0.87 |
| 1:D:199:TYR:HA | 1:D:276:VAL:HG12 | 1.57 | 0.87 |
| 1:H:166:MET:HE2 | 1:H:171:LYS:HA | 1.55 | 0.87 |
| 1:J:16:MET:O | 1:J:20:VAL:HG12 | 1.75 | 0.87 |
| 1:K:359:ASP:HA | 1:K:362:ARG:NH1 | 1.88 | 0.86 |
| 1:A:219:PHE:HD1 | 1:A:319:GLN:HE21 | 1.22 | 0.86 |
| 1:E:215:LEU:HB3 | 1:E:246:PRO:HB2 | 1.57 | 0.86 |
| 1:L:249:ILE:HB | 1:L:275:ALA:CB | 2.05 | 0.86 |
| 1:D:305:ILE:HG22 | 1:D:306:GLY:N | 1.89 | 0.86 |
| 1:I:69:MET:HE2 | 1:I:522:THR:HB | 1.55 | 0.86 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:149:THR:HG23 | 1:K:159:GLY:HA3 | 1.55 | 0.86 |
| 1:F:82:ASN:ND2 | 1:F:86:GLY:HA2 | 1.90 | 0.86 |
| 1:I:256:GLY:HA2 | 1:I:259:LEU:HB3 | 1.56 | 0.86 |
| 1:I:266:THR:HG22 | 1:I:272:LYS:HA | 1.58 | 0.86 |
| 1:C:322:ARG:HG2 | 1:C:323:VAL:H | 1.41 | 0.86 |
| 1:F:199:TYR:HA | 1:F:276:VAL:HG12 | 1.58 | 0.86 |
| 1:D:273:VAL:HG12 | 1:D:274:ALA:H | 1.41 | 0.86 |
| 1:B:34:LYS:HD2 | 1:B:458:CYS:SG | 2.14 | 0.86 |
| 2:P:55:LYS:CE | 2:P:55:LYS:H | 1.89 | 0.86 |
| 2:S:17:VAL:HG21 | 2:S:34:LYS:HD2 | 1.57 | 0.86 |
| 1:G:245:LYS:HA | 1:G:245:LYS:HE2 | 1.56 | 0.86 |
| 1:G:273:VAL:HG12 | 1:G:274:ALA:H | 1.40 | 0.85 |
| 1:N:193:MET:HG2 | 1:N:194:GLN:N | 1.91 | 0.85 |
| 1:I:381:VAL:HG21 | 1:I:393:LYS:HA | 1.56 | 0.85 |
| 1:C:256:GLY:HA2 | 1:C:259:LEU:HB2 | 1.56 | 0.85 |
| 1:D:360:TYR:HA | 1:D:363:GLU:OE1 | 1.76 | 0.85 |
| 1:H:284:ARG:HH11 | 1:H:284:ARG:HB2 | 1.40 | 0.85 |
| 1:L:169:VAL:HG13 | 1:L:173:GLY:HA3 | 1.57 | 0.85 |
| 1:C:34:LYS:HD2 | 1:C:458:CYS:SG | 2.16 | 0.85 |
| 1:D:226:LYS:C | 1:D:227:ILE:HD12 | 1.96 | 0.85 |
| 1:K:356:ALA:HB1 | 1:K:362:ARG:HE | 1.41 | 0.85 |
| 1:N:434:GLU:HA | 1:N:437:ASN:ND2 | 1.92 | 0.85 |
| 1:D:349:ILE:HA | 1:D:352:GLN:NE2 | 1.90 | 0.85 |
| 1:M:434:GLU:HA | 1:M:437:ASN:ND2 | 1.91 | 0.85 |
| 1:B:74:VAL:O | 1:B:77:VAL:HG13 | 1.76 | 0.85 |
| 1:C:33:PRO:HA | 1:C:153:ASN:HD21 | 1.42 | 0.85 |
| 1:J:143:ALA:O | 1:J:147:VAL:HG12 | 1.75 | 0.85 |
| 1:J:229:ASN:ND2 | 1:J:231:ARG:HH12 | 1.75 | 0.85 |
| 1:L:65:LYS:O | 1:L:66:PHE:HB2 | 1.75 | 0.85 |
| 2:S:14:ARG:HG2 | 2:S:15:LYS:H | 1.40 | 0.85 |
| 1:B:411:VAL:HG12 | 1:B:496:PRO:HA | 1.58 | 0.85 |
| 1:I:284:ARG:NH1 | 1:I:284:ARG:HB2 | 1.91 | 0.85 |
| 1:L:222:LEU:HD22 | 1:L:289:LEU:HD11 | 1.58 | 0.85 |
| 1:D:265:ASN:HA | 1:D:270:ILE:HD12 | 1.57 | 0.84 |
| 1:G:64:ASP:HB3 | 1:G:67:GLU:HB2 | 1.59 | 0.84 |
| 1:L:166:MET:HE2 | 1:L:171:LYS:HA | 1.56 | 0.84 |
| 1:E:314:LEU:HD12 | 1:E:315:GLU:N | 1.92 | 0.84 |
| 1:F:18:ARG:NH1 | 1:F:18:ARG:HB3 | 1.92 | 0.84 |
| 1:D:234:LEU:HD12 | 1:D:234:LEU:H | 1.40 | 0.84 |
| 1:B:265:ASN:HA | 1:B:270:ILE:HD12 | 1.58 | 0.84 |
| 1:C:234:LEU:HD12 | 1:C:234:LEU:H | 1.41 | 0.84 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:224:ASP:HB2 | 1:E:303:GLU:HB3 | 1.59 | 0.84 |
| 1:E:131:LEU:CD2 | 1:E:422:VAL:HG11 | 2.06 | 0.84 |
| 1:J:247:LEU:O | 1:J:273:VAL:HB | 1.78 | 0.84 |
| 1:J:284:ARG:HB2 | 1:J:284:ARG:HH11 | 1.43 | 0.84 |
| 1:C:249:ILE:HB | 1:C:275:ALA:CB | 2.07 | 0.84 |
| 1:K:449:ALA:HB3 | 1:K:450:PRO:HD3 | 1.58 | 0.84 |
| 1:M:169:VAL:HG13 | 1:M:173:GLY:HA3 | 1.58 | 0.84 |
| 2:T:47:ARG:HD3 | 2:T:49:LEU:HD12 | 1.60 | 0.84 |
| 1:A:215:LEU:HB3 | 1:A:246:PRO:HB2 | 1.58 | 0.84 |
| 1:E:33:PRO:HA | 1:E:153:ASN:HD21 | 1.42 | 0.84 |
| 1:M:359:ASP:HA | 1:M:362:ARG:NH1 | 1.92 | 0.84 |
| 1:N:314:LEU:H | 1:N:314:LEU:HD12 | 1.42 | 0.84 |
| 1:G:452:ARG:HB2 | 1:G:462:PRO:HB3 | 1.59 | 0.84 |
| 1:D:233:MET:C | 1:D:235:PRO:HD2 | 1.97 | 0.84 |
| 1:E:305:ILE:HG22 | 1:E:306:GLY:H | 1.43 | 0.84 |
| 1:I:286:LYS:HA | 1:I:286:LYS:HE2 | 1.59 | 0.84 |
| 1:N:230:ILE:N | 1:N:230:ILE:HD12 | 1.93 | 0.84 |
| 1:L:230:ILE:HD12 | 1:L:230:ILE:H | 1.42 | 0.84 |
| 1:A:82:ASN:HD22 | 1:A:86:GLY:HA2 | 1.42 | 0.83 |
| 1:E:417:VAL:O | 1:E:420:ILE:HG22 | 1.77 | 0.83 |
| 1:F:34:LYS:HD2 | 1:F:458:CYS:SG | 2.18 | 0.83 |
| 1:N:449:ALA:HB3 | 1:N:450:PRO:HD3 | 1.58 | 0.83 |
| 1:A:452:ARG:HB2 | 1:A:462:PRO:HB3 | 1.58 | 0.83 |
| 1:B:233:MET:C | 1:B:235:PRO:HD2 | 1.98 | 0.83 |
| 1:H:249:ILE:HB | 1:H:275:ALA:CB | 2.07 | 0.83 |
| 1:J:381:VAL:HG21 | 1:J:393:LYS:HA | 1.60 | 0.83 |
| 1:N:403:THR:O | 1:N:407:VAL:HG23 | 1.76 | 0.83 |
| 1:E:295:LEU:O | 1:E:337:GLY:HA3 | 1.79 | 0.83 |
| 1:F:414:GLY:O | 1:F:417:VAL:HG12 | 1.78 | 0.83 |
| 1:B:360:TYR:HA | 1:B:363:GLU:OE1 | 1.79 | 0.83 |
| 1:I:415:GLY:H | 1:I:417:VAL:HG23 | 1.43 | 0.83 |
| 1:A:266:THR:HG22 | 1:A:271:VAL:O | 1.78 | 0.83 |
| 1:B:417:VAL:O | 1:B:420:ILE:HG22 | 1.77 | 0.83 |
| 1:E:452:ARG:HB2 | 1:E:462:PRO:HB3 | 1.59 | 0.83 |
| 1:F:349:ILE:O | 1:F:353:ILE:HG13 | 1.79 | 0.83 |
| 1:G:18:ARG:NH1 | 1:G:18:ARG:HB3 | 1.92 | 0.83 |
| 1:E:273:VAL:HG12 | 1:E:274:ALA:N | 1.93 | 0.83 |
| 1:H:314:LEU:HA | 1:H:317:LEU:HD13 | 1.59 | 0.83 |
| 1:K:198:GLY:HA3 | 1:K:328:ASP:HA | 1.59 | 0.83 |
| 1:K:69:MET:HE1 | 1:K:522:THR:HB | 1.60 | 0.83 |
| 1:D:296:THR:HG22 | 1:D:335:GLY:HA3 | 1.60 | 0.83 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:359:ASP:HA | 1:H:362:ARG:HH12 | 1.44 | 0.83 |
| 1:M:356:ALA:HB1 | 1:M:362:ARG:HE | 1.43 | 0.83 |
| 2:P:55:LYS:HE2 | 2:P:55:LYS:H | 1.44 | 0.83 |
| 1:F:74:VAL:O | 1:F:77:VAL:HG13 | 1.77 | 0.83 |
| 1:G:174:VAL:HG21 | 1:G:367:GLU:HA | 1.61 | 0.83 |
| 1:M:69:MET:CE | 1:M:522:THR:HB | 2.08 | 0.83 |
| 1:N:308:GLU:HB3 | 1:N:311:LYS:HD3 | 1.60 | 0.83 |
| 2:S:14:ARG:HD3 | 2:S:35:SER:HB3 | 1.58 | 0.83 |
| 1:C:360:TYR:O | 1:C:364:LYS:HE2 | 1.78 | 0.83 |
| 1:H:100:ILE:O | 1:H:104:LEU:HB2 | 1.79 | 0.83 |
| 1:J:223:ALA:HB3 | 1:J:251:ALA:HB2 | 1.61 | 0.83 |
| 1:A:314:LEU:HD12 | 1:A:315:GLU:N | 1.94 | 0.83 |
| 1:H:254:VAL:HG12 | 1:H:259:LEU:HB2 | 1.59 | 0.83 |
| 1:I:169:VAL:HG13 | 1:I:173:GLY:HA3 | 1.57 | 0.83 |
| 2:Q:68:ASN:HD22 | 2:R:74:LYS:HE3 | 1.43 | 0.83 |
| 1:A:64:ASP:HB3 | 1:A:67:GLU:HB2 | 1.61 | 0.82 |
| 1:F:346:VAL:HG12 | 1:F:350:ARG:HH22 | 1.44 | 0.82 |
| 1:A:174:VAL:HG21 | 1:A:367:GLU:HA | 1.60 | 0.82 |
| 1:A:487:ASN:O | 1:A:491:MET:HG3 | 1.78 | 0.82 |
| 1:F:223:ALA:HB3 | 1:F:251:ALA:HB2 | 1.62 | 0.82 |
| 1:H:69:MET:CE | 1:H:522:THR:HB | 2.09 | 0.82 |
| 1:J:299:THR:N | 1:J:316:ASP:O | 2.11 | 0.82 |
| 1:K:381:VAL:HG21 | 1:K:393:LYS:HA | 1.60 | 0.82 |
| 1:A:214:GLU:HB3 | 1:A:322:ARG:HD3 | 1.61 | 0.82 |
| 1:G:461:GLU:HB2 | 1:G:464:VAL:HB | 1.60 | 0.82 |
| 1:N:16:MET:O | 1:N:20:VAL:HG12 | 1.80 | 0.82 |
| 1:B:277:LYS:HD3 | 1:B:285:ARG:HH22 | 1.43 | 0.82 |
| 1:N:433:ASN:HB3 | 1:N:436:GLN:HG3 | 1.62 | 0.82 |
| 1:C:249:ILE:HB | 1:C:275:ALA:HB2 | 1.60 | 0.82 |
| 1:I:199:TYR:HA | 1:I:276:VAL:HG12 | 1.61 | 0.82 |
| 1:J:100:ILE:O | 1:J:104:LEU:HB2 | 1.79 | 0.82 |
| 1:H:149:THR:HG23 | 1:H:159:GLY:HA3 | 1.61 | 0.82 |
| 1:I:230:ILE:N | 1:I:230:ILE:HD12 | 1.95 | 0.82 |
| 2:O:14:ARG:HG2 | 2:O:15:LYS:H | 1.45 | 0.82 |
| 1:F:33:PRO:HA | 1:F:153:ASN:ND2 | 1.94 | 0.82 |
| 1:N:69:MET:CE | 1:N:522:THR:HB | 2.09 | 0.82 |
| 1:B:487:ASN:O | 1:B:491:MET:HG3 | 1.80 | 0.82 |
| 1:C:199:TYR:HA | 1:C:276:VAL:HG12 | 1.62 | 0.82 |
| 1:C:226:LYS:C | 1:C:227:ILE:HD12 | 2.01 | 0.82 |
| 1:G:273:VAL:HG12 | 1:G:274:ALA:N | 1.95 | 0.82 |
| 1:H:194:GLN:HG3 | 1:H:331:THR:HB | 1.62 | 0.82 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:436:GLN:O | 1:J:440:ILE:HG13 | 1.80 | 0.82 |
| 2:T:17:VAL:HG21 | 2:T:34:LYS:HD2 | 1.62 | 0.82 |
| 1:A:33:PRO:HA | 1:A:153:ASN:HD21 | 1.45 | 0.81 |
| 1:B:215:LEU:O | 1:B:218:PRO:HD3 | 1.79 | 0.81 |
| 1:E:199:TYR:HA | 1:E:276:VAL:HG12 | 1.61 | 0.81 |
| 1:F:411:VAL:HG12 | 1:F:496:PRO:HA | 1.60 | 0.81 |
| 1:L:314:LEU:HA | 1:L:317:LEU:HD13 | 1.62 | 0.81 |
| 2:T:65:VAL:HG12 | 2:T:94:ILE:HG12 | 1.61 | 0.81 |
| 1:G:265:ASN:HA | 1:G:270:ILE:HD12 | 1.61 | 0.81 |
| 1:C:411:VAL:HG12 | 1:C:496:PRO:HA | 1.62 | 0.81 |
| 1:J:249:ILE:HB | 1:J:275:ALA:HB2 | 1.62 | 0.81 |
| 1:M:205:ILE:HA | 1:M:213:VAL:HG22 | 1.61 | 0.81 |
| 2:Q:11:ILE:HB | 2:Q:42:ALA:HB3 | 1.60 | 0.81 |
| 1:A:277:LYS:HD3 | 1:A:285:ARG:HH22 | 1.44 | 0.81 |
| 1:C:349:ILE:HA | 1:C:352:GLN:NE2 | 1.95 | 0.81 |
| 1:E:360:TYR:HA | 1:E:363:GLU:OE1 | 1.79 | 0.81 |
| 1:E:414:GLY:O | 1:E:417:VAL:HG12 | 1.80 | 0.81 |
| 1:I:433:ASN:HB3 | 1:I:436:GLN:HG3 | 1.60 | 0.81 |
| 1:I:85:ALA:HB1 | 1:I:499:VAL:HG12 | 1.60 | 0.81 |
| 1:L:359:ASP:HA | 1:L:362:ARG:NH1 | 1.94 | 0.81 |
| 2:Q:78:ILE:HD13 | 2:Q:83:VAL:HG21 | 1.63 | 0.81 |
| 1:D:417:VAL:O | 1:D:420:ILE:HG22 | 1.79 | 0.81 |
| 1:E:233:MET:C | 1:E:235:PRO:HD2 | 2.00 | 0.81 |
| 1:C:461:GLU:HB2 | 1:C:464:VAL:HB | 1.62 | 0.81 |
| 1:D:322:ARG:HB3 | 1:D:333:ILE:CD1 | 2.10 | 0.81 |
| 1:G:233:MET:C | 1:G:235:PRO:HD2 | 2.01 | 0.81 |
| 1:H:143:ALA:O | 1:H:147:VAL:HG12 | 1.81 | 0.81 |
| 1:H:426:LEU:HD23 | 1:H:426:LEU:H | 1.44 | 0.81 |
| 1:I:436:GLN:O | 1:I:440:ILE:HG13 | 1.80 | 0.81 |
| 1:M:286:LYS:HA | 1:M:286:LYS:HE2 | 1.60 | 0.81 |
| 1:K:284:ARG:HB2 | 1:K:284:ARG:NH1 | 1.95 | 0.81 |
| 1:A:18:ARG:NH1 | 1:A:18:ARG:HB3 | 1.94 | 0.81 |
| 1:F:82:ASN:HD22 | 1:F:86:GLY:HA2 | 1.45 | 0.81 |
| 1:K:284:ARG:HB2 | 1:K:284:ARG:HH11 | 1.44 | 0.81 |
| 1:D:249:ILE:HB | 1:D:275:ALA:HB2 | 1.61 | 0.81 |
| 1:D:291:ASP:OD1 | 1:D:292:ILE:HG13 | 1.81 | 0.81 |
| 1:F:368:ARG:HG2 | 1:F:372:LEU:HG | 1.62 | 0.81 |
| 1:J:351:GLN:HG2 | 1:J:354:GLU:OE2 | 1.80 | 0.81 |
| 1:M:199:TYR:HA | 1:M:276:VAL:HG12 | 1.63 | 0.81 |
| 2:Q:14:ARG:HG2 | 2:Q:15:LYS:H | 1.44 | 0.81 |
| 1:B:107:VAL:HG13 | 1:B:113:PRO:HG3 | 1.63 | 0.81 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:349:ILE:HA | 1:B:352:GLN:NE2 | 1.95 | 0.81 |
| 1:C:278:ALA:HB1 | 1:C:279:PRO:CD | 2.11 | 0.81 |
| 1:J:494:LEU:HD23 | 1:J:494:LEU:N | 1.95 | 0.81 |
| 1:N:230:ILE:H | 1:N:230:ILE:CD1 | 1.94 | 0.81 |
| 1:L:217:SER:HA | 1:L:320:ALA:O | 1.80 | 0.80 |
| 1:M:143:ALA:O | 1:M:147:VAL:HG12 | 1.79 | 0.80 |
| 1:B:33:PRO:HA | 1:B:153:ASN:ND2 | 1.94 | 0.80 |
| 1:D:273:VAL:HG12 | 1:D:274:ALA:N | 1.95 | 0.80 |
| 1:F:280:GLY:HA3 | 1:F:284:ARG:HH11 | 1.43 | 0.80 |
| 1:F:44:PHE:CD1 | 1:F:44:PHE:N | 2.46 | 0.80 |
| 1:M:385:THR:HG23 | 1:M:388:GLU:H | 1.46 | 0.80 |
| 1:C:449:ALA:HB3 | 1:C:450:PRO:HD3 | 1.64 | 0.80 |
| 1:D:64:ASP:HB3 | 1:D:67:GLU:HB2 | 1.63 | 0.80 |
| 1:F:215:LEU:HB3 | 1:F:246:PRO:HB2 | 1.62 | 0.80 |
| 1:K:249:ILE:HB | 1:K:275:ALA:CB | 2.10 | 0.80 |
| 1:L:5:ASP:HB2 | 1:L:524:LEU:HD23 | 1.62 | 0.80 |
| 2:S:18:GLU:CD | 2:S:33:ALA:HB3 | 2.02 | 0.80 |
| 1:B:273:VAL:HG12 | 1:B:274:ALA:H | 1.45 | 0.80 |
| 1:C:273:VAL:HG12 | 1:C:274:ALA:N | 1.96 | 0.80 |
| 1:E:34:LYS:HD2 | 1:E:458:CYS:SG | 2.22 | 0.80 |
| 1:I:143:ALA:O | 1:I:146:GLN:HB3 | 1.81 | 0.80 |
| 1:C:302:SER:HB2 | 1:C:305:ILE:HD13 | 1.62 | 0.80 |
| 1:I:223:ALA:HB3 | 1:I:251:ALA:HB2 | 1.64 | 0.80 |
| 1:K:254:VAL:HG12 | 1:K:259:LEU:HB2 | 1.63 | 0.80 |
| 1:K:69:MET:CE | 1:K:522:THR:HB | 2.10 | 0.80 |
| 1:L:199:TYR:HA | 1:L:276:VAL:HG12 | 1.64 | 0.80 |
| 1:L:34:LYS:HB2 | 1:L:458:CYS:SG | 2.21 | 0.80 |
| 1:M:433:ASN:HB3 | 1:M:436:GLN:HG3 | 1.62 | 0.80 |
| 2:Q:17:VAL:HG21 | 2:Q:34:LYS:HD2 | 1.64 | 0.80 |
| 1:A:417:VAL:O | 1:A:420:ILE:HG22 | 1.81 | 0.80 |
| 1:G:74:VAL:O | 1:G:77:VAL:HG13 | 1.80 | 0.80 |
| 2:O:65:VAL:HG12 | 2:O:94:ILE:HG12 | 1.62 | 0.80 |
| 1:G:417:VAL:O | 1:G:420:ILE:HG22 | 1.81 | 0.80 |
| 1:K:215:LEU:HB3 | 1:K:218:PRO:HG2 | 1.61 | 0.80 |
| 1:J:308:GLU:HG2 | 1:J:309:LEU:N | 1.95 | 0.80 |
| 1:K:143:ALA:O | 1:K:147:VAL:HG12 | 1.80 | 0.80 |
| 1:K:5:ASP:HB2 | 1:K:524:LEU:HD23 | 1.63 | 0.80 |
| 1:L:198:GLY:HA3 | 1:L:328:ASP:HA | 1.64 | 0.80 |
| 1:F:64:ASP:HB3 | 1:F:67:GLU:HB2 | 1.64 | 0.80 |
| 2:S:14:ARG:HG2 | 2:S:15:LYS:N | 1.97 | 0.80 |
| 1:A:74:VAL:O | 1:A:77:VAL:HG13 | 1.80 | 0.80 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:18:ARG:CB | 1:C:18:ARG:HH11 | 1.90 | 0.80 |
| 1:E:33:PRO:HA | 1:E:153:ASN:ND2 | 1.97 | 0.80 |
| 1:G:33:PRO:HA | 1:G:153:ASN:ND2 | 1.95 | 0.80 |
| 1:A:234:LEU:HD12 | 1:A:234:LEU:H | 1.47 | 0.79 |
| 1:B:351:GLN:HG2 | 1:C:210:THR:OG1 | 1.82 | 0.79 |
| 1:G:234:LEU:HD12 | 1:G:234:LEU:H | 1.46 | 0.79 |
| 1:C:325:ILE:HG13 | 1:C:330:THR:HG23 | 1.64 | 0.79 |
| 1:C:414:GLY:O | 1:C:417:VAL:HG12 | 1.81 | 0.79 |
| 1:F:277:LYS:HD3 | 1:F:285:ARG:HH22 | 1.48 | 0.79 |
| 1:H:286:LYS:HE2 | 1:H:286:LYS:HA | 1.64 | 0.79 |
| 1:B:224:ASP:HB2 | 1:B:303:GLU:HB3 | 1.64 | 0.79 |
| 1:H:284:ARG:NH1 | 1:H:284:ARG:HB2 | 1.97 | 0.79 |
| 1:B:278:ALA:HB1 | 1:B:279:PRO:CD | 2.11 | 0.79 |
| 1:G:349:ILE:O | 1:G:353:ILE:HG13 | 1.82 | 0.79 |
| 1:G:34:LYS:HD2 | 1:G:458:CYS:SG | 2.23 | 0.79 |
| 1:H:85:ALA:HB1 | 1:H:499:VAL:HG12 | 1.64 | 0.79 |
| 1:L:161:LEU:HD12 | 1:L:161:LEU:H | 1.47 | 0.79 |
| 2:R:47:ARG:HD3 | 2:R:49:LEU:HD12 | 1.64 | 0.79 |
| 1:B:314:LEU:HD12 | 1:B:315:GLU:N | 1.97 | 0.79 |
| 1:D:249:ILE:HB | 1:D:275:ALA:CB | 2.12 | 0.79 |
| 1:H:266:THR:HG22 | 1:H:272:LYS:HA | 1.63 | 0.79 |
| 1:I:230:ILE:H | 1:I:230:ILE:CD1 | 1.94 | 0.79 |
| 1:J:198:GLY:HA3 | 1:J:328:ASP:HA | 1.63 | 0.79 |
| 1:K:96:ALA:O | 1:K:100:ILE:HG13 | 1.82 | 0.79 |
| 1:M:436:GLN:O | 1:M:440:ILE:HG13 | 1.81 | 0.79 |
| 1:N:287:ALA:HB1 | 1:N:368:ARG:CZ | 2.12 | 0.79 |
| 1:A:273:VAL:HG12 | 1:A:274:ALA:N | 1.98 | 0.79 |
| 1:A:82:ASN:ND2 | 1:A:86:GLY:HA2 | 1.97 | 0.79 |
| 1:D:235:PRO:HG3 | 1:D:310:GLU:HB3 | 1.62 | 0.79 |
| 1:G:360:TYR:O | 1:G:364:LYS:HE2 | 1.82 | 0.79 |
| 1:J:169:VAL:HG13 | 1:J:173:GLY:HA3 | 1.64 | 0.79 |
| 1:J:403:THR:O | 1:J:407:VAL:HG23 | 1.81 | 0.79 |
| 1:K:256:GLY:HA2 | 1:K:259:LEU:HB3 | 1.64 | 0.79 |
| 1:K:436:GLN:O | 1:K:440:ILE:HG13 | 1.81 | 0.79 |
| 1:N:100:ILE:O | 1:N:104:LEU:HB2 | 1.82 | 0.79 |
| 1:N:85:ALA:HB1 | 1:N:499:VAL:HG12 | 1.65 | 0.79 |
| 2:R:14:ARG:HG2 | 2:R:15:LYS:H | 1.48 | 0.79 |
| 1:A:20:VAL:HG13 | 1:A:74:VAL:HG11 | 1.63 | 0.79 |
| 1:C:233:MET:C | 1:C:235:PRO:HD2 | 2.02 | 0.79 |
| 1:E:349:ILE:O | 1:E:353:ILE:HG13 | 1.81 | 0.79 |
| 1:H:233:MET:HA | 1:H:233:MET:HE2 | 1.65 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:415:GLY:H | 1:J:417:VAL:HG23 | 1.47 | 0.79 |
| 1:J:85:ALA:HB1 | 1:J:499:VAL:HG12 | 1.63 | 0.79 |
| 2:S:55:LYS:H | 2:S:55:LYS:HE2 | 1.47 | 0.79 |
| 1:A:322:ARG:HG2 | 1:A:323:VAL:H | 1.46 | 0.79 |
| 1:A:414:GLY:O | 1:A:417:VAL:HG12 | 1.82 | 0.79 |
| 1:A:131:LEU:CD2 | 1:A:422:VAL:HG11 | 2.12 | 0.79 |
| 1:E:123:ALA:HB2 | 1:E:440:ILE:HG23 | 1.65 | 0.79 |
| 1:J:286:LYS:HE2 | 1:J:286:LYS:HA | 1.65 | 0.79 |
| 1:N:124:VAL:HG13 | 1:N:504:LEU:CD1 | 2.13 | 0.79 |
| 1:A:215:LEU:O | 1:A:218:PRO:HD3 | 1.83 | 0.79 |
| 1:A:233:MET:C | 1:A:235:PRO:HD2 | 2.02 | 0.79 |
| 1:B:414:GLY:HA2 | 1:B:495:ASP:OD2 | 1.83 | 0.79 |
| 1:C:281:PHE:O | 1:C:285:ARG:HG2 | 1.83 | 0.79 |
| 1:K:221:LEU:HD12 | 1:K:249:ILE:HG23 | 1.65 | 0.79 |
| 1:L:308:GLU:HG2 | 1:L:309:LEU:N | 1.97 | 0.79 |
| 1:N:143:ALA:O | 1:N:146:GLN:HB3 | 1.83 | 0.79 |
| 1:B:219:PHE:HD1 | 1:B:319:GLN:HE21 | 1.29 | 0.79 |
| 1:B:295:LEU:O | 1:B:337:GLY:HA3 | 1.83 | 0.79 |
| 1:B:461:GLU:HB2 | 1:B:464:VAL:HB | 1.65 | 0.79 |
| 1:C:305:ILE:HD12 | 1:C:305:ILE:N | 1.99 | 0.79 |
| 1:F:234:LEU:HD12 | 1:F:234:LEU:H | 1.46 | 0.79 |
| 1:I:326:ASN:OD1 | 1:I:329:THR:HB | 1.83 | 0.79 |
| 1:A:206:ASN:CB | 1:A:214:GLU:H | 1.96 | 0.78 |
| 1:D:215:LEU:O | 1:D:218:PRO:HD3 | 1.82 | 0.78 |
| 1:L:415:GLY:H | 1:L:417:VAL:HG23 | 1.46 | 0.78 |
| 1:L:433:ASN:HB3 | 1:L:436:GLN:HG3 | 1.64 | 0.78 |
| 1:N:436:GLN:O | 1:N:440:ILE:HG13 | 1.84 | 0.78 |
| 2:U:14:ARG:HG2 | 2:U:15:LYS:H | 1.48 | 0.78 |
| 1:C:214:GLU:HB3 | 1:C:322:ARG:HD3 | 1.65 | 0.78 |
| 1:G:295:LEU:O | 1:G:337:GLY:HA3 | 1.84 | 0.78 |
| 1:J:284:ARG:HB2 | 1:J:284:ARG:NH1 | 1.98 | 0.78 |
| 1:F:360:TYR:HA | 1:F:363:GLU:OE1 | 1.83 | 0.78 |
| 1:A:199:TYR:HA | 1:A:276:VAL:HG12 | 1.65 | 0.78 |
| 1:E:368:ARG:HG2 | 1:E:372:LEU:HG | 1.63 | 0.78 |
| 1:J:235:PRO:HG3 | 1:J:310:GLU:HA | 1.66 | 0.78 |
| 1:B:414:GLY:O | 1:B:417:VAL:HG12 | 1.83 | 0.78 |
| 1:H:217:SER:HA | 1:H:320:ALA:O | 1.84 | 0.78 |
| 1:A:350:ARG:HD3 | 1:A:353:ILE:HD12 | 1.66 | 0.78 |
| 1:B:273:VAL:HG12 | 1:B:274:ALA:N | 1.99 | 0.78 |
| 1:E:411:VAL:HG12 | 1:E:496:PRO:HA | 1.65 | 0.78 |
| 1:F:222:LEU:HD22 | 1:F:300:VAL:HG22 | 1.66 | 0.78 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:78:ILE:HD13 | 2:T:83:VAL:HG21 | 1.66 | 0.78 |
| 1:B:64:ASP:HB3 | 1:B:67:GLU:HB2 | 1.65 | 0.78 |
| 1:E:44:PHE:N | 1:E:44:PHE:CD1 | 2.50 | 0.78 |
| 1:M:287:ALA:HB1 | 1:M:368:ARG:NH2 | 1.98 | 0.78 |
| 1:D:305:ILE:HD12 | 1:D:305:ILE:N | 1.98 | 0.78 |
| 1:G:314:LEU:HD12 | 1:G:315:GLU:N | 1.99 | 0.78 |
| 1:K:100:ILE:O | 1:K:104:LEU:HB2 | 1.83 | 0.78 |
| 1:N:166:MET:HE2 | 1:N:171:LYS:HA | 1.64 | 0.78 |
| 1:N:415:GLY:H | 1:N:417:VAL:HG23 | 1.48 | 0.78 |
| 2:T:34:LYS:HG3 | 2:T:35:SER:H | 1.47 | 0.78 |
| 1:G:305:ILE:N | 1:G:305:ILE:HD12 | 1.99 | 0.78 |
| 1:A:449:ALA:HB3 | 1:A:450:PRO:HD3 | 1.65 | 0.78 |
| 1:G:305:ILE:HG22 | 1:G:306:GLY:N | 1.97 | 0.78 |
| 1:K:16:MET:O | 1:K:20:VAL:HG12 | 1.83 | 0.78 |
| 1:A:322:ARG:HB3 | 1:A:333:ILE:CD1 | 2.14 | 0.77 |
| 1:G:360:TYR:HA | 1:G:363:GLU:OE1 | 1.85 | 0.77 |
| 1:N:247:LEU:O | 1:N:273:VAL:HB | 1.83 | 0.77 |
| 1:N:284:ARG:HH11 | 1:N:284:ARG:HB2 | 1.49 | 0.77 |
| 1:N:284:ARG:NH1 | 1:N:284:ARG:HB2 | 1.99 | 0.77 |
| 1:B:44:PHE:N | 1:B:44:PHE:CD1 | 2.50 | 0.77 |
| 1:E:245:LYS:HA | 1:E:245:LYS:HE2 | 1.66 | 0.77 |
| 1:E:305:ILE:N | 1:E:305:ILE:HD12 | 1.99 | 0.77 |
| 1:E:322:ARG:HB3 | 1:E:333:ILE:CD1 | 2.14 | 0.77 |
| 1:G:322:ARG:HG2 | 1:G:323:VAL:N | 1.98 | 0.77 |
| 1:I:5:ASP:HB2 | 1:I:524:LEU:HD23 | 1.64 | 0.77 |
| 1:N:249:ILE:HB | 1:N:275:ALA:HB2 | 1.65 | 0.77 |
| 2:O:14:ARG:HG2 | 2:O:15:LYS:N | 1.99 | 0.77 |
| 2:T:14:ARG:HD3 | 2:T:35:SER:HB3 | 1.63 | 0.77 |
| 2:U:55:LYS:HE2 | 2:U:55:LYS:N | 1.94 | 0.77 |
| 1:F:247:LEU:HD12 | 1:F:249:ILE:HD11 | 1.67 | 0.77 |
| 1:F:417:VAL:O | 1:F:420:ILE:HG22 | 1.84 | 0.77 |
| 1:G:350:ARG:HD3 | 1:G:353:ILE:HD12 | 1.64 | 0.77 |
| 1:I:308:GLU:HG2 | 1:I:309:LEU:N | 1.98 | 0.77 |
| 1:J:5:ASP:HB2 | 1:J:524:LEU:HD23 | 1.66 | 0.77 |
| 1:M:219:PHE:HE1 | 1:M:245:LYS:HB2 | 1.49 | 0.77 |
| 1:N:235:PRO:HG3 | 1:N:310:GLU:HA | 1.67 | 0.77 |
| 1:A:247:LEU:HD12 | 1:A:249:ILE:HD11 | 1.67 | 0.77 |
| 1:A:291:ASP:OD1 | 1:A:292:ILE:HG13 | 1.84 | 0.77 |
| 1:A:310:GLU:CD | 1:A:310:GLU:H | 1.85 | 0.77 |
| 1:K:191:GLU:HB3 | 1:K:295:LEU:HD11 | 1.66 | 0.77 |
| 1:M:351:GLN:HG2 | 1:M:354:GLU:OE2 | 1.84 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:S:20:LYS:H | 2:S:20:LYS:HD2 | 1.49 | 0.77 |
| 1:D:252:GLU:HA | 1:D:285:ARG:NH1 | 2.00 | 0.77 |
| 1:E:487:ASN:O | 1:E:491:MET:HG3 | 1.83 | 0.77 |
| 1:G:237:LEU:HD22 | 2:U:26:VAL:HG22 | 1.66 | 0.77 |
| 1:H:206:ASN:OD1 | 1:H:213:VAL:HA | 1.85 | 0.77 |
| 1:M:85:ALA:HB1 | 1:M:499:VAL:HG12 | 1.65 | 0.77 |
| 2:S:65:VAL:HG12 | 2:S:94:ILE:HG12 | 1.66 | 0.77 |
| 1:F:131:LEU:CD2 | 1:F:422:VAL:HG11 | 2.15 | 0.77 |
| 1:H:359:ASP:HA | 1:H:362:ARG:NH1 | 1.99 | 0.77 |
| 2:O:97:ALA:O | 2:P:1:MET:HA | 1.83 | 0.77 |
| 1:E:233:MET:HA | 1:E:310:GLU:HG3 | 1.64 | 0.77 |
| 1:H:122:LYS:HE2 | 1:H:429:LEU:HD11 | 1.67 | 0.77 |
| 1:H:230:ILE:HD12 | 1:H:230:ILE:N | 1.99 | 0.77 |
| 1:M:230:ILE:N | 1:M:230:ILE:HD12 | 2.00 | 0.77 |
| 1:N:143:ALA:O | 1:N:147:VAL:HG12 | 1.84 | 0.77 |
| 2:S:7:HIS:O | 2:S:8:ASP:HB3 | 1.84 | 0.77 |
| 1:A:44:PHE:N | 1:A:44:PHE:CD1 | 2.47 | 0.77 |
| 1:M:248:LEU:HD22 | 1:M:249:ILE:H | 1.49 | 0.77 |
| 1:M:122:LYS:HE2 | 1:M:429:LEU:HD11 | 1.67 | 0.77 |
| 1:N:200:LEU:CD1 | 1:N:276:VAL:HA | 2.15 | 0.77 |
| 1:A:289:LEU:HA | 1:A:292:ILE:HD12 | 1.67 | 0.77 |
| 1:L:356:ALA:HB1 | 1:L:362:ARG:HE | 1.50 | 0.77 |
| 1:M:266:THR:HG22 | 1:M:272:LYS:HA | 1.66 | 0.77 |
| 1:M:284:ARG:HB2 | 1:M:284:ARG:HH11 | 1.50 | 0.77 |
| 2:O:48:ILE:HG23 | 2:O:54:VAL:HG22 | 1.67 | 0.77 |
| 1:A:131:LEU:HD21 | 1:A:422:VAL:HG11 | 1.67 | 0.77 |
| 1:C:215:LEU:O | 1:C:218:PRO:HD3 | 1.84 | 0.77 |
| 1:E:74:VAL:O | 1:E:77:VAL:HG13 | 1.84 | 0.77 |
| 1:K:85:ALA:HB1 | 1:K:499:VAL:HG12 | 1.66 | 0.77 |
| 1:L:230:ILE:N | 1:L:230:ILE:HD12 | 1.99 | 0.76 |
| 1:B:266:THR:HG22 | 1:B:271:VAL:O | 1.85 | 0.76 |
| 1:H:16:MET:O | 1:H:20:VAL:HG12 | 1.85 | 0.76 |
| 1:H:235:PRO:HG3 | 1:H:310:GLU:HA | 1.66 | 0.76 |
| 1:J:230:ILE:HD12 | 1:J:230:ILE:N | 1.99 | 0.76 |
| 1:M:111:MET:HG2 | 1:M:435:ASP:OD1 | 1.85 | 0.76 |
| 1:B:281:PHE:O | 1:B:285:ARG:HG2 | 1.84 | 0.76 |
| 1:H:356:ALA:HB1 | 1:H:362:ARG:HE | 1.49 | 0.76 |
| 1:I:34:LYS:HB2 | 1:I:458:CYS:SG | 2.25 | 0.76 |
| 1:M:124:VAL:O | 1:M:128:VAL:HG23 | 1.84 | 0.76 |
| 1:M:326:ASN:OD1 | 1:M:329:THR:HB | 1.85 | 0.76 |
| 2:Q:48:ILE:HG12 | 2:Q:54:VAL:HG13 | 1.68 | 0.76 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:219:PHE:HB3 | 1:A:317:LEU:HD13 | 1.66 | 0.76 |
| 1:A:339:GLU:HB3 | 1:A:343:GLN:OE1 | 1.86 | 0.76 |
| 1:B:305:ILE:HG22 | 1:B:306:GLY:N | 2.00 | 0.76 |
| 1:H:169:VAL:HG13 | 1:H:173:GLY:HA3 | 1.65 | 0.76 |
| 1:M:308:GLU:HG2 | 1:M:309:LEU:N | 2.01 | 0.76 |
| 2:O:18:GLU:CD | 2:O:33:ALA:HB3 | 2.06 | 0.76 |
| 2:P:78:ILE:HD13 | 2:P:83:VAL:HG21 | 1.68 | 0.76 |
| 1:B:342:ILE:O | 1:B:346:VAL:HG23 | 1.85 | 0.76 |
| 1:B:355:GLU:HG3 | 1:B:357:THR:H | 1.48 | 0.76 |
| 1:D:33:PRO:HA | 1:D:153:ASN:HD21 | 1.50 | 0.76 |
| 1:G:215:LEU:O | 1:G:218:PRO:HD3 | 1.85 | 0.76 |
| 1:H:69:MET:HE1 | 1:H:522:THR:HB | 1.67 | 0.76 |
| 1:I:301:ILE:N | 1:I:301:ILE:HD12 | 2.00 | 0.76 |
| 1:E:82:ASN:ND2 | 1:E:86:GLY:HA2 | 2.01 | 0.76 |
| 1:A:346:VAL:CG1 | 1:A:350:ARG:HH22 | 1.98 | 0.76 |
| 1:D:414:GLY:O | 1:D:417:VAL:HG12 | 1.85 | 0.76 |
| 1:J:166:MET:HE2 | 1:J:171:LYS:HA | 1.67 | 0.76 |
| 1:N:200:LEU:HD13 | 1:N:276:VAL:HA | 1.67 | 0.76 |
| 1:N:111:MET:HG2 | 1:N:435:ASP:OD1 | 1.85 | 0.76 |
| 2:R:92:LEU:O | 2:S:6:LEU:HB2 | 1.85 | 0.76 |
| 1:F:20:VAL:HG13 | 1:F:74:VAL:HG11 | 1.66 | 0.76 |
| 2:S:47:ARG:HD3 | 2:S:49:LEU:HD12 | 1.67 | 0.76 |
| 1:A:411:VAL:HA | 1:A:497:THR:H | 1.50 | 0.76 |
| 1:B:360:TYR:O | 1:B:364:LYS:HE2 | 1.86 | 0.76 |
| 1:E:234:LEU:H | 1:E:234:LEU:HD12 | 1.48 | 0.76 |
| 1:G:302:SER:HB2 | 1:G:305:ILE:HD13 | 1.68 | 0.76 |
| 1:J:434:GLU:HA | 1:J:437:ASN:ND2 | 2.01 | 0.76 |
| 1:L:248:LEU:HD13 | 1:L:249:ILE:N | 2.01 | 0.76 |
| 1:L:284:ARG:NH1 | 1:L:284:ARG:HB2 | 2.00 | 0.76 |
| 1:L:32:GLY:HA2 | 1:L:454:ILE:HD12 | 1.68 | 0.76 |
| 1:J:199:TYR:HA | 1:J:276:VAL:HG12 | 1.67 | 0.75 |
| 2:Q:55:LYS:HE2 | 2:Q:55:LYS:N | 1.98 | 0.75 |
| 1:F:273:VAL:HG12 | 1:F:274:ALA:N | 1.99 | 0.75 |
| 1:F:281:PHE:O | 1:F:285:ARG:HG2 | 1.87 | 0.75 |
| 1:M:215:LEU:HB3 | 1:M:218:PRO:HG2 | 1.67 | 0.75 |
| 1:N:249:ILE:HB | 1:N:275:ALA:CB | 2.16 | 0.75 |
| 1:D:321:LYS:HD2 | 1:D:333:ILE:HG22 | 1.69 | 0.75 |
| 1:G:226:LYS:C | 1:G:227:ILE:HD12 | 2.06 | 0.75 |
| 1:A:346:VAL:HG12 | 1:A:350:ARG:NH2 | 2.00 | 0.75 |
| 1:D:199:TYR:HE1 | 1:D:327:LYS:HG3 | 1.50 | 0.75 |
| 1:F:273:VAL:HG12 | 1:F:274:ALA:H | 1.49 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:239:ALA:O | 1:G:242:LYS:HB3 | 1.87 | 0.75 |
| 1:M:256:GLY:HA2 | 1:M:259:LEU:HB3 | 1.67 | 0.75 |
| 1:A:234:LEU:N | 1:A:235:PRO:HD2 | 2.02 | 0.75 |
| 1:L:365:LEU:O | 1:L:369:VAL:HG23 | 1.85 | 0.75 |
| 1:B:215:LEU:HB3 | 1:B:246:PRO:HB2 | 1.67 | 0.75 |
| 1:D:214:GLU:HA | 1:D:323:VAL:O | 1.86 | 0.75 |
| 1:E:461:GLU:HB2 | 1:E:464:VAL:HB | 1.68 | 0.75 |
| 1:F:449:ALA:HB3 | 1:F:450:PRO:HD3 | 1.68 | 0.75 |
| 1:F:461:GLU:HB2 | 1:F:464:VAL:HB | 1.67 | 0.75 |
| 1:H:5:ASP:HB2 | 1:H:524:LEU:HD23 | 1.69 | 0.75 |
| 1:L:124:VAL:O | 1:L:128:VAL:HG23 | 1.87 | 0.75 |
| 1:L:203:TYR:HB2 | 1:L:263:VAL:HG13 | 1.68 | 0.75 |
| 1:N:254:VAL:HG12 | 1:N:259:LEU:HB2 | 1.68 | 0.75 |
| 1:B:223:ALA:HB3 | 1:B:251:ALA:HB2 | 1.69 | 0.75 |
| 1:B:322:ARG:HG2 | 1:B:323:VAL:N | 2.01 | 0.75 |
| 1:C:342:ILE:O | 1:C:346:VAL:HG23 | 1.86 | 0.75 |
| 1:K:169:VAL:HG13 | 1:K:173:GLY:HA3 | 1.67 | 0.75 |
| 1:L:434:GLU:HA | 1:L:437:ASN:ND2 | 2.00 | 0.75 |
| 2:O:5:PRO:HD3 | 2:O:42:ALA:HB1 | 1.69 | 0.75 |
| 1:C:208:PRO:HB2 | 1:C:212:ALA:CB | 2.16 | 0.75 |
| 1:C:291:ASP:HB3 | 1:C:345:ARG:HH21 | 1.52 | 0.75 |
| 1:H:198:GLY:HA3 | 1:H:328:ASP:HA | 1.69 | 0.75 |
| 1:M:100:ILE:O | 1:M:104:LEU:HB2 | 1.86 | 0.75 |
| 2:R:48:ILE:HG23 | 2:R:54:VAL:HG22 | 1.69 | 0.75 |
| 1:A:147:VAL:O | 1:A:150:ILE:HG22 | 1.86 | 0.75 |
| 1:B:18:ARG:HH11 | 1:B:18:ARG:CB | 1.97 | 0.75 |
| 1:B:237:LEU:HD22 | 2:P:26:VAL:HG22 | 1.69 | 0.75 |
| 1:B:235:PRO:HG3 | 1:B:310:GLU:HB3 | 1.69 | 0.75 |
| 1:C:296:THR:HG22 | 1:C:335:GLY:HA3 | 1.66 | 0.75 |
| 1:D:44:PHE:CD1 | 1:D:44:PHE:N | 2.50 | 0.75 |
| 1:E:252:GLU:HA | 1:E:285:ARG:NH1 | 2.02 | 0.75 |
| 2:O:7:HIS:O | 2:O:8:ASP:HB3 | 1.85 | 0.75 |
| 1:B:392:LYS:O | 1:B:396:VAL:HG23 | 1.86 | 0.74 |
| 1:D:247:LEU:HD12 | 1:D:249:ILE:HD11 | 1.67 | 0.74 |
| 1:E:82:ASN:HD22 | 1:E:86:GLY:HA2 | 1.52 | 0.74 |
| 1:I:157:THR:O | 1:I:160:LYS:HB3 | 1.86 | 0.74 |
| 1:K:157:THR:O | 1:K:160:LYS:HB3 | 1.86 | 0.74 |
| 1:L:205:ILE:HD13 | 1:L:211:GLY:HA2 | 1.68 | 0.74 |
| 2:O:14:ARG:HD3 | 2:O:35:SER:HB3 | 1.68 | 0.74 |
| 2:Q:14:ARG:HD3 | 2:Q:35:SER:HB3 | 1.67 | 0.74 |
| 1:A:229:ASN:HA | 1:A:257:GLU:OE2 | 1.87 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:302:SER:HB2 | 1:B:305:ILE:HB | 1.69 | 0.74 |
| 1:F:322:ARG:HB3 | 1:F:333:ILE:CD1 | 2.11 | 0.74 |
| 1:I:415:GLY:N | 1:I:417:VAL:HG23 | 2.02 | 0.74 |
| 1:J:149:THR:HG23 | 1:J:159:GLY:HA3 | 1.67 | 0.74 |
| 2:Q:20:LYS:H | 2:Q:20:LYS:HD2 | 1.52 | 0.74 |
| 1:C:235:PRO:HG3 | 1:C:310:GLU:HB3 | 1.68 | 0.74 |
| 1:D:461:GLU:HB2 | 1:D:464:VAL:HB | 1.69 | 0.74 |
| 1:E:265:ASN:HA | 1:E:270:ILE:HD12 | 1.69 | 0.74 |
| 1:G:215:LEU:HB3 | 1:G:246:PRO:HB2 | 1.68 | 0.74 |
| 2:S:5:PRO:HD3 | 2:S:42:ALA:HB1 | 1.70 | 0.74 |
| 1:C:252:GLU:HA | 1:C:285:ARG:NH1 | 2.02 | 0.74 |
| 1:E:449:ALA:HB3 | 1:E:450:PRO:HD3 | 1.70 | 0.74 |
| 1:C:360:TYR:HA | 1:C:363:GLU:OE1 | 1.87 | 0.74 |
| 1:D:314:LEU:HD12 | 1:D:315:GLU:N | 2.01 | 0.74 |
| 1:I:351:GLN:HG2 | 1:I:354:GLU:OE2 | 1.88 | 0.74 |
| 1:L:287:ALA:HB1 | 1:L:368:ARG:NH2 | 2.02 | 0.74 |
| 1:N:359:ASP:HA | 1:N:362:ARG:NH1 | 2.02 | 0.74 |
| 1:E:305:ILE:HG22 | 1:E:306:GLY:N | 2.02 | 0.74 |
| 1:I:100:ILE:O | 1:I:104:LEU:HB2 | 1.87 | 0.74 |
| 1:L:124:VAL:HG13 | 1:L:504:LEU:CD1 | 2.18 | 0.74 |
| 1:M:284:ARG:NH1 | 1:M:284:ARG:HB2 | 2.03 | 0.74 |
| 2:P:77:LYS:HG3 | 2:P:80:ASN:HA | 1.68 | 0.74 |
| 1:B:202:PRO:O | 1:B:205:ILE:HG13 | 1.87 | 0.74 |
| 1:F:308:GLU:HB2 | 1:F:311:LYS:HB2 | 1.68 | 0.74 |
| 1:G:220:ILE:HG23 | 1:G:248:LEU:HD12 | 1.68 | 0.74 |
| 1:I:82:ASN:HB2 | 1:I:89:THR:OG1 | 1.87 | 0.74 |
| 1:M:345:ARG:HA | 1:M:348:GLN:NE2 | 2.02 | 0.74 |
| 1:N:284:ARG:HH11 | 1:N:284:ARG:H | 1.33 | 0.74 |
| 2:Q:14:ARG:HG2 | 2:Q:15:LYS:N | 2.03 | 0.74 |
| 2:T:11:ILE:HB | 2:T:42:ALA:HB3 | 1.68 | 0.74 |
| 1:B:234:LEU:N | 1:B:235:PRO:HD2 | 2.03 | 0.74 |
| 1:C:74:VAL:O | 1:C:77:VAL:HG13 | 1.88 | 0.74 |
| 1:E:127:ALA:O | 1:E:130:GLU:HB2 | 1.86 | 0.74 |
| 1:G:291:ASP:HB3 | 1:G:345:ARG:NH2 | 2.03 | 0.74 |
| 1:G:44:PHE:CD1 | 1:G:44:PHE:N | 2.48 | 0.74 |
| 1:I:149:THR:CG2 | 1:I:156:GLU:HA | 2.18 | 0.74 |
| 1:J:494:LEU:HD23 | 1:J:494:LEU:H | 1.52 | 0.74 |
| 2:O:6:LEU:HB2 | 2:U:92:LEU:O | 1.88 | 0.74 |
| 1:C:237:LEU:HD22 | 2:Q:26:VAL:HG22 | 1.68 | 0.74 |
| 2:U:40:VAL:HB | 2:U:62:GLY:H | 1.51 | 0.74 |
| 1:B:229:ASN:HA | 1:B:257:GLU:OE2 | 1.88 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:226:LYS:C | 1:E:227:ILE:HD12 | 2.07 | 0.74 |
| 1:E:360:TYR:O | 1:E:364:LYS:HE2 | 1.87 | 0.74 |
| 1:E:135:SER:HB2 | 1:E:497:THR:HG21 | 1.69 | 0.74 |
| 1:H:249:ILE:HB | 1:H:275:ALA:HB2 | 1.69 | 0.74 |
| 1:I:339:GLU:O | 1:I:343:GLN:HG2 | 1.88 | 0.74 |
| 1:N:149:THR:HG23 | 1:N:159:GLY:HA3 | 1.68 | 0.74 |
| 1:E:321:LYS:HD2 | 1:E:333:ILE:HG22 | 1.67 | 0.74 |
| 1:H:256:GLY:HA2 | 1:H:259:LEU:HB3 | 1.68 | 0.74 |
| 1:J:66:PHE:H | 1:J:69:MET:HG3 | 1.51 | 0.74 |
| 1:K:124:VAL:HG13 | 1:K:504:LEU:CD1 | 2.18 | 0.74 |
| 1:K:124:VAL:O | 1:K:128:VAL:HG23 | 1.88 | 0.74 |
| 1:L:213:VAL:O | 1:L:324:VAL:HA | 1.88 | 0.74 |
| 1:M:301:ILE:HD12 | 1:M:301:ILE:N | 2.03 | 0.74 |
| 1:N:66:PHE:H | 1:N:69:MET:HG3 | 1.51 | 0.74 |
| 1:C:314:LEU:HD12 | 1:C:315:GLU:N | 2.01 | 0.73 |
| 1:C:325:ILE:N | 1:C:325:ILE:HD12 | 2.03 | 0.73 |
| 1:J:287:ALA:HB1 | 1:J:368:ARG:NH2 | 2.02 | 0.73 |
| 1:A:235:PRO:HG3 | 1:A:310:GLU:HB3 | 1.70 | 0.73 |
| 1:D:302:SER:HB2 | 1:D:305:ILE:HB | 1.70 | 0.73 |
| 1:K:287:ALA:HB1 | 1:K:368:ARG:NH2 | 2.03 | 0.73 |
| 1:N:233:MET:HA | 1:N:233:MET:HE2 | 1.69 | 0.73 |
| 1:A:273:VAL:HG12 | 1:A:274:ALA:H | 1.50 | 0.73 |
| 1:A:308:GLU:HB2 | 1:A:311:LYS:HB2 | 1.70 | 0.73 |
| 1:B:131:LEU:CD2 | 1:B:422:VAL:HG11 | 2.18 | 0.73 |
| 1:B:449:ALA:HB3 | 1:B:450:PRO:HD3 | 1.70 | 0.73 |
| 1:E:280:GLY:HA3 | 1:E:284:ARG:HH11 | 1.53 | 0.73 |
| 1:G:414:GLY:HA2 | 1:G:495:ASP:OD2 | 1.88 | 0.73 |
| 1:H:230:ILE:CD1 | 1:H:230:ILE:H | 1.97 | 0.73 |
| 1:L:228:SER:O | 1:L:257:GLU:HB3 | 1.88 | 0.73 |
| 1:A:226:LYS:C | 1:A:227:ILE:HD12 | 2.09 | 0.73 |
| 1:A:510:VAL:HG23 | 1:A:511:ALA:N | 2.03 | 0.73 |
| 1:C:346:VAL:HG12 | 1:C:350:ARG:HH22 | 1.53 | 0.73 |
| 1:F:233:MET:C | 1:F:235:PRO:HD2 | 2.08 | 0.73 |
| 1:G:281:PHE:O | 1:G:285:ARG:HG2 | 1.87 | 0.73 |
| 1:J:314:LEU:HA | 1:J:317:LEU:HD13 | 1.70 | 0.73 |
| 1:K:249:ILE:HB | 1:K:275:ALA:HB2 | 1.70 | 0.73 |
| 1:M:157:THR:O | 1:M:160:LYS:HB3 | 1.88 | 0.73 |
| 1:N:320:ALA:HA | 1:N:334:ASP:O | 1.88 | 0.73 |
| 1:D:34:LYS:HD2 | 1:D:458:CYS:SG | 2.29 | 0.73 |
| 1:G:256:GLY:O | 1:G:260:ALA:N | 2.21 | 0.73 |
| 1:C:33:PRO:HA | 1:C:153:ASN:ND2 | 2.03 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:266:THR:HG22 | 1:D:271:VAL:O | 1.89 | 0.73 |
| 1:D:351:GLN:HG2 | 1:E:210:THR:OG1 | 1.88 | 0.73 |
| 1:E:131:LEU:HD23 | 1:E:422:VAL:HG11 | 1.71 | 0.73 |
| 1:E:234:LEU:N | 1:E:235:PRO:HD2 | 2.02 | 0.73 |
| 1:E:291:ASP:HB3 | 1:E:345:ARG:HH21 | 1.52 | 0.73 |
| 1:F:310:GLU:H | 1:F:310:GLU:CD | 1.92 | 0.73 |
| 1:H:215:LEU:HB3 | 1:H:218:PRO:HG2 | 1.68 | 0.73 |
| 1:I:434:GLU:HA | 1:I:437:ASN:ND2 | 2.03 | 0.73 |
| 1:E:229:ASN:HA | 1:E:257:GLU:OE2 | 1.89 | 0.73 |
| 1:E:277:LYS:HD3 | 1:E:285:ARG:HH22 | 1.53 | 0.73 |
| 1:F:342:ILE:O | 1:F:346:VAL:HG23 | 1.89 | 0.73 |
| 1:N:169:VAL:HG13 | 1:N:173:GLY:HA3 | 1.69 | 0.73 |
| 1:N:199:TYR:HA | 1:N:276:VAL:HG12 | 1.69 | 0.73 |
| 2:R:17:VAL:CG2 | 2:R:34:LYS:HD2 | 2.18 | 0.73 |
| 1:G:296:THR:HG22 | 1:G:335:GLY:HA3 | 1.71 | 0.73 |
| 1:L:100:ILE:O | 1:L:104:LEU:HB2 | 1.87 | 0.73 |
| 1:E:237:LEU:HD22 | 2:S:26:VAL:HG22 | 1.68 | 0.73 |
| 1:B:219:PHE:O | 1:B:247:LEU:HD22 | 1.89 | 0.73 |
| 1:C:202:PRO:O | 1:C:205:ILE:HG13 | 1.88 | 0.73 |
| 1:E:20:VAL:HG13 | 1:E:74:VAL:HG11 | 1.71 | 0.73 |
| 1:I:32:GLY:HA2 | 1:I:454:ILE:HD12 | 1.71 | 0.73 |
| 1:L:107:VAL:HG23 | 1:L:108:ALA:N | 2.04 | 0.73 |
| 1:N:149:THR:CG2 | 1:N:156:GLU:HA | 2.18 | 0.73 |
| 1:D:324:VAL:C | 1:D:325:ILE:HD12 | 2.09 | 0.73 |
| 1:J:385:THR:HG23 | 1:J:388:GLU:H | 1.52 | 0.73 |
| 2:R:14:ARG:HG2 | 2:R:15:LYS:N | 2.04 | 0.73 |
| 2:U:40:VAL:HG21 | 2:U:63:ASP:HB2 | 1.71 | 0.73 |
| 1:A:220:ILE:N | 1:A:220:ILE:HD12 | 2.04 | 0.72 |
| 1:A:295:LEU:O | 1:A:337:GLY:HA3 | 1.89 | 0.72 |
| 1:D:229:ASN:HA | 1:D:257:GLU:OE2 | 1.89 | 0.72 |
| 1:H:149:THR:CG2 | 1:H:156:GLU:HA | 2.17 | 0.72 |
| 1:L:494:LEU:HD23 | 1:L:494:LEU:N | 2.04 | 0.72 |
| 1:N:124:VAL:O | 1:N:128:VAL:HG23 | 1.90 | 0.72 |
| 1:A:70:GLY:O | 1:A:74:VAL:HG22 | 1.88 | 0.72 |
| 1:C:249:ILE:HD12 | 1:C:249:ILE:N | 2.04 | 0.72 |
| 1:D:131:LEU:CD2 | 1:D:422:VAL:HG11 | 2.19 | 0.72 |
| 1:H:247:LEU:HD22 | 1:H:248:LEU:H | 1.54 | 0.72 |
| 1:J:175:ILE:HD12 | 1:J:175:ILE:N | 2.04 | 0.72 |
| 1:B:291:ASP:HB3 | 1:B:345:ARG:HH21 | 1.54 | 0.72 |
| 1:C:305:ILE:HG22 | 1:C:306:GLY:N | 2.03 | 0.72 |
| 1:C:82:ASN:ND2 | 1:C:86:GLY:HA2 | 2.04 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:285:ARG:HG3 | 1:D:286:LYS:H | 1.54 | 0.72 |
| 1:D:291:ASP:HB3 | 1:D:345:ARG:HH21 | 1.54 | 0.72 |
| 1:E:219:PHE:HB3 | 1:E:317:LEU:HD13 | 1.69 | 0.72 |
| 1:F:305:ILE:HG22 | 1:F:306:GLY:H | 1.51 | 0.72 |
| 1:G:249:ILE:HB | 1:G:275:ALA:HB2 | 1.72 | 0.72 |
| 1:M:411:VAL:HG21 | 1:M:494:LEU:HD12 | 1.72 | 0.72 |
| 1:N:494:LEU:HD23 | 1:N:494:LEU:N | 2.04 | 0.72 |
| 2:Q:7:HIS:O | 2:Q:8:ASP:HB3 | 1.88 | 0.72 |
| 1:D:202:PRO:O | 1:D:205:ILE:HG13 | 1.89 | 0.72 |
| 1:G:233:MET:CA | 1:G:310:GLU:HG3 | 2.11 | 0.72 |
| 1:I:217:SER:HA | 1:I:320:ALA:O | 1.89 | 0.72 |
| 1:K:32:GLY:HA2 | 1:K:454:ILE:HD12 | 1.69 | 0.72 |
| 1:L:206:ASN:OD1 | 1:L:213:VAL:HA | 1.88 | 0.72 |
| 2:P:43:VAL:HG23 | 2:P:61:VAL:HG22 | 1.71 | 0.72 |
| 1:A:349:ILE:O | 1:A:353:ILE:HG13 | 1.88 | 0.72 |
| 1:C:339:GLU:HB3 | 1:C:343:GLN:OE1 | 1.90 | 0.72 |
| 1:F:124:VAL:HG13 | 1:F:504:LEU:CD1 | 2.19 | 0.72 |
| 1:F:169:VAL:HB | 1:F:173:GLY:HA3 | 1.72 | 0.72 |
| 1:G:510:VAL:HG23 | 1:G:511:ALA:N | 2.04 | 0.72 |
| 1:K:223:ALA:HB3 | 1:K:251:ALA:CB | 2.19 | 0.72 |
| 1:L:69:MET:HE2 | 1:L:522:THR:HB | 1.71 | 0.72 |
| 1:M:247:LEU:H | 1:M:273:VAL:HG12 | 1.53 | 0.72 |
| 1:N:287:ALA:HB1 | 1:N:368:ARG:NH2 | 2.05 | 0.72 |
| 1:F:247:LEU:HD12 | 1:F:249:ILE:CD1 | 2.19 | 0.72 |
| 1:L:143:ALA:O | 1:L:146:GLN:HB3 | 1.89 | 0.72 |
| 1:N:308:GLU:HG2 | 1:N:309:LEU:N | 2.04 | 0.72 |
| 2:O:17:VAL:CG2 | 2:O:34:LYS:HD2 | 2.18 | 0.72 |
| 1:C:266:THR:HG22 | 1:C:271:VAL:O | 1.89 | 0.72 |
| 1:C:351:GLN:HG2 | 1:D:210:THR:OG1 | 1.90 | 0.72 |
| 1:H:494:LEU:HD23 | 1:H:494:LEU:N | 2.05 | 0.72 |
| 1:J:149:THR:CG2 | 1:J:156:GLU:HA | 2.19 | 0.72 |
| 1:C:195:PHE:O | 1:C:329:THR:HG23 | 1.89 | 0.72 |
| 1:D:248:LEU:C | 1:D:249:ILE:HD12 | 2.09 | 0.72 |
| 1:J:124:VAL:HG13 | 1:J:504:LEU:CD1 | 2.19 | 0.72 |
| 1:L:248:LEU:HD22 | 1:L:249:ILE:H | 1.53 | 0.72 |
| 1:M:175:ILE:HD12 | 1:M:175:ILE:N | 2.04 | 0.72 |
| 1:A:202:PRO:O | 1:A:205:ILE:HG13 | 1.90 | 0.72 |
| 1:B:234:LEU:HD12 | 1:B:234:LEU:H | 1.54 | 0.72 |
| 1:D:487:ASN:O | 1:D:491:MET:HG3 | 1.89 | 0.72 |
| 1:F:134:LEU:O | 1:F:136:VAL:HG13 | 1.90 | 0.72 |
| 1:J:359:ASP:HA | 1:J:362:ARG:NH1 | 2.05 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:345:ARG:HA | 1:N:348:GLN:NE2 | 2.04 | 0.72 |
| 1:A:349:ILE:HA | 1:A:352:GLN:NE2 | 2.05 | 0.72 |
| 1:B:291:ASP:OD1 | 1:B:292:ILE:HG13 | 1.90 | 0.72 |
| 1:D:219:PHE:HB3 | 1:D:317:LEU:HD13 | 1.70 | 0.72 |
| 1:D:346:VAL:HG12 | 1:D:350:ARG:HH22 | 1.55 | 0.72 |
| 1:G:228:SER:HA | 1:G:255:GLU:CB | 2.19 | 0.72 |
| 1:I:221:LEU:HD13 | 1:I:222:LEU:N | 2.05 | 0.72 |
| 1:N:385:THR:HG23 | 1:N:388:GLU:H | 1.54 | 0.72 |
| 1:C:253:ASP:CG | 1:C:254:VAL:H | 1.93 | 0.71 |
| 1:N:217:SER:HA | 1:N:320:ALA:O | 1.90 | 0.71 |
| 1:C:44:PHE:N | 1:C:44:PHE:CD1 | 2.46 | 0.71 |
| 1:F:305:ILE:HD12 | 1:F:305:ILE:N | 2.04 | 0.71 |
| 1:K:25:ASP:HA | 1:K:28:LYS:HE2 | 1.72 | 0.71 |
| 1:M:5:ASP:HB2 | 1:M:524:LEU:HD23 | 1.72 | 0.71 |
| 1:A:299:THR:HB | 1:A:316:ASP:HB3 | 1.72 | 0.71 |
| 1:E:206:ASN:CB | 1:E:214:GLU:H | 2.03 | 0.71 |
| 1:I:149:THR:HG23 | 1:I:159:GLY:HA3 | 1.69 | 0.71 |
| 1:L:436:GLN:O | 1:L:440:ILE:HG13 | 1.90 | 0.71 |
| 1:N:219:PHE:HE1 | 1:N:245:LYS:HB2 | 1.55 | 0.71 |
| 1:A:305:ILE:HD12 | 1:A:305:ILE:N | 2.05 | 0.71 |
| 1:B:310:GLU:H | 1:B:310:GLU:CD | 1.94 | 0.71 |
| 1:C:228:SER:O | 1:C:257:GLU:HB3 | 1.89 | 0.71 |
| 1:C:350:ARG:HD3 | 1:C:353:ILE:HD12 | 1.71 | 0.71 |
| 1:C:392:LYS:O | 1:C:396:VAL:HG23 | 1.89 | 0.71 |
| 1:D:147:VAL:O | 1:D:150:ILE:HG22 | 1.90 | 0.71 |
| 1:F:365:LEU:HD22 | 1:F:366:GLN:HE22 | 1.55 | 0.71 |
| 1:K:301:ILE:HD12 | 1:K:301:ILE:N | 2.06 | 0.71 |
| 2:Q:47:ARG:HD3 | 2:Q:49:LEU:CD1 | 2.18 | 0.71 |
| 2:U:18:GLU:CD | 2:U:33:ALA:HB3 | 2.10 | 0.71 |
| 1:H:32:GLY:HA2 | 1:H:454:ILE:HD12 | 1.72 | 0.71 |
| 1:K:247:LEU:O | 1:K:273:VAL:HB | 1.90 | 0.71 |
| 2:Q:48:ILE:HG23 | 2:Q:54:VAL:HG22 | 1.70 | 0.71 |
| 1:E:235:PRO:HG2 | 1:E:236:VAL:H | 1.55 | 0.71 |
| 1:G:392:LYS:O | 1:G:396:VAL:HG23 | 1.90 | 0.71 |
| 1:J:392:LYS:O | 1:J:396:VAL:HG23 | 1.90 | 0.71 |
| 1:K:161:LEU:H | 1:K:161:LEU:HD12 | 1.55 | 0.71 |
| 1:F:237:LEU:HD22 | 2:T:26:VAL:HG22 | 1.72 | 0.71 |
| 1:E:64:ASP:HB3 | 1:E:67:GLU:HB2 | 1.73 | 0.71 |
| 1:F:355:GLU:O | 1:F:362:ARG:NH2 | 2.24 | 0.71 |
| 1:M:494:LEU:HD23 | 1:M:494:LEU:N | 2.06 | 0.71 |
| 1:N:215:LEU:HB3 | 1:N:218:PRO:HG2 | 1.73 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:5:PRO:HD3 | 2:Q:42:ALA:HB1 | 1.71 | 0.71 |
| 1:A:252:GLU:O | 1:A:253:ASP:HB2 | 1.89 | 0.71 |
| 1:A:5:ASP:HB2 | 1:A:524:LEU:HD23 | 1.72 | 0.71 |
| 1:F:350:ARG:HA | 1:F:353:ILE:HD12 | 1.73 | 0.71 |
| 1:H:116:LEU:HD23 | 1:H:435:ASP:O | 1.89 | 0.71 |
| 1:I:161:LEU:H | 1:I:161:LEU:HD12 | 1.54 | 0.71 |
| 1:K:123:ALA:HB2 | 1:K:440:ILE:HG23 | 1.73 | 0.71 |
| 1:K:230:ILE:N | 1:K:230:ILE:HD12 | 2.04 | 0.71 |
| 1:L:194:GLN:HG3 | 1:L:331:THR:HB | 1.72 | 0.71 |
| 1:M:206:ASN:OD1 | 1:M:213:VAL:HA | 1.90 | 0.71 |
| 2:S:40:VAL:HB | 2:S:62:GLY:H | 1.56 | 0.71 |
| 1:B:368:ARG:HG2 | 1:B:372:LEU:HG | 1.71 | 0.71 |
| 1:G:131:LEU:CD2 | 1:G:422:VAL:HG11 | 2.20 | 0.71 |
| 1:G:234:LEU:N | 1:G:235:PRO:HD2 | 2.06 | 0.71 |
| 1:G:247:LEU:HD12 | 1:G:249:ILE:HD11 | 1.73 | 0.71 |
| 1:H:193:MET:HG2 | 1:H:194:GLN:N | 2.04 | 0.71 |
| 1:H:308:GLU:HG2 | 1:H:309:LEU:N | 2.04 | 0.71 |
| 1:I:215:LEU:HB3 | 1:I:218:PRO:HG2 | 1.73 | 0.71 |
| 1:J:200:LEU:CD1 | 1:J:276:VAL:HA | 2.20 | 0.71 |
| 1:K:240:VAL:HA | 1:K:243:ALA:HB3 | 1.72 | 0.71 |
| 1:K:286:LYS:HE2 | 1:K:286:LYS:HA | 1.72 | 0.71 |
| 2:R:47:ARG:HD2 | 2:R:55:LYS:HD2 | 1.72 | 0.71 |
| 1:A:252:GLU:HA | 1:A:285:ARG:NH1 | 2.06 | 0.71 |
| 1:F:248:LEU:C | 1:F:249:ILE:HD12 | 2.11 | 0.71 |
| 2:S:34:LYS:HG3 | 2:S:35:SER:H | 1.55 | 0.71 |
| 1:A:278:ALA:HB1 | 1:A:279:PRO:CD | 2.21 | 0.70 |
| 1:B:195:PHE:O | 1:B:329:THR:HG23 | 1.91 | 0.70 |
| 1:D:277:LYS:HD3 | 1:D:285:ARG:NH2 | 2.04 | 0.70 |
| 1:E:266:THR:HG22 | 1:E:271:VAL:O | 1.91 | 0.70 |
| 1:E:349:ILE:HG21 | 1:E:369:VAL:HG22 | 1.73 | 0.70 |
| 1:F:322:ARG:HG2 | 1:F:323:VAL:N | 2.04 | 0.70 |
| 1:G:18:ARG:HB2 | 1:G:67:GLU:HG2 | 1.73 | 0.70 |
| 1:J:417:VAL:HG21 | 1:J:488:MET:HG3 | 1.73 | 0.70 |
| 1:K:230:ILE:CD1 | 1:K:230:ILE:H | 2.03 | 0.70 |
| 1:M:69:MET:HE2 | 1:M:522:THR:HB | 1.71 | 0.70 |
| 1:A:305:ILE:HG22 | 1:A:306:GLY:N | 2.05 | 0.70 |
| 1:D:510:VAL:HG23 | 1:D:511:ALA:N | 2.05 | 0.70 |
| 1:H:265:ASN:O | 1:H:269:GLY:HA3 | 1.91 | 0.70 |
| 1:J:40:LEU:N | 1:J:40:LEU:HD22 | 2.05 | 0.70 |
| 1:L:487:ASN:HB3 | 1:L:490:ASP:HB2 | 1.73 | 0.70 |
| 1:M:254:VAL:HG12 | 1:M:259:LEU:HB2 | 1.73 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:7:HIS:HB3 | 2:P:45:ASN:HD22 | 1.55 | 0.70 |
| 1:F:324:VAL:C | 1:F:325:ILE:HD12 | 2.12 | 0.70 |
| 1:F:325:ILE:HG13 | 1:F:330:THR:HG23 | 1.73 | 0.70 |
| 1:F:77:VAL:HG12 | 1:F:510:VAL:HG21 | 1.71 | 0.70 |
| 1:K:219:PHE:HE1 | 1:K:245:LYS:HB2 | 1.55 | 0.70 |
| 1:L:175:ILE:HD12 | 1:L:175:ILE:N | 2.05 | 0.70 |
| 1:N:282:GLY:O | 1:N:285:ARG:HG2 | 1.92 | 0.70 |
| 1:N:32:GLY:HA2 | 1:N:454:ILE:HD12 | 1.71 | 0.70 |
| 1:C:234:LEU:N | 1:C:235:PRO:HD2 | 2.05 | 0.70 |
| 1:D:449:ALA:HB3 | 1:D:450:PRO:HD3 | 1.72 | 0.70 |
| 1:F:44:PHE:H | 1:F:44:PHE:HD1 | 1.35 | 0.70 |
| 1:G:252:GLU:O | 1:G:253:ASP:HB2 | 1.91 | 0.70 |
| 1:G:162:ILE:HG21 | 1:G:403:THR:HG21 | 1.74 | 0.70 |
| 1:I:111:MET:HG2 | 1:I:435:ASP:OD1 | 1.91 | 0.70 |
| 1:J:404:ARG:O | 1:J:408:GLU:HG3 | 1.91 | 0.70 |
| 1:E:346:VAL:CG1 | 1:E:350:ARG:HH22 | 2.03 | 0.70 |
| 1:F:226:LYS:C | 1:F:227:ILE:HD12 | 2.12 | 0.70 |
| 1:F:346:VAL:HG12 | 1:F:350:ARG:NH2 | 2.06 | 0.70 |
| 1:F:486:GLY:HA3 | 1:F:491:MET:CE | 2.22 | 0.70 |
| 1:G:322:ARG:HB3 | 1:G:333:ILE:CD1 | 2.17 | 0.70 |
| 1:A:16:MET:O | 1:A:20:VAL:HG23 | 1.92 | 0.70 |
| 1:E:339:GLU:HB3 | 1:E:343:GLN:OE1 | 1.90 | 0.70 |
| 1:H:257:GLU:OE2 | 1:N:270:ILE:HA | 1.91 | 0.70 |
| 1:J:270:ILE:HG23 | 1:K:229:ASN:HD21 | 1.55 | 0.70 |
| 1:L:326:ASN:OD1 | 1:L:329:THR:HB | 1.91 | 0.70 |
| 1:N:116:LEU:HD23 | 1:N:435:ASP:O | 1.91 | 0.70 |
| 2:R:34:LYS:HG3 | 2:R:35:SER:H | 1.56 | 0.70 |
| 2:T:68:ASN:HD22 | 2:U:74:LYS:HE3 | 1.56 | 0.70 |
| 1:D:213:VAL:O | 1:D:324:VAL:HA | 1.91 | 0.70 |
| 1:D:214:GLU:CB | 1:D:322:ARG:HD3 | 2.17 | 0.70 |
| 1:D:411:VAL:HA | 1:D:497:THR:H | 1.55 | 0.70 |
| 1:E:199:TYR:CZ | 1:E:202:PRO:HA | 2.27 | 0.70 |
| 1:L:143:ALA:O | 1:L:147:VAL:HG12 | 1.90 | 0.70 |
| 1:L:17:LEU:O | 1:L:20:VAL:HG13 | 1.91 | 0.70 |
| 1:M:263:VAL:O | 1:M:267:MET:HG2 | 1.92 | 0.70 |
| 1:N:93:THR:O | 1:N:96:ALA:HB3 | 1.90 | 0.70 |
| 1:D:237:LEU:HD22 | 2:R:26:VAL:HG22 | 1.73 | 0.70 |
| 1:C:510:VAL:HG23 | 1:C:511:ALA:N | 2.07 | 0.70 |
| 1:J:339:GLU:O | 1:J:343:GLN:HG2 | 1.92 | 0.70 |
| 1:L:264:VAL:HA | 1:L:267:MET:HG2 | 1.74 | 0.70 |
| 1:A:218:PRO:HA | 1:A:246:PRO:HG2 | 1.74 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:249:ILE:HD12 | 1:B:249:ILE:N | 2.07 | 0.70 |
| 1:C:349:ILE:O | 1:C:353:ILE:HG13 | 1.91 | 0.70 |
| 1:D:310:GLU:CD | 1:D:310:GLU:H | 1.95 | 0.70 |
| 1:H:205:ILE:HD13 | 1:H:211:GLY:HA2 | 1.72 | 0.70 |
| 1:J:230:ILE:CD1 | 1:J:230:ILE:H | 2.03 | 0.70 |
| 1:J:226:LYS:HD2 | 1:J:252:GLU:HG3 | 1.74 | 0.70 |
| 1:K:116:LEU:HD23 | 1:K:435:ASP:O | 1.90 | 0.70 |
| 1:K:386:GLU:HG2 | 1:K:390:LYS:HE2 | 1.73 | 0.70 |
| 1:A:233:MET:CA | 1:A:310:GLU:HG3 | 2.17 | 0.70 |
| 1:F:365:LEU:HD22 | 1:F:366:GLN:NE2 | 2.05 | 0.70 |
| 1:F:392:LYS:O | 1:F:396:VAL:HG23 | 1.92 | 0.70 |
| 1:H:398:ASP:O | 1:H:401:HIS:HB2 | 1.92 | 0.70 |
| 1:L:314:LEU:H | 1:L:314:LEU:CD1 | 2.04 | 0.70 |
| 1:M:288:MET:CE | 1:M:288:MET:HA | 2.22 | 0.70 |
| 1:M:190:VAL:HG21 | 1:M:334:ASP:CG | 2.11 | 0.70 |
| 2:S:17:VAL:HG13 | 2:S:34:LYS:HA | 1.74 | 0.70 |
| 1:B:134:LEU:HD12 | 1:B:134:LEU:N | 2.06 | 0.69 |
| 1:B:305:ILE:HD12 | 1:B:305:ILE:N | 2.07 | 0.69 |
| 1:E:348:GLN:NE2 | 1:E:352:GLN:NE2 | 2.40 | 0.69 |
| 1:F:206:ASN:CB | 1:F:214:GLU:H | 2.04 | 0.69 |
| 1:F:487:ASN:O | 1:F:491:MET:HG3 | 1.92 | 0.69 |
| 1:J:198:GLY:CA | 1:J:328:ASP:HA | 2.20 | 0.69 |
| 1:J:230:ILE:HD11 | 1:J:257:GLU:O | 1.92 | 0.69 |
| 1:L:115:ASP:HB3 | 1:L:436:GLN:HG2 | 1.74 | 0.69 |
| 1:L:215:LEU:HB3 | 1:L:218:PRO:HG2 | 1.72 | 0.69 |
| 1:L:219:PHE:HB2 | 1:L:247:LEU:HD23 | 1.74 | 0.69 |
| 1:F:249:ILE:HD12 | 1:F:249:ILE:N | 2.08 | 0.69 |
| 1:G:279:PRO:HB3 | 1:G:288:MET:HE3 | 1.72 | 0.69 |
| 1:G:449:ALA:HB3 | 1:G:450:PRO:HD3 | 1.72 | 0.69 |
| 1:I:219:PHE:HE1 | 1:I:245:LYS:HB2 | 1.57 | 0.69 |
| 1:M:325:ILE:N | 1:M:325:ILE:HD12 | 2.07 | 0.69 |
| 1:N:193:MET:HG2 | 1:N:194:GLN:H | 1.55 | 0.69 |
| 2:Q:65:VAL:HG12 | 2:Q:94:ILE:HG12 | 1.73 | 0.69 |
| 2:S:5:PRO:CD | 2:S:42:ALA:HB1 | 2.21 | 0.69 |
| 1:A:235:PRO:HG2 | 1:A:236:VAL:H | 1.57 | 0.69 |
| 1:B:325:ILE:HD12 | 1:B:325:ILE:N | 2.07 | 0.69 |
| 1:C:285:ARG:HG3 | 1:C:286:LYS:H | 1.56 | 0.69 |
| 1:E:266:THR:HG22 | 1:E:273:VAL:H | 1.55 | 0.69 |
| 1:E:392:LYS:O | 1:E:396:VAL:HG23 | 1.91 | 0.69 |
| 1:E:486:GLY:HA3 | 1:E:491:MET:CE | 2.22 | 0.69 |
| 1:I:324:VAL:C | 1:I:325:ILE:HD12 | 2.13 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:155:ASP:OD1 | 1:K:158:VAL:HG23 | 1.91 | 0.69 |
| 1:C:194:GLN:HG3 | 1:C:330:THR:O | 1.92 | 0.69 |
| 1:D:219:PHE:HD1 | 1:D:319:GLN:HE21 | 1.38 | 0.69 |
| 1:E:169:VAL:HB | 1:E:173:GLY:HA3 | 1.74 | 0.69 |
| 1:G:249:ILE:N | 1:G:249:ILE:HD12 | 2.07 | 0.69 |
| 1:H:301:ILE:N | 1:H:301:ILE:HD12 | 2.06 | 0.69 |
| 1:L:221:LEU:HD13 | 1:L:222:LEU:N | 2.08 | 0.69 |
| 1:M:107:VAL:HG23 | 1:M:108:ALA:N | 2.07 | 0.69 |
| 1:N:198:GLY:HA3 | 1:N:328:ASP:HA | 1.73 | 0.69 |
| 1:E:346:VAL:HG12 | 1:E:350:ARG:NH2 | 2.07 | 0.69 |
| 1:I:17:LEU:O | 1:I:20:VAL:HG13 | 1.92 | 0.69 |
| 1:I:206:ASN:OD1 | 1:I:213:VAL:HA | 1.93 | 0.69 |
| 1:J:219:PHE:HB3 | 1:J:317:LEU:HD23 | 1.73 | 0.69 |
| 1:L:200:LEU:CD1 | 1:L:276:VAL:HA | 2.23 | 0.69 |
| 1:L:286:LYS:HE2 | 1:L:286:LYS:HA | 1.74 | 0.69 |
| 1:M:277:LYS:HB2 | 1:M:277:LYS:NZ | 2.07 | 0.69 |
| 2:O:20:LYS:HB3 | 2:O:27:LEU:HG | 1.73 | 0.69 |
| 2:O:92:LEU:O | 2:P:6:LEU:HB2 | 1.91 | 0.69 |
| 1:A:264:VAL:HA | 1:A:267:MET:HB2 | 1.72 | 0.69 |
| 1:B:248:LEU:HD13 | 1:B:249:ILE:N | 2.07 | 0.69 |
| 1:C:235:PRO:HG2 | 1:C:236:VAL:H | 1.57 | 0.69 |
| 1:C:365:LEU:HD22 | 1:C:366:GLN:NE2 | 2.07 | 0.69 |
| 1:F:350:ARG:O | 1:F:354:GLU:HG2 | 1.93 | 0.69 |
| 1:G:288:MET:HA | 1:G:291:ASP:OD2 | 1.92 | 0.69 |
| 1:H:96:ALA:O | 1:H:100:ILE:HG13 | 1.92 | 0.69 |
| 1:H:205:ILE:HA | 1:H:213:VAL:HG22 | 1.74 | 0.69 |
| 1:H:465:VAL:O | 1:H:469:VAL:HG23 | 1.93 | 0.69 |
| 1:I:247:LEU:O | 1:I:273:VAL:HB | 1.93 | 0.69 |
| 1:N:239:ALA:CB | 1:N:314:LEU:HD11 | 2.22 | 0.69 |
| 1:A:219:PHE:HB2 | 1:A:247:LEU:HD22 | 1.74 | 0.69 |
| 1:C:324:VAL:C | 1:C:325:ILE:HD12 | 2.13 | 0.69 |
| 1:D:123:ALA:HB2 | 1:D:440:ILE:HG23 | 1.74 | 0.69 |
| 1:D:234:LEU:CD1 | 1:D:234:LEU:H | 2.05 | 0.69 |
| 1:E:273:VAL:CG1 | 1:E:274:ALA:H | 2.04 | 0.69 |
| 1:F:291:ASP:OD1 | 1:F:292:ILE:HG13 | 1.93 | 0.69 |
| 1:J:205:ILE:HD13 | 1:J:211:GLY:HA2 | 1.74 | 0.69 |
| 1:J:422:VAL:O | 1:J:425:LYS:HB2 | 1.93 | 0.69 |
| 1:L:122:LYS:HE2 | 1:L:429:LEU:HD11 | 1.73 | 0.69 |
| 1:L:69:MET:HE1 | 1:L:522:THR:HB | 1.73 | 0.69 |
| 1:A:404:ARG:HG3 | 1:A:404:ARG:HH11 | 1.58 | 0.69 |
| 1:B:134:LEU:O | 1:B:136:VAL:HG13 | 1.93 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:233:MET:CA | 1:B:310:GLU:HG3 | 2.18 | 0.69 |
| 1:D:278:ALA:HB1 | 1:D:279:PRO:CD | 2.22 | 0.69 |
| 1:K:434:GLU:HA | 1:K:437:ASN:ND2 | 2.08 | 0.69 |
| 1:B:219:PHE:HB2 | 1:B:247:LEU:CD2 | 2.22 | 0.69 |
| 1:C:169:VAL:HB | 1:C:173:GLY:HA3 | 1.75 | 0.69 |
| 1:D:135:SER:HB2 | 1:D:497:THR:HG21 | 1.74 | 0.69 |
| 1:F:259:LEU:O | 1:F:263:VAL:HG23 | 1.92 | 0.69 |
| 1:F:291:ASP:HB3 | 1:F:345:ARG:HH21 | 1.57 | 0.69 |
| 1:J:116:LEU:HD23 | 1:J:435:ASP:O | 1.92 | 0.69 |
| 1:K:270:ILE:HG23 | 1:L:229:ASN:ND2 | 2.08 | 0.69 |
| 1:L:403:THR:O | 1:L:407:VAL:HG23 | 1.93 | 0.69 |
| 1:N:301:ILE:HD12 | 1:N:301:ILE:N | 2.08 | 0.69 |
| 1:N:34:LYS:HB2 | 1:N:458:CYS:SG | 2.33 | 0.69 |
| 2:P:7:HIS:O | 2:P:8:ASP:HB3 | 1.93 | 0.69 |
| 1:A:248:LEU:HD13 | 1:A:249:ILE:N | 2.08 | 0.69 |
| 1:C:242:LYS:C | 1:C:242:LYS:HD3 | 2.13 | 0.69 |
| 1:D:325:ILE:N | 1:D:325:ILE:HD12 | 2.08 | 0.69 |
| 1:F:234:LEU:N | 1:F:235:PRO:HD2 | 2.07 | 0.69 |
| 1:F:266:THR:HG22 | 1:F:271:VAL:O | 1.92 | 0.69 |
| 1:H:175:ILE:HD12 | 1:H:175:ILE:N | 2.08 | 0.69 |
| 1:J:32:GLY:HA2 | 1:J:454:ILE:HD12 | 1.75 | 0.69 |
| 1:K:345:ARG:HA | 1:K:348:GLN:NE2 | 2.07 | 0.69 |
| 1:K:417:VAL:HG21 | 1:K:488:MET:HG3 | 1.75 | 0.69 |
| 1:N:96:ALA:O | 1:N:100:ILE:HG13 | 1.93 | 0.69 |
| 1:A:239:ALA:O | 1:A:242:LYS:HB3 | 1.93 | 0.69 |
| 1:A:256:GLY:HA2 | 1:A:259:LEU:HB2 | 1.75 | 0.69 |
| 1:A:296:THR:HG22 | 1:A:335:GLY:HA3 | 1.74 | 0.69 |
| 1:B:124:VAL:HG13 | 1:B:504:LEU:CD1 | 2.23 | 0.69 |
| 1:E:259:LEU:O | 1:E:262:LEU:HB3 | 1.93 | 0.69 |
| 1:F:305:ILE:HG22 | 1:F:306:GLY:N | 2.08 | 0.69 |
| 1:G:20:VAL:HG13 | 1:G:74:VAL:HG11 | 1.74 | 0.69 |
| 1:J:455:VAL:HG13 | 1:J:460:GLU:HB2 | 1.75 | 0.69 |
| 2:S:20:LYS:HD2 | 2:S:20:LYS:N | 2.07 | 0.69 |
| 1:B:228:SER:O | 1:B:257:GLU:HB3 | 1.93 | 0.68 |
| 1:D:194:GLN:HG2 | 1:D:195:PHE:N | 2.07 | 0.68 |
| 1:D:264:VAL:HA | 1:D:267:MET:HB2 | 1.74 | 0.68 |
| 1:D:5:ASP:HB2 | 1:D:524:LEU:HD23 | 1.75 | 0.68 |
| 1:G:290:GLN:N | 1:G:290:GLN:OE1 | 2.26 | 0.68 |
| 1:H:221:LEU:HD13 | 1:H:222:LEU:N | 2.07 | 0.68 |
| 1:H:345:ARG:HA | 1:H:348:GLN:HE21 | 1.58 | 0.68 |
| 1:I:32:GLY:HA3 | 1:I:454:ILE:HG23 | 1.76 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:66:PHE:H | 1:I:69:MET:HG3 | 1.57 | 0.68 |
| 1:C:82:ASN:HD22 | 1:C:86:GLY:HA2 | 1.58 | 0.68 |
| 1:D:234:LEU:N | 1:D:235:PRO:HD2 | 2.07 | 0.68 |
| 1:D:257:GLU:O | 1:D:261:THR:HG22 | 1.94 | 0.68 |
| 1:D:199:TYR:CE1 | 1:D:327:LYS:HG3 | 2.28 | 0.68 |
| 1:H:415:GLY:H | 1:H:417:VAL:HG23 | 1.56 | 0.68 |
| 1:H:66:PHE:H | 1:H:69:MET:HG3 | 1.58 | 0.68 |
| 1:K:362:ARG:O | 1:K:366:GLN:HB2 | 1.93 | 0.68 |
| 1:M:149:THR:CG2 | 1:M:156:GLU:HA | 2.22 | 0.68 |
| 1:A:218:PRO:CA | 1:A:246:PRO:HG2 | 2.23 | 0.68 |
| 1:A:247:LEU:HD12 | 1:A:249:ILE:CD1 | 2.23 | 0.68 |
| 1:A:325:ILE:N | 1:A:325:ILE:HD12 | 2.09 | 0.68 |
| 1:G:404:ARG:HG3 | 1:G:404:ARG:HH11 | 1.58 | 0.68 |
| 1:H:82:ASN:HB2 | 1:H:89:THR:OG1 | 1.92 | 0.68 |
| 1:I:248:LEU:HD13 | 1:I:249:ILE:N | 2.09 | 0.68 |
| 1:K:270:ILE:HG23 | 1:L:229:ASN:HD21 | 1.58 | 0.68 |
| 1:L:254:VAL:HG12 | 1:L:259:LEU:HB2 | 1.74 | 0.68 |
| 1:L:82:ASN:HB2 | 1:L:89:THR:OG1 | 1.92 | 0.68 |
| 2:R:7:HIS:O | 2:R:8:ASP:HB3 | 1.93 | 0.68 |
| 1:B:365:LEU:HD22 | 1:B:366:GLN:NE2 | 2.08 | 0.68 |
| 1:D:18:ARG:HH11 | 1:D:18:ARG:CB | 2.01 | 0.68 |
| 1:D:256:GLY:HA2 | 1:D:259:LEU:HB2 | 1.76 | 0.68 |
| 1:E:249:ILE:HB | 1:E:275:ALA:CB | 2.24 | 0.68 |
| 1:F:325:ILE:HD12 | 1:F:325:ILE:N | 2.09 | 0.68 |
| 1:F:5:ASP:HB2 | 1:F:524:LEU:HD23 | 1.75 | 0.68 |
| 1:K:82:ASN:HB2 | 1:K:89:THR:OG1 | 1.93 | 0.68 |
| 1:M:365:LEU:O | 1:M:369:VAL:HG23 | 1.93 | 0.68 |
| 1:N:455:VAL:HG13 | 1:N:460:GLU:HB2 | 1.76 | 0.68 |
| 1:A:248:LEU:C | 1:A:249:ILE:HD12 | 2.13 | 0.68 |
| 1:B:123:ALA:HB2 | 1:B:440:ILE:HG23 | 1.74 | 0.68 |
| 1:J:247:LEU:H | 1:J:273:VAL:HG12 | 1.58 | 0.68 |
| 1:L:111:MET:HG2 | 1:L:435:ASP:OD1 | 1.93 | 0.68 |
| 1:M:225:LYS:HE2 | 1:M:309:LEU:HD11 | 1.76 | 0.68 |
| 2:T:20:LYS:HD2 | 2:T:20:LYS:N | 2.07 | 0.68 |
| 1:A:302:SER:HB2 | 1:A:305:ILE:HD13 | 1.75 | 0.68 |
| 1:C:219:PHE:HB3 | 1:C:317:LEU:HD13 | 1.75 | 0.68 |
| 1:D:220:ILE:HD12 | 1:D:220:ILE:N | 2.08 | 0.68 |
| 1:F:233:MET:CA | 1:F:310:GLU:HG3 | 2.18 | 0.68 |
| 1:A:456:LEU:HD13 | 1:A:462:PRO:CG | 2.24 | 0.68 |
| 1:F:241:ALA:HA | 1:F:271:VAL:HG12 | 1.74 | 0.68 |
| 1:G:278:ALA:HB1 | 1:G:279:PRO:CD | 2.24 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:115:ASP:HB3 | 1:I:436:GLN:HG2 | 1.73 | 0.68 |
| 1:C:417:VAL:O | 1:C:420:ILE:HG22 | 1.94 | 0.68 |
| 1:C:44:PHE:HD1 | 1:C:44:PHE:H | 1.35 | 0.68 |
| 1:D:310:GLU:O | 1:D:312:ALA:N | 2.26 | 0.68 |
| 1:E:247:LEU:HD12 | 1:E:249:ILE:HD11 | 1.76 | 0.68 |
| 1:E:342:ILE:O | 1:E:346:VAL:HG23 | 1.92 | 0.68 |
| 1:F:222:LEU:N | 1:F:222:LEU:HD12 | 2.08 | 0.68 |
| 1:G:273:VAL:CG1 | 1:G:274:ALA:H | 2.05 | 0.68 |
| 1:H:404:ARG:O | 1:H:408:GLU:HG3 | 1.94 | 0.68 |
| 2:Q:68:ASN:ND2 | 2:R:74:LYS:HE3 | 2.09 | 0.68 |
| 2:U:34:LYS:HG3 | 2:U:35:SER:H | 1.58 | 0.68 |
| 1:A:177:VAL:HG11 | 1:A:397:GLU:HG2 | 1.75 | 0.68 |
| 1:G:247:LEU:HD12 | 1:G:249:ILE:CD1 | 2.24 | 0.68 |
| 1:K:199:TYR:HA | 1:K:276:VAL:HG12 | 1.76 | 0.68 |
| 1:L:149:THR:CG2 | 1:L:156:GLU:HA | 2.24 | 0.68 |
| 1:L:301:ILE:HD12 | 1:L:301:ILE:N | 2.09 | 0.68 |
| 1:N:326:ASN:OD1 | 1:N:329:THR:HB | 1.94 | 0.68 |
| 1:N:434:GLU:HA | 1:N:437:ASN:HD22 | 1.58 | 0.68 |
| 2:Q:37:ARG:HH11 | 2:Q:37:ARG:HG2 | 1.59 | 0.68 |
| 2:U:17:VAL:HG13 | 2:U:34:LYS:HA | 1.76 | 0.68 |
| 1:A:259:LEU:O | 1:A:262:LEU:HB3 | 1.94 | 0.68 |
| 1:B:146:GLN:NE2 | 1:B:494:LEU:HD11 | 2.08 | 0.68 |
| 1:D:404:ARG:HG3 | 1:D:404:ARG:HH11 | 1.59 | 0.68 |
| 1:E:195:PHE:O | 1:E:329:THR:HG23 | 1.95 | 0.68 |
| 1:E:27:VAL:HG12 | 1:E:90:THR:HG23 | 1.76 | 0.68 |
| 1:G:219:PHE:HB2 | 1:G:247:LEU:HD22 | 1.76 | 0.68 |
| 1:G:325:ILE:HD12 | 1:G:325:ILE:N | 2.08 | 0.68 |
| 1:G:475:ASN:HD22 | 1:G:475:ASN:N | 1.91 | 0.68 |
| 1:H:381:VAL:HB | 1:H:389:MET:HE3 | 1.76 | 0.68 |
| 1:I:398:ASP:O | 1:I:401:HIS:HB2 | 1.93 | 0.68 |
| 1:I:417:VAL:HG21 | 1:I:488:MET:HG3 | 1.75 | 0.68 |
| 1:J:200:LEU:HD13 | 1:J:276:VAL:HA | 1.76 | 0.68 |
| 1:J:298:GLY:HA2 | 1:J:317:LEU:O | 1.93 | 0.68 |
| 1:L:200:LEU:HD13 | 1:L:276:VAL:HA | 1.76 | 0.68 |
| 1:M:455:VAL:HG13 | 1:M:460:GLU:HB2 | 1.76 | 0.68 |
| 1:N:247:LEU:H | 1:N:273:VAL:HG12 | 1.59 | 0.68 |
| 1:N:5:ASP:HB2 | 1:N:524:LEU:HD23 | 1.76 | 0.68 |
| 2:U:37:ARG:HG2 | 2:U:37:ARG:HH11 | 1.58 | 0.68 |
| 1:A:194:GLN:HG2 | 1:A:195:PHE:N | 2.09 | 0.67 |
| 1:A:224:ASP:HB2 | 1:A:303:GLU:HB3 | 1.76 | 0.67 |
| 1:C:234:LEU:CD1 | 1:C:234:LEU:H | 2.06 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:339:GLU:HA | 1:E:342:ILE:HB | 1.76 | 0.67 |
| 1:G:219:PHE:HD1 | 1:G:319:GLN:HE21 | 1.42 | 0.67 |
| 1:G:277:LYS:HD3 | 1:G:285:ARG:HH22 | 1.56 | 0.67 |
| 1:G:194:GLN:HG3 | 1:G:330:THR:O | 1.94 | 0.67 |
| 1:H:157:THR:O | 1:H:160:LYS:HB3 | 1.93 | 0.67 |
| 1:H:413:ALA:HB1 | 1:H:417:VAL:HB | 1.76 | 0.67 |
| 1:D:256:GLY:O | 1:D:260:ALA:N | 2.26 | 0.67 |
| 1:D:82:ASN:ND2 | 1:D:86:GLY:HA2 | 2.09 | 0.67 |
| 1:E:202:PRO:O | 1:E:205:ILE:HG13 | 1.94 | 0.67 |
| 1:F:349:ILE:HA | 1:F:352:GLN:NE2 | 2.08 | 0.67 |
| 1:G:411:VAL:HA | 1:G:497:THR:H | 1.60 | 0.67 |
| 1:H:267:MET:HG3 | 1:H:267:MET:O | 1.93 | 0.67 |
| 1:I:175:ILE:N | 1:I:175:ILE:HD12 | 2.10 | 0.67 |
| 1:J:157:THR:O | 1:J:160:LYS:HB3 | 1.94 | 0.67 |
| 1:L:219:PHE:CE1 | 1:L:245:LYS:HD2 | 2.29 | 0.67 |
| 1:M:229:ASN:ND2 | 1:M:231:ARG:HH12 | 1.92 | 0.67 |
| 2:O:49:LEU:O | 2:O:55:LYS:NZ | 2.27 | 0.67 |
| 1:B:264:VAL:HA | 1:B:267:MET:HB2 | 1.75 | 0.67 |
| 1:B:349:ILE:O | 1:B:353:ILE:HG13 | 1.94 | 0.67 |
| 1:C:273:VAL:CG1 | 1:C:274:ALA:H | 2.07 | 0.67 |
| 1:D:281:PHE:O | 1:D:285:ARG:HG2 | 1.94 | 0.67 |
| 1:D:322:ARG:HG2 | 1:D:323:VAL:N | 2.10 | 0.67 |
| 1:E:247:LEU:HD12 | 1:E:249:ILE:CD1 | 2.25 | 0.67 |
| 1:E:309:LEU:HD12 | 1:E:309:LEU:H | 1.58 | 0.67 |
| 1:F:339:GLU:HB3 | 1:F:343:GLN:OE1 | 1.93 | 0.67 |
| 1:I:494:LEU:HD23 | 1:I:494:LEU:N | 2.10 | 0.67 |
| 1:J:143:ALA:O | 1:J:146:GLN:HB3 | 1.94 | 0.67 |
| 1:J:206:ASN:ND2 | 1:J:207:LYS:HE2 | 2.09 | 0.67 |
| 1:J:270:ILE:HG22 | 1:J:271:VAL:N | 2.09 | 0.67 |
| 1:L:499:VAL:HG23 | 1:L:500:THR:N | 2.10 | 0.67 |
| 1:M:82:ASN:HB2 | 1:M:89:THR:OG1 | 1.95 | 0.67 |
| 2:O:40:VAL:HB | 2:O:62:GLY:N | 2.10 | 0.67 |
| 2:Q:92:LEU:O | 2:R:6:LEU:HB2 | 1.94 | 0.67 |
| 1:B:169:VAL:HB | 1:B:173:GLY:HA3 | 1.75 | 0.67 |
| 1:C:239:ALA:HB1 | 1:C:314:LEU:HD23 | 1.76 | 0.67 |
| 1:C:70:GLY:O | 1:C:74:VAL:HG22 | 1.95 | 0.67 |
| 1:D:432:GLN:NE2 | 1:D:436:GLN:HE22 | 1.92 | 0.67 |
| 1:G:249:ILE:HB | 1:G:275:ALA:CB | 2.24 | 0.67 |
| 1:J:359:ASP:HA | 1:J:362:ARG:HH12 | 1.57 | 0.67 |
| 1:L:96:ALA:O | 1:L:100:ILE:HG13 | 1.94 | 0.67 |
| 1:N:175:ILE:HD12 | 1:N:175:ILE:N | 2.09 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:226:LYS:HD2 | 1:N:252:GLU:HG3 | 1.75 | 0.67 |
| 2:U:77:LYS:C | 2:U:78:ILE:HD12 | 2.14 | 0.67 |
| 1:C:248:LEU:C | 1:C:249:ILE:HD12 | 2.15 | 0.67 |
| 1:D:414:GLY:HA2 | 1:D:495:ASP:OD2 | 1.95 | 0.67 |
| 1:F:321:LYS:HD2 | 1:F:333:ILE:HG22 | 1.76 | 0.67 |
| 1:H:34:LYS:HB2 | 1:H:458:CYS:SG | 2.35 | 0.67 |
| 1:J:221:LEU:C | 1:J:221:LEU:HD13 | 2.14 | 0.67 |
| 1:J:422:VAL:O | 1:J:426:LEU:HD23 | 1.95 | 0.67 |
| 1:K:487:ASN:HB3 | 1:K:490:ASP:HB2 | 1.77 | 0.67 |
| 2:O:17:VAL:HG13 | 2:O:34:LYS:HA | 1.76 | 0.67 |
| 1:C:247:LEU:O | 1:C:273:VAL:HG13 | 1.94 | 0.67 |
| 1:C:224:ASP:HB2 | 1:C:303:GLU:HB3 | 1.75 | 0.67 |
| 1:E:288:MET:HA | 1:E:291:ASP:OD2 | 1.94 | 0.67 |
| 1:F:123:ALA:HB2 | 1:F:440:ILE:HG23 | 1.76 | 0.67 |
| 1:F:208:PRO:HB2 | 1:F:212:ALA:HB3 | 1.76 | 0.67 |
| 1:G:456:LEU:HD13 | 1:G:462:PRO:CG | 2.25 | 0.67 |
| 1:K:365:LEU:O | 1:K:369:VAL:HG23 | 1.95 | 0.67 |
| 1:K:66:PHE:H | 1:K:69:MET:HG3 | 1.60 | 0.67 |
| 1:N:247:LEU:HD13 | 1:N:247:LEU:C | 2.15 | 0.67 |
| 1:N:417:VAL:HG21 | 1:N:488:MET:HG3 | 1.77 | 0.67 |
| 1:E:350:ARG:O | 1:E:354:GLU:HG2 | 1.95 | 0.67 |
| 1:A:228:SER:O | 1:A:257:GLU:HB3 | 1.94 | 0.67 |
| 1:C:350:ARG:O | 1:C:354:GLU:HG2 | 1.94 | 0.67 |
| 1:E:239:ALA:O | 1:E:242:LYS:HB3 | 1.94 | 0.67 |
| 1:J:326:ASN:OD1 | 1:J:329:THR:HB | 1.94 | 0.67 |
| 1:J:415:GLY:N | 1:J:417:VAL:HG23 | 2.09 | 0.67 |
| 1:K:198:GLY:CA | 1:K:328:ASP:HA | 2.25 | 0.67 |
| 1:K:233:MET:HA | 1:K:233:MET:HE2 | 1.76 | 0.67 |
| 1:M:339:GLU:O | 1:M:343:GLN:HG2 | 1.95 | 0.67 |
| 1:M:465:VAL:O | 1:M:469:VAL:HG23 | 1.94 | 0.67 |
| 2:R:65:VAL:HG12 | 2:R:94:ILE:HG12 | 1.76 | 0.67 |
| 2:U:14:ARG:HG2 | 2:U:15:LYS:N | 2.10 | 0.67 |
| 1:A:220:ILE:HG23 | 1:A:248:LEU:HD12 | 1.77 | 0.67 |
| 1:E:325:ILE:HG13 | 1:E:330:THR:HG23 | 1.76 | 0.67 |
| 1:F:456:LEU:HD13 | 1:F:462:PRO:CG | 2.24 | 0.67 |
| 1:G:247:LEU:O | 1:G:273:VAL:HG13 | 1.95 | 0.67 |
| 1:I:107:VAL:HG23 | 1:I:108:ALA:N | 2.10 | 0.67 |
| 1:K:111:MET:HG2 | 1:K:435:ASP:OD1 | 1.94 | 0.67 |
| 1:L:404:ARG:O | 1:L:408:GLU:HG3 | 1.92 | 0.67 |
| 2:O:47:ARG:O | 2:O:55:LYS:HE3 | 1.94 | 0.67 |
| 2:P:14:ARG:HG2 | 2:P:15:LYS:N | 2.09 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:14:ARG:HG2 | 2:T:15:LYS:N | 2.10 | 0.67 |
| 1:B:214:GLU:HA | 1:B:323:VAL:O | 1.95 | 0.67 |
| 1:B:227:ILE:HD12 | 1:B:227:ILE:N | 2.10 | 0.67 |
| 1:B:288:MET:HA | 1:B:291:ASP:OD2 | 1.94 | 0.67 |
| 1:C:219:PHE:HB2 | 1:C:247:LEU:HD22 | 1.76 | 0.67 |
| 1:C:247:LEU:HD12 | 1:C:249:ILE:HD11 | 1.76 | 0.67 |
| 1:E:291:ASP:HB2 | 1:E:372:LEU:HD21 | 1.77 | 0.67 |
| 1:E:325:ILE:N | 1:E:325:ILE:HD12 | 2.09 | 0.67 |
| 1:F:227:ILE:N | 1:F:227:ILE:HD12 | 2.10 | 0.67 |
| 1:H:219:PHE:HE1 | 1:H:245:LYS:HB2 | 1.58 | 0.67 |
| 1:J:270:ILE:HG23 | 1:K:229:ASN:ND2 | 2.09 | 0.67 |
| 1:K:249:ILE:HB | 1:K:275:ALA:HB1 | 1.77 | 0.67 |
| 1:K:353:ILE:HD11 | 1:K:369:VAL:HG21 | 1.75 | 0.67 |
| 1:A:362:ARG:HA | 1:A:365:LEU:HD13 | 1.77 | 0.66 |
| 1:E:472:GLY:HA3 | 1:E:476:TYR:CD2 | 2.29 | 0.66 |
| 1:F:248:LEU:HD13 | 1:F:249:ILE:N | 2.10 | 0.66 |
| 1:K:107:VAL:HG23 | 1:K:108:ALA:N | 2.09 | 0.66 |
| 1:L:72:GLN:NE2 | 1:L:72:GLN:HA | 2.10 | 0.66 |
| 1:M:205:ILE:HD13 | 1:M:211:GLY:HA2 | 1.76 | 0.66 |
| 1:M:218:PRO:HB3 | 1:M:246:PRO:C | 2.15 | 0.66 |
| 2:R:96:GLU:OE1 | 2:S:4:ARG:HB2 | 1.96 | 0.66 |
| 1:B:326:ASN:ND2 | 1:B:328:ASP:H | 1.92 | 0.66 |
| 1:E:220:ILE:N | 1:E:220:ILE:HD12 | 2.10 | 0.66 |
| 1:F:349:ILE:HG21 | 1:F:369:VAL:HG22 | 1.77 | 0.66 |
| 1:F:124:VAL:HG13 | 1:F:504:LEU:HD12 | 1.77 | 0.66 |
| 1:I:213:VAL:O | 1:I:324:VAL:HA | 1.95 | 0.66 |
| 1:K:213:VAL:O | 1:K:324:VAL:HA | 1.96 | 0.66 |
| 2:U:17:VAL:HG21 | 2:U:34:LYS:HD2 | 1.77 | 0.66 |
| 1:B:247:LEU:HD13 | 1:B:248:LEU:N | 2.10 | 0.66 |
| 1:C:234:LEU:HD12 | 1:C:234:LEU:N | 2.09 | 0.66 |
| 1:C:215:LEU:HB3 | 1:C:246:PRO:HB2 | 1.76 | 0.66 |
| 1:I:266:THR:HB | 1:I:272:LYS:HG3 | 1.77 | 0.66 |
| 1:I:356:ALA:HB1 | 1:I:362:ARG:HE | 1.60 | 0.66 |
| 1:I:385:THR:HG23 | 1:I:388:GLU:H | 1.58 | 0.66 |
| 1:J:247:LEU:C | 1:J:247:LEU:HD13 | 2.15 | 0.66 |
| 1:L:191:GLU:O | 1:L:334:ASP:HA | 1.96 | 0.66 |
| 1:L:313:THR:HG22 | 1:L:314:LEU:N | 2.10 | 0.66 |
| 1:M:434:GLU:HA | 1:M:437:ASN:HD22 | 1.57 | 0.66 |
| 1:H:229:ASN:ND2 | 1:N:270:ILE:HG23 | 2.09 | 0.66 |
| 2:Q:17:VAL:CG2 | 2:Q:34:LYS:HD2 | 2.26 | 0.66 |
| 1:A:461:GLU:HB2 | 1:A:464:VAL:HB | 1.78 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:284:ARG:HG2 | 1:F:288:MET:HE2 | 1.76 | 0.66 |
| 1:F:302:SER:HB2 | 1:F:305:ILE:HB | 1.78 | 0.66 |
| 1:F:302:SER:HB2 | 1:F:305:ILE:HD13 | 1.76 | 0.66 |
| 1:G:234:LEU:CD1 | 1:G:234:LEU:H | 2.09 | 0.66 |
| 1:K:314:LEU:H | 1:K:314:LEU:CD1 | 2.02 | 0.66 |
| 1:M:161:LEU:HD12 | 1:M:161:LEU:H | 1.60 | 0.66 |
| 1:A:146:GLN:NE2 | 1:A:494:LEU:HD11 | 2.10 | 0.66 |
| 1:C:194:GLN:HG2 | 1:C:195:PHE:N | 2.09 | 0.66 |
| 1:C:20:VAL:HG13 | 1:C:74:VAL:HG11 | 1.78 | 0.66 |
| 1:F:247:LEU:HB3 | 1:F:273:VAL:HG13 | 1.77 | 0.66 |
| 1:H:247:LEU:HD22 | 1:H:248:LEU:N | 2.10 | 0.66 |
| 1:H:226:LYS:HA | 1:H:252:GLU:HB2 | 1.76 | 0.66 |
| 1:I:219:PHE:HB2 | 1:I:247:LEU:HD23 | 1.78 | 0.66 |
| 1:I:249:ILE:HB | 1:I:275:ALA:HB1 | 1.77 | 0.66 |
| 1:K:270:ILE:HG22 | 1:K:271:VAL:N | 2.11 | 0.66 |
| 1:L:494:LEU:H | 1:L:494:LEU:HD23 | 1.60 | 0.66 |
| 1:D:233:MET:CE | 1:D:237:LEU:HB2 | 2.25 | 0.66 |
| 1:F:228:SER:HA | 1:F:255:GLU:CB | 2.18 | 0.66 |
| 1:L:415:GLY:N | 1:L:417:VAL:HG23 | 2.09 | 0.66 |
| 2:P:20:LYS:HG2 | 2:P:27:LEU:HD23 | 1.77 | 0.66 |
| 2:Q:84:LEU:N | 2:Q:84:LEU:HD12 | 2.10 | 0.66 |
| 2:T:37:ARG:HH11 | 2:T:37:ARG:HG2 | 1.61 | 0.66 |
| 1:A:349:ILE:HG21 | 1:A:369:VAL:HG22 | 1.76 | 0.66 |
| 1:E:253:ASP:CG | 1:E:254:VAL:H | 1.99 | 0.66 |
| 1:E:302:SER:HB2 | 1:E:305:ILE:HB | 1.78 | 0.66 |
| 1:F:131:LEU:HD21 | 1:F:422:VAL:HG11 | 1.76 | 0.66 |
| 1:G:18:ARG:CB | 1:G:18:ARG:HH11 | 2.02 | 0.66 |
| 1:G:220:ILE:HD12 | 1:G:220:ILE:N | 2.09 | 0.66 |
| 1:H:270:ILE:HG23 | 1:I:229:ASN:HD21 | 1.61 | 0.66 |
| 1:J:249:ILE:HB | 1:J:275:ALA:HB1 | 1.77 | 0.66 |
| 1:M:356:ALA:CB | 1:M:362:ARG:HE | 2.07 | 0.66 |
| 2:O:20:LYS:HG2 | 2:O:27:LEU:CD2 | 2.26 | 0.66 |
| 2:R:84:LEU:N | 2:R:84:LEU:HD12 | 2.11 | 0.66 |
| 1:B:206:ASN:CB | 1:B:214:GLU:H | 2.09 | 0.66 |
| 1:F:381:VAL:HG21 | 1:F:393:LYS:HA | 1.77 | 0.66 |
| 1:G:246:PRO:HA | 1:G:272:LYS:O | 1.95 | 0.66 |
| 1:I:124:VAL:O | 1:I:128:VAL:HG23 | 1.94 | 0.66 |
| 1:J:324:VAL:C | 1:J:325:ILE:HD12 | 2.16 | 0.66 |
| 1:N:155:ASP:OD1 | 1:N:158:VAL:HG23 | 1.95 | 0.66 |
| 1:N:160:LYS:HG2 | 1:N:164:GLU:OE2 | 1.95 | 0.66 |
| 1:N:345:ARG:HA | 1:N:348:GLN:HE21 | 1.60 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:29:VAL:HG23 | 1:A:30:THR:HG23 | 1.78 | 0.66 |
| 1:A:44:PHE:H | 1:A:44:PHE:HD1 | 1.40 | 0.66 |
| 1:F:253:ASP:CG | 1:F:254:VAL:H | 1.99 | 0.66 |
| 1:F:29:VAL:HG23 | 1:F:30:THR:HG23 | 1.78 | 0.66 |
| 1:G:10:ASN:O | 1:G:14:VAL:HG23 | 1.96 | 0.66 |
| 1:K:247:LEU:H | 1:K:273:VAL:HG12 | 1.61 | 0.66 |
| 1:L:256:GLY:CA | 1:L:259:LEU:HB3 | 2.25 | 0.66 |
| 1:M:249:ILE:HB | 1:M:275:ALA:HB1 | 1.76 | 0.66 |
| 2:T:48:ILE:HG23 | 2:T:54:VAL:HG22 | 1.78 | 0.66 |
| 1:B:355:GLU:O | 1:B:362:ARG:NH2 | 2.28 | 0.66 |
| 1:D:70:GLY:O | 1:D:74:VAL:HG22 | 1.96 | 0.66 |
| 1:E:219:PHE:HB2 | 1:E:247:LEU:CD2 | 2.25 | 0.66 |
| 1:G:124:VAL:HG13 | 1:G:504:LEU:CD1 | 2.26 | 0.66 |
| 1:G:169:VAL:HB | 1:G:173:GLY:HA3 | 1.78 | 0.66 |
| 1:H:199:TYR:HA | 1:H:276:VAL:HG12 | 1.77 | 0.66 |
| 1:I:143:ALA:O | 1:I:147:VAL:HG12 | 1.96 | 0.66 |
| 1:J:25:ASP:HA | 1:J:28:LYS:HE2 | 1.78 | 0.66 |
| 1:L:161:LEU:CD1 | 1:L:161:LEU:H | 2.08 | 0.66 |
| 1:L:449:ALA:HB3 | 1:L:450:PRO:HD3 | 1.78 | 0.66 |
| 1:M:301:ILE:HG21 | 1:M:309:LEU:HD23 | 1.77 | 0.66 |
| 1:A:27:VAL:HG12 | 1:A:90:THR:HG23 | 1.78 | 0.65 |
| 1:D:360:TYR:O | 1:D:364:LYS:HE2 | 1.96 | 0.65 |
| 1:E:249:ILE:N | 1:E:249:ILE:HD12 | 2.10 | 0.65 |
| 1:E:214:GLU:CB | 1:E:322:ARG:HD3 | 2.23 | 0.65 |
| 1:F:222:LEU:HD22 | 1:F:293:ALA:HB2 | 1.76 | 0.65 |
| 1:L:413:ALA:CB | 1:L:417:VAL:HB | 2.26 | 0.65 |
| 1:N:301:ILE:HG21 | 1:N:309:LEU:HD23 | 1.78 | 0.65 |
| 1:D:223:ALA:HB3 | 1:D:251:ALA:HB2 | 1.78 | 0.65 |
| 1:E:146:GLN:NE2 | 1:E:494:LEU:HD11 | 2.10 | 0.65 |
| 1:F:218:PRO:CA | 1:F:246:PRO:HG2 | 2.26 | 0.65 |
| 1:F:499:VAL:HG23 | 1:F:500:THR:N | 2.10 | 0.65 |
| 1:F:35:GLY:HA3 | 1:F:51:LYS:HE2 | 1.78 | 0.65 |
| 1:G:206:ASN:CB | 1:G:214:GLU:H | 2.09 | 0.65 |
| 1:G:82:ASN:ND2 | 1:G:86:GLY:HA2 | 2.11 | 0.65 |
| 1:J:122:LYS:HE2 | 1:J:429:LEU:HD11 | 1.77 | 0.65 |
| 1:K:221:LEU:C | 1:K:221:LEU:HD13 | 2.16 | 0.65 |
| 1:K:385:THR:HG23 | 1:K:388:GLU:H | 1.62 | 0.65 |
| 1:K:494:LEU:HD23 | 1:K:494:LEU:N | 2.11 | 0.65 |
| 1:N:115:ASP:HB3 | 1:N:436:GLN:HG2 | 1.77 | 0.65 |
| 1:N:499:VAL:HG23 | 1:N:500:THR:N | 2.10 | 0.65 |
| 2:O:68:ASN:ND2 | 2:P:74:LYS:HE3 | 2.12 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:353:ILE:HG12 | 1:B:366:GLN:NE2 | 2.12 | 0.65 |
| 1:D:124:VAL:HG22 | 1:D:504:LEU:HD11 | 1.76 | 0.65 |
| 1:F:239:ALA:O | 1:F:242:LYS:HB3 | 1.96 | 0.65 |
| 1:K:191:GLU:OE1 | 1:K:342:ILE:HG21 | 1.95 | 0.65 |
| 1:L:247:LEU:HD13 | 1:L:247:LEU:C | 2.16 | 0.65 |
| 1:L:417:VAL:HG21 | 1:L:488:MET:HG3 | 1.79 | 0.65 |
| 1:M:123:ALA:HB2 | 1:M:440:ILE:HG23 | 1.78 | 0.65 |
| 1:N:494:LEU:HD23 | 1:N:494:LEU:H | 1.60 | 0.65 |
| 2:P:20:LYS:HG2 | 2:P:27:LEU:CD2 | 2.26 | 0.65 |
| 2:R:14:ARG:CD | 2:R:35:SER:HB3 | 2.25 | 0.65 |
| 1:B:257:GLU:O | 1:B:261:THR:HG22 | 1.97 | 0.65 |
| 1:B:472:GLY:HA3 | 1:B:476:TYR:CD2 | 2.31 | 0.65 |
| 1:C:290:GLN:OE1 | 1:C:290:GLN:N | 2.29 | 0.65 |
| 1:D:10:ASN:O | 1:D:14:VAL:HG23 | 1.97 | 0.65 |
| 1:G:219:PHE:HB2 | 1:G:247:LEU:CD2 | 2.26 | 0.65 |
| 1:H:107:VAL:HG23 | 1:H:108:ALA:N | 2.10 | 0.65 |
| 1:H:249:ILE:HB | 1:H:275:ALA:HB1 | 1.78 | 0.65 |
| 1:H:277:LYS:NZ | 1:H:277:LYS:HB2 | 2.11 | 0.65 |
| 1:K:313:THR:HG22 | 1:K:314:LEU:N | 2.11 | 0.65 |
| 1:L:30:THR:HB | 1:L:51:LYS:O | 1.97 | 0.65 |
| 1:M:417:VAL:HG21 | 1:M:488:MET:HG3 | 1.78 | 0.65 |
| 1:N:23:LEU:O | 1:N:27:VAL:HG12 | 1.96 | 0.65 |
| 1:A:348:GLN:NE2 | 1:A:352:GLN:NE2 | 2.45 | 0.65 |
| 1:B:456:LEU:HD13 | 1:B:462:PRO:CG | 2.27 | 0.65 |
| 1:C:123:ALA:HB2 | 1:C:440:ILE:HG23 | 1.78 | 0.65 |
| 1:F:284:ARG:HG2 | 1:F:288:MET:CE | 2.25 | 0.65 |
| 1:G:205:ILE:CD1 | 1:G:211:GLY:HA2 | 2.25 | 0.65 |
| 1:G:248:LEU:C | 1:G:249:ILE:HD12 | 2.17 | 0.65 |
| 1:H:256:GLY:HA2 | 1:H:260:ALA:H | 1.61 | 0.65 |
| 1:K:398:ASP:O | 1:K:401:HIS:HB2 | 1.96 | 0.65 |
| 1:N:256:GLY:HA2 | 1:N:259:LEU:HB3 | 1.78 | 0.65 |
| 1:A:265:ASN:HB3 | 1:A:271:VAL:HG22 | 1.77 | 0.65 |
| 1:B:247:LEU:HD12 | 1:B:249:ILE:HD11 | 1.79 | 0.65 |
| 1:D:249:ILE:N | 1:D:249:ILE:HD12 | 2.11 | 0.65 |
| 1:D:131:LEU:HD23 | 1:D:422:VAL:HG11 | 1.78 | 0.65 |
| 1:F:193:MET:O | 1:F:331:THR:HG23 | 1.97 | 0.65 |
| 1:G:326:ASN:ND2 | 1:G:328:ASP:H | 1.95 | 0.65 |
| 1:J:115:ASP:HB3 | 1:J:436:GLN:HG2 | 1.77 | 0.65 |
| 1:K:235:PRO:HG3 | 1:K:310:GLU:HA | 1.76 | 0.65 |
| 1:K:308:GLU:HG2 | 1:K:309:LEU:H | 1.62 | 0.65 |
| 1:M:240:VAL:HA | 1:M:243:ALA:HB3 | 1.77 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:205:ILE:HD13 | 1:N:211:GLY:HA2 | 1.78 | 0.65 |
| 1:A:302:SER:HB2 | 1:A:305:ILE:HB | 1.77 | 0.65 |
| 1:A:499:VAL:HG23 | 1:A:500:THR:N | 2.11 | 0.65 |
| 1:C:321:LYS:HD2 | 1:C:333:ILE:HG22 | 1.78 | 0.65 |
| 1:F:360:TYR:H | 1:F:363:GLU:CD | 2.00 | 0.65 |
| 1:G:313:THR:CG2 | 1:G:315:GLU:HG3 | 2.27 | 0.65 |
| 1:H:155:ASP:OD1 | 1:H:158:VAL:HG23 | 1.97 | 0.65 |
| 1:H:326:ASN:OD1 | 1:H:329:THR:HB | 1.97 | 0.65 |
| 1:I:175:ILE:HD13 | 1:I:404:ARG:NH2 | 2.12 | 0.65 |
| 1:I:282:GLY:O | 1:I:285:ARG:HG2 | 1.97 | 0.65 |
| 1:J:193:MET:HG2 | 1:J:194:GLN:N | 2.11 | 0.65 |
| 1:K:303:GLU:C | 1:K:305:ILE:H | 2.00 | 0.65 |
| 1:K:367:GLU:O | 1:K:370:ALA:HB3 | 1.97 | 0.65 |
| 1:L:325:ILE:HD12 | 1:L:325:ILE:N | 2.11 | 0.65 |
| 1:L:66:PHE:H | 1:L:69:MET:HG3 | 1.62 | 0.65 |
| 1:N:122:LYS:HE2 | 1:N:429:LEU:HD11 | 1.79 | 0.65 |
| 1:N:65:LYS:O | 1:N:66:PHE:CB | 2.38 | 0.65 |
| 2:R:78:ILE:HD13 | 2:R:83:VAL:HG21 | 1.78 | 0.65 |
| 2:S:55:LYS:CE | 2:S:55:LYS:H | 2.09 | 0.65 |
| 2:S:78:ILE:HD13 | 2:S:83:VAL:CG2 | 2.26 | 0.65 |
| 2:T:20:LYS:HD2 | 2:T:20:LYS:H | 1.62 | 0.65 |
| 1:A:135:SER:HB2 | 1:A:497:THR:HG21 | 1.79 | 0.65 |
| 1:D:222:LEU:N | 1:D:222:LEU:HD12 | 2.12 | 0.65 |
| 1:D:350:ARG:HA | 1:D:353:ILE:HD12 | 1.78 | 0.65 |
| 1:D:368:ARG:CD | 1:D:372:LEU:HD11 | 2.27 | 0.65 |
| 1:E:350:ARG:HA | 1:E:353:ILE:HD12 | 1.78 | 0.65 |
| 1:F:229:ASN:C | 1:F:231:ARG:H | 1.96 | 0.65 |
| 1:I:160:LYS:HG2 | 1:I:164:GLU:OE2 | 1.97 | 0.65 |
| 1:J:325:ILE:N | 1:J:325:ILE:HD12 | 2.11 | 0.65 |
| 1:K:115:ASP:HB3 | 1:K:436:GLN:HG2 | 1.79 | 0.65 |
| 1:K:314:LEU:HA | 1:K:317:LEU:HD13 | 1.77 | 0.65 |
| 1:M:217:SER:HA | 1:M:320:ALA:O | 1.96 | 0.65 |
| 1:N:415:GLY:N | 1:N:417:VAL:HG23 | 2.12 | 0.65 |
| 2:P:20:LYS:HG3 | 2:P:28:THR:O | 1.95 | 0.65 |
| 1:B:228:SER:HA | 1:B:255:GLU:CB | 2.17 | 0.65 |
| 1:E:353:ILE:HG12 | 1:E:366:GLN:HE22 | 1.62 | 0.65 |
| 1:E:499:VAL:HG23 | 1:E:500:THR:N | 2.10 | 0.65 |
| 1:E:510:VAL:HG23 | 1:E:511:ALA:N | 2.10 | 0.65 |
| 1:F:242:LYS:C | 1:F:242:LYS:HD3 | 2.16 | 0.65 |
| 1:F:30:THR:HB | 1:F:51:LYS:HG3 | 1.79 | 0.65 |
| 1:F:352:GLN:C | 1:F:365:LEU:HD11 | 2.18 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:510:VAL:HG23 | 1:F:511:ALA:N | 2.12 | 0.65 |
| 1:F:52:ASP:OD1 | 1:F:54:VAL:HG12 | 1.96 | 0.65 |
| 1:G:235:PRO:HG2 | 1:G:236:VAL:H | 1.60 | 0.65 |
| 1:H:226:LYS:HG3 | 1:H:252:GLU:HB3 | 1.78 | 0.65 |
| 1:I:320:ALA:HA | 1:I:334:ASP:O | 1.96 | 0.65 |
| 1:L:263:VAL:O | 1:L:267:MET:HG2 | 1.97 | 0.65 |
| 2:O:40:VAL:HB | 2:O:62:GLY:H | 1.61 | 0.65 |
| 1:A:123:ALA:HB2 | 1:A:440:ILE:HG23 | 1.77 | 0.65 |
| 1:A:338:GLU:O | 1:A:341:ALA:HB3 | 1.97 | 0.65 |
| 1:A:348:GLN:HE22 | 1:A:352:GLN:NE2 | 1.95 | 0.65 |
| 1:B:321:LYS:HD2 | 1:B:333:ILE:HG22 | 1.78 | 0.65 |
| 1:C:247:LEU:HD12 | 1:C:249:ILE:CD1 | 2.27 | 0.65 |
| 1:D:346:VAL:CG1 | 1:D:350:ARG:HH22 | 2.10 | 0.65 |
| 1:D:368:ARG:HG2 | 1:D:372:LEU:HG | 1.79 | 0.65 |
| 1:F:213:VAL:O | 1:F:324:VAL:HA | 1.97 | 0.65 |
| 1:F:219:PHE:HB2 | 1:F:247:LEU:HD22 | 1.77 | 0.65 |
| 1:F:249:ILE:HB | 1:F:275:ALA:HB2 | 1.79 | 0.65 |
| 1:G:279:PRO:HB2 | 1:G:285:ARG:HA | 1.78 | 0.65 |
| 1:I:314:LEU:CD1 | 1:I:314:LEU:H | 2.06 | 0.65 |
| 1:I:359:ASP:CA | 1:I:362:ARG:HH12 | 2.07 | 0.65 |
| 1:I:365:LEU:O | 1:I:369:VAL:HG23 | 1.97 | 0.65 |
| 1:K:325:ILE:N | 1:K:325:ILE:HD12 | 2.12 | 0.65 |
| 1:L:116:LEU:HD23 | 1:L:435:ASP:O | 1.97 | 0.65 |
| 1:N:157:THR:O | 1:N:160:LYS:HB3 | 1.97 | 0.65 |
| 2:O:12:VAL:HG23 | 2:O:84:LEU:HB2 | 1.79 | 0.65 |
| 2:S:12:VAL:HG23 | 2:S:84:LEU:HB2 | 1.78 | 0.65 |
| 2:T:47:ARG:HD2 | 2:T:55:LYS:HD2 | 1.77 | 0.65 |
| 1:B:366:GLN:HA | 1:B:369:VAL:CG2 | 2.27 | 0.64 |
| 1:B:411:VAL:HA | 1:B:497:THR:H | 1.61 | 0.64 |
| 1:C:262:LEU:HD11 | 1:C:273:VAL:HB | 1.79 | 0.64 |
| 1:C:281:PHE:H | 1:C:284:ARG:HD2 | 1.61 | 0.64 |
| 1:F:214:GLU:HA | 1:F:323:VAL:O | 1.96 | 0.64 |
| 1:F:326:ASN:ND2 | 1:F:328:ASP:H | 1.94 | 0.64 |
| 1:G:234:LEU:HD12 | 1:G:234:LEU:N | 2.12 | 0.64 |
| 1:I:254:VAL:HG12 | 1:I:259:LEU:HB2 | 1.79 | 0.64 |
| 1:I:25:ASP:HA | 1:I:28:LYS:HE2 | 1.78 | 0.64 |
| 1:L:214:GLU:HA | 1:L:324:VAL:HG12 | 1.78 | 0.64 |
| 2:S:84:LEU:N | 2:S:84:LEU:HD12 | 2.12 | 0.64 |
| 1:D:18:ARG:HB2 | 1:D:67:GLU:HG2 | 1.80 | 0.64 |
| 1:D:233:MET:HE2 | 1:D:237:LEU:HB2 | 1.79 | 0.64 |
| 1:D:234:LEU:HD12 | 1:D:234:LEU:N | 2.11 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:273:VAL:CG1 | 1:D:274:ALA:H | 2.09 | 0.64 |
| 1:F:346:VAL:CG1 | 1:F:350:ARG:HH22 | 2.09 | 0.64 |
| 1:K:205:ILE:HA | 1:K:213:VAL:HG22 | 1.78 | 0.64 |
| 1:L:351:GLN:HG2 | 1:L:354:GLU:OE2 | 1.97 | 0.64 |
| 1:L:400:LEU:HD23 | 1:L:400:LEU:C | 2.18 | 0.64 |
| 1:M:34:LYS:HB2 | 1:M:458:CYS:SG | 2.37 | 0.64 |
| 1:A:249:ILE:HD12 | 1:A:249:ILE:N | 2.12 | 0.64 |
| 1:G:207:LYS:NZ | 1:G:207:LYS:HB2 | 2.12 | 0.64 |
| 1:H:417:VAL:HG21 | 1:H:488:MET:HG3 | 1.79 | 0.64 |
| 1:I:200:LEU:CD1 | 1:I:276:VAL:HA | 2.27 | 0.64 |
| 1:I:265:ASN:O | 1:I:269:GLY:HA3 | 1.96 | 0.64 |
| 1:I:287:ALA:HB1 | 1:I:368:ARG:CZ | 2.27 | 0.64 |
| 1:I:69:MET:HE1 | 1:I:522:THR:HB | 1.79 | 0.64 |
| 1:M:403:THR:O | 1:M:407:VAL:HG23 | 1.96 | 0.64 |
| 1:B:207:LYS:HB2 | 1:B:207:LYS:NZ | 2.13 | 0.64 |
| 1:B:313:THR:HB | 1:B:315:GLU:OE2 | 1.96 | 0.64 |
| 1:B:472:GLY:HA3 | 1:B:476:TYR:HD2 | 1.63 | 0.64 |
| 1:C:368:ARG:HG2 | 1:C:372:LEU:HG | 1.80 | 0.64 |
| 1:E:310:GLU:O | 1:E:312:ALA:N | 2.30 | 0.64 |
| 1:F:249:ILE:HB | 1:F:275:ALA:CB | 2.28 | 0.64 |
| 1:K:415:GLY:H | 1:K:417:VAL:HG23 | 1.62 | 0.64 |
| 1:L:155:ASP:OD1 | 1:L:158:VAL:HG23 | 1.97 | 0.64 |
| 1:N:123:ALA:HB2 | 1:N:440:ILE:HG23 | 1.80 | 0.64 |
| 2:P:20:LYS:HD2 | 2:P:20:LYS:N | 2.12 | 0.64 |
| 1:A:247:LEU:O | 1:A:273:VAL:HG13 | 1.97 | 0.64 |
| 1:B:248:LEU:C | 1:B:249:ILE:HD12 | 2.18 | 0.64 |
| 1:D:247:LEU:HD12 | 1:D:249:ILE:CD1 | 2.28 | 0.64 |
| 1:F:207:LYS:CB | 1:F:208:PRO:HD3 | 2.27 | 0.64 |
| 1:F:291:ASP:HB3 | 1:F:345:ARG:NH2 | 2.12 | 0.64 |
| 1:F:414:GLY:HA2 | 1:F:495:ASP:OD2 | 1.98 | 0.64 |
| 1:G:123:ALA:HB2 | 1:G:440:ILE:HG23 | 1.80 | 0.64 |
| 1:I:256:GLY:CA | 1:I:259:LEU:HB3 | 2.27 | 0.64 |
| 1:I:403:THR:O | 1:I:407:VAL:HG23 | 1.97 | 0.64 |
| 1:I:135:SER:HA | 1:I:412:VAL:HG12 | 1.79 | 0.64 |
| 1:L:205:ILE:HA | 1:L:213:VAL:HG22 | 1.78 | 0.64 |
| 1:L:422:VAL:O | 1:L:425:LYS:HB2 | 1.97 | 0.64 |
| 1:M:115:ASP:HB3 | 1:M:436:GLN:HG2 | 1.80 | 0.64 |
| 2:O:68:ASN:HD22 | 2:P:74:LYS:HE3 | 1.62 | 0.64 |
| 2:Q:20:LYS:HD2 | 2:Q:20:LYS:N | 2.12 | 0.64 |
| 2:R:20:LYS:HG3 | 2:R:28:THR:O | 1.97 | 0.64 |
| 1:B:160:LYS:HE3 | 1:B:164:GLU:OE2 | 1.97 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:206:ASN:CB | 1:D:214:GLU:H | 2.11 | 0.64 |
| 1:E:219:PHE:HB2 | 1:E:247:LEU:HD22 | 1.77 | 0.64 |
| 1:G:229:ASN:HA | 1:G:257:GLU:OE2 | 1.98 | 0.64 |
| 1:K:385:THR:O | 1:K:389:MET:HB2 | 1.97 | 0.64 |
| 1:N:265:ASN:O | 1:N:269:GLY:HA3 | 1.97 | 0.64 |
| 2:O:78:ILE:HD13 | 2:O:83:VAL:CG2 | 2.26 | 0.64 |
| 2:Q:50:GLU:OE1 | 2:R:50:GLU:HA | 1.98 | 0.64 |
| 1:A:195:PHE:O | 1:A:329:THR:HG23 | 1.98 | 0.64 |
| 1:A:5:ASP:HB2 | 1:A:524:LEU:CD2 | 2.28 | 0.64 |
| 1:B:349:ILE:HG21 | 1:B:369:VAL:HG22 | 1.79 | 0.64 |
| 1:C:368:ARG:O | 1:C:372:LEU:HG | 1.97 | 0.64 |
| 1:D:27:VAL:HG12 | 1:D:90:THR:HG23 | 1.78 | 0.64 |
| 1:E:130:GLU:O | 1:E:134:LEU:HD13 | 1.97 | 0.64 |
| 1:E:18:ARG:HH11 | 1:E:18:ARG:CB | 2.01 | 0.64 |
| 1:E:322:ARG:HG2 | 1:E:323:VAL:N | 2.09 | 0.64 |
| 1:G:130:GLU:O | 1:G:133:ALA:HB3 | 1.98 | 0.64 |
| 1:I:267:MET:O | 1:I:267:MET:HG3 | 1.97 | 0.64 |
| 1:J:111:MET:HG2 | 1:J:435:ASP:OD1 | 1.98 | 0.64 |
| 1:K:175:ILE:N | 1:K:175:ILE:HD12 | 2.12 | 0.64 |
| 1:K:254:VAL:O | 1:K:259:LEU:HD12 | 1.98 | 0.64 |
| 1:K:339:GLU:O | 1:K:343:GLN:HG2 | 1.98 | 0.64 |
| 1:K:351:GLN:HG2 | 1:K:354:GLU:OE2 | 1.98 | 0.64 |
| 2:O:47:ARG:HD3 | 2:O:49:LEU:CD1 | 2.26 | 0.64 |
| 2:U:47:ARG:HD3 | 2:U:49:LEU:CD1 | 2.20 | 0.64 |
| 1:A:291:ASP:HB3 | 1:A:345:ARG:NH2 | 2.13 | 0.64 |
| 1:A:417:VAL:HA | 1:A:420:ILE:HG22 | 1.79 | 0.64 |
| 1:C:280:GLY:HA3 | 1:C:284:ARG:HH11 | 1.62 | 0.64 |
| 1:D:320:ALA:HA | 1:D:335:GLY:HA2 | 1.78 | 0.64 |
| 1:D:345:ARG:O | 1:D:349:ILE:HG13 | 1.98 | 0.64 |
| 1:E:228:SER:O | 1:E:257:GLU:HB3 | 1.97 | 0.64 |
| 1:E:291:ASP:OD1 | 1:E:292:ILE:HG13 | 1.98 | 0.64 |
| 1:E:499:VAL:CG2 | 1:E:500:THR:N | 2.59 | 0.64 |
| 1:H:32:GLY:HA3 | 1:H:454:ILE:HG23 | 1.80 | 0.64 |
| 1:I:222:LEU:HD22 | 1:I:289:LEU:HD11 | 1.80 | 0.64 |
| 1:I:302:SER:HB2 | 1:I:305:ILE:HD12 | 1.80 | 0.64 |
| 1:J:313:THR:HG22 | 1:J:314:LEU:N | 2.12 | 0.64 |
| 1:K:149:THR:CG2 | 1:K:156:GLU:HA | 2.27 | 0.64 |
| 1:M:25:ASP:HA | 1:M:28:LYS:HE2 | 1.79 | 0.64 |
| 1:N:221:LEU:C | 1:N:221:LEU:HD13 | 2.18 | 0.64 |
| 1:B:220:ILE:HD12 | 1:B:220:ILE:N | 2.13 | 0.64 |
| 1:B:31:LEU:HD12 | 4:B:1:ADP:O1A | 1.98 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:20:VAL:HG13 | 1:B:74:VAL:HG11 | 1.80 | 0.64 |
| 1:B:82:ASN:HD22 | 1:B:86:GLY:HA2 | 1.63 | 0.64 |
| 1:B:82:ASN:ND2 | 1:B:86:GLY:HA2 | 2.12 | 0.64 |
| 1:D:350:ARG:O | 1:D:354:GLU:HG2 | 1.97 | 0.64 |
| 1:I:66:PHE:HA | 1:I:520:MET:HE1 | 1.80 | 0.64 |
| 1:N:161:LEU:HD12 | 1:N:161:LEU:H | 1.63 | 0.64 |
| 2:Q:5:PRO:CD | 2:Q:42:ALA:HB1 | 2.28 | 0.64 |
| 1:A:33:PRO:HA | 1:A:153:ASN:ND2 | 2.11 | 0.64 |
| 1:C:310:GLU:O | 1:C:312:ALA:N | 2.31 | 0.64 |
| 1:D:20:VAL:HG13 | 1:D:74:VAL:HG11 | 1.78 | 0.64 |
| 1:E:391:GLU:O | 1:E:394:ALA:HB3 | 1.98 | 0.64 |
| 1:F:135:SER:HB2 | 1:F:497:THR:HG21 | 1.79 | 0.64 |
| 1:F:264:VAL:HA | 1:F:267:MET:HB2 | 1.79 | 0.64 |
| 1:F:44:PHE:HD1 | 1:F:44:PHE:N | 1.92 | 0.64 |
| 1:G:325:ILE:HG13 | 1:G:330:THR:HG23 | 1.80 | 0.64 |
| 1:A:210:THR:OG1 | 1:G:351:GLN:HG2 | 1.97 | 0.64 |
| 1:I:499:VAL:HG23 | 1:I:500:THR:N | 2.12 | 0.64 |
| 1:L:385:THR:HG23 | 1:L:388:GLU:H | 1.63 | 0.64 |
| 1:M:198:GLY:HA3 | 1:M:328:ASP:HA | 1.80 | 0.64 |
| 2:S:17:VAL:CG1 | 2:S:34:LYS:HA | 2.27 | 0.64 |
| 1:B:324:VAL:C | 1:B:325:ILE:HD12 | 2.18 | 0.63 |
| 1:D:322:ARG:HG2 | 1:D:323:VAL:H | 1.63 | 0.63 |
| 1:E:247:LEU:HB3 | 1:E:273:VAL:HG13 | 1.79 | 0.63 |
| 1:F:18:ARG:HH11 | 1:F:18:ARG:CB | 2.05 | 0.63 |
| 1:I:232:GLU:HB2 | 1:I:233:MET:HE1 | 1.80 | 0.63 |
| 1:L:277:LYS:HB2 | 1:L:277:LYS:NZ | 2.12 | 0.63 |
| 1:M:116:LEU:HD23 | 1:M:435:ASP:O | 1.98 | 0.63 |
| 2:P:47:ARG:HG2 | 2:P:49:LEU:H | 1.63 | 0.63 |
| 1:B:235:PRO:HG2 | 1:B:236:VAL:H | 1.63 | 0.63 |
| 1:B:29:VAL:HG23 | 1:B:30:THR:HG23 | 1.80 | 0.63 |
| 1:D:248:LEU:HD13 | 1:D:249:ILE:N | 2.13 | 0.63 |
| 1:E:147:VAL:O | 1:E:150:ILE:HG22 | 1.97 | 0.63 |
| 1:F:278:ALA:HB1 | 1:F:279:PRO:CD | 2.27 | 0.63 |
| 1:G:213:VAL:O | 1:G:324:VAL:HA | 1.98 | 0.63 |
| 1:H:325:ILE:N | 1:H:325:ILE:HD12 | 2.13 | 0.63 |
| 1:I:287:ALA:HB1 | 1:I:368:ARG:NH2 | 2.13 | 0.63 |
| 1:J:107:VAL:HG23 | 1:J:108:ALA:N | 2.13 | 0.63 |
| 1:M:265:ASN:O | 1:M:269:GLY:HA3 | 1.99 | 0.63 |
| 2:T:49:LEU:O | 2:T:55:LYS:NZ | 2.32 | 0.63 |
| 1:B:279:PRO:HG2 | 1:B:288:MET:HE3 | 1.81 | 0.63 |
| 1:B:219:PHE:HB3 | 1:B:317:LEU:HD13 | 1.80 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:499:VAL:HG23 | 1:C:500:THR:N | 2.14 | 0.63 |
| 1:D:219:PHE:HB2 | 1:D:247:LEU:HD22 | 1.80 | 0.63 |
| 1:D:456:LEU:HD13 | 1:D:462:PRO:CG | 2.28 | 0.63 |
| 1:E:324:VAL:C | 1:E:325:ILE:HD12 | 2.18 | 0.63 |
| 1:F:224:ASP:HB2 | 1:F:303:GLU:HB3 | 1.80 | 0.63 |
| 1:F:195:PHE:O | 1:F:329:THR:HG23 | 1.98 | 0.63 |
| 1:H:171:LYS:HD3 | 1:H:407:VAL:HG11 | 1.79 | 0.63 |
| 1:J:194:GLN:HG2 | 1:J:195:PHE:N | 2.13 | 0.63 |
| 1:J:213:VAL:O | 1:J:324:VAL:HA | 1.98 | 0.63 |
| 1:J:499:VAL:HG23 | 1:J:500:THR:N | 2.13 | 0.63 |
| 1:L:363:GLU:O | 1:L:366:GLN:HB3 | 1.97 | 0.63 |
| 1:N:326:ASN:ND2 | 1:N:328:ASP:H | 1.95 | 0.63 |
| 2:P:37:ARG:HG2 | 2:P:37:ARG:HH11 | 1.63 | 0.63 |
| 2:S:43:VAL:HG23 | 2:S:61:VAL:HG22 | 1.80 | 0.63 |
| 1:A:368:ARG:HG2 | 1:A:372:LEU:HG | 1.81 | 0.63 |
| 1:B:222:LEU:N | 1:B:222:LEU:HD12 | 2.14 | 0.63 |
| 1:C:131:LEU:CD2 | 1:C:422:VAL:HG11 | 2.27 | 0.63 |
| 1:E:70:GLY:O | 1:E:74:VAL:HG22 | 1.99 | 0.63 |
| 1:G:228:SER:O | 1:G:257:GLU:HB3 | 1.98 | 0.63 |
| 1:H:422:VAL:O | 1:H:426:LEU:HD23 | 1.98 | 0.63 |
| 1:I:247:LEU:H | 1:I:273:VAL:HG12 | 1.64 | 0.63 |
| 1:J:197:ARG:HG2 | 1:J:277:LYS:O | 1.99 | 0.63 |
| 1:L:282:GLY:O | 1:L:285:ARG:HG2 | 1.98 | 0.63 |
| 1:M:324:VAL:C | 1:M:325:ILE:HD12 | 2.19 | 0.63 |
| 1:M:415:GLY:H | 1:M:417:VAL:HG23 | 1.62 | 0.63 |
| 2:T:17:VAL:CG2 | 2:T:34:LYS:HD2 | 2.29 | 0.63 |
| 2:U:14:ARG:HD3 | 2:U:35:SER:HB3 | 1.79 | 0.63 |
| 1:D:160:LYS:HE3 | 1:D:164:GLU:OE2 | 1.98 | 0.63 |
| 1:D:219:PHE:HB2 | 1:D:247:LEU:CD2 | 2.28 | 0.63 |
| 1:D:228:SER:HA | 1:D:255:GLU:CB | 2.27 | 0.63 |
| 1:D:349:ILE:O | 1:D:353:ILE:HG13 | 1.99 | 0.63 |
| 1:E:310:GLU:H | 1:E:310:GLU:CD | 2.02 | 0.63 |
| 1:F:280:GLY:HA3 | 1:F:284:ARG:NH1 | 2.13 | 0.63 |
| 1:G:235:PRO:HG3 | 1:G:310:GLU:HB3 | 1.80 | 0.63 |
| 1:H:145:ALA:HA | 1:H:159:GLY:O | 1.99 | 0.63 |
| 1:I:124:VAL:HG13 | 1:I:504:LEU:CD1 | 2.28 | 0.63 |
| 1:J:218:PRO:HB3 | 1:J:246:PRO:C | 2.18 | 0.63 |
| 1:K:326:ASN:OD1 | 1:K:329:THR:HB | 1.98 | 0.63 |
| 2:P:20:LYS:HD2 | 2:P:20:LYS:H | 1.63 | 0.63 |
| 1:A:199:TYR:HE2 | 1:A:205:ILE:HG12 | 1.63 | 0.63 |
| 1:C:288:MET:HA | 1:C:291:ASP:OD2 | 1.99 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:404:ARG:HG3 | 1:C:404:ARG:HH11 | 1.63 | 0.63 |
| 1:D:233:MET:CA | 1:D:310:GLU:HG3 | 2.24 | 0.63 |
| 1:F:229:ASN:HA | 1:F:257:GLU:OE2 | 1.99 | 0.63 |
| 1:F:313:THR:HB | 1:F:315:GLU:OE2 | 1.99 | 0.63 |
| 1:K:200:LEU:CD1 | 1:K:276:VAL:HA | 2.28 | 0.63 |
| 1:N:31:LEU:HG | 1:N:454:ILE:HD11 | 1.81 | 0.63 |
| 1:N:82:ASN:HB2 | 1:N:89:THR:OG1 | 1.97 | 0.63 |
| 2:T:84:LEU:N | 2:T:84:LEU:HD12 | 2.13 | 0.63 |
| 1:A:223:ALA:HB3 | 1:A:251:ALA:CB | 2.28 | 0.63 |
| 1:A:54:VAL:HB | 1:A:89:THR:HG21 | 1.79 | 0.63 |
| 1:C:207:LYS:CB | 1:C:208:PRO:HD3 | 2.27 | 0.63 |
| 1:F:208:PRO:HB2 | 1:F:212:ALA:CB | 2.28 | 0.63 |
| 1:F:348:GLN:HE22 | 1:F:352:GLN:NE2 | 1.96 | 0.63 |
| 1:H:365:LEU:O | 1:H:369:VAL:HG23 | 1.99 | 0.63 |
| 1:H:413:ALA:CB | 1:H:417:VAL:HB | 2.28 | 0.63 |
| 1:I:166:MET:HE2 | 1:I:171:LYS:HA | 1.80 | 0.63 |
| 1:I:232:GLU:HB3 | 1:I:309:LEU:CB | 2.26 | 0.63 |
| 1:K:194:GLN:HG2 | 1:K:195:PHE:N | 2.12 | 0.63 |
| 1:K:265:ASN:O | 1:K:269:GLY:HA3 | 1.99 | 0.63 |
| 1:M:385:THR:O | 1:M:389:MET:HB2 | 1.98 | 0.63 |
| 1:M:450:PRO:O | 1:M:454:ILE:HG12 | 1.99 | 0.63 |
| 2:R:77:LYS:HG3 | 2:R:80:ASN:HA | 1.80 | 0.63 |
| 2:T:97:ALA:O | 2:U:1:MET:HA | 1.99 | 0.63 |
| 1:C:433:ASN:HD21 | 1:C:435:ASP:HB2 | 1.63 | 0.63 |
| 1:I:266:THR:CG2 | 1:I:273:VAL:H | 2.12 | 0.63 |
| 1:K:478:TYR:HB2 | 1:K:485:TYR:CD2 | 2.34 | 0.63 |
| 1:K:72:GLN:HA | 1:K:72:GLN:NE2 | 2.14 | 0.63 |
| 2:Q:77:LYS:HG3 | 2:Q:80:ASN:HA | 1.81 | 0.63 |
| 2:S:49:LEU:O | 2:S:55:LYS:NZ | 2.32 | 0.63 |
| 1:A:199:TYR:HE1 | 1:A:327:LYS:HG3 | 1.64 | 0.63 |
| 1:B:226:LYS:C | 1:B:227:ILE:HD12 | 2.19 | 0.63 |
| 1:B:291:ASP:HB3 | 1:B:345:ARG:NH2 | 2.12 | 0.63 |
| 1:C:365:LEU:HD22 | 1:C:366:GLN:HE22 | 1.63 | 0.63 |
| 1:C:499:VAL:CG2 | 1:C:500:THR:N | 2.62 | 0.63 |
| 1:D:309:LEU:HD12 | 1:D:309:LEU:H | 1.64 | 0.63 |
| 1:G:348:GLN:NE2 | 1:G:352:GLN:NE2 | 2.45 | 0.63 |
| 1:J:367:GLU:O | 1:J:370:ALA:HB3 | 1.98 | 0.63 |
| 1:K:287:ALA:HB1 | 1:K:368:ARG:CZ | 2.29 | 0.63 |
| 1:K:422:VAL:O | 1:K:425:LYS:HB2 | 1.99 | 0.63 |
| 1:E:353:ILE:HG12 | 1:E:366:GLN:NE2 | 2.14 | 0.62 |
| 1:G:365:LEU:O | 1:G:369:VAL:HG23 | 1.99 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:157:THR:O | 1:H:161:LEU:HD13 | 1.98 | 0.62 |
| 1:H:434:GLU:HA | 1:H:437:ASN:ND2 | 2.14 | 0.62 |
| 1:I:411:VAL:HG21 | 1:I:494:LEU:HD12 | 1.80 | 0.62 |
| 1:I:422:VAL:O | 1:I:425:LYS:HB2 | 1.99 | 0.62 |
| 1:J:248:LEU:HD22 | 1:J:249:ILE:H | 1.63 | 0.62 |
| 1:K:217:SER:N | 1:K:218:PRO:HD3 | 2.14 | 0.62 |
| 1:L:265:ASN:O | 1:L:269:GLY:HA3 | 1.98 | 0.62 |
| 1:N:264:VAL:HA | 1:N:267:MET:HG2 | 1.80 | 0.62 |
| 1:E:280:GLY:HA3 | 1:E:284:ARG:NH1 | 2.13 | 0.62 |
| 1:F:215:LEU:O | 1:F:218:PRO:HD3 | 1.98 | 0.62 |
| 1:G:242:LYS:HD3 | 1:G:242:LYS:C | 2.20 | 0.62 |
| 1:G:305:ILE:CG2 | 1:G:306:GLY:H | 2.02 | 0.62 |
| 1:I:122:LYS:HE2 | 1:I:429:LEU:HD11 | 1.81 | 0.62 |
| 1:J:138:CYS:SG | 1:J:144:ILE:HD13 | 2.39 | 0.62 |
| 1:J:478:TYR:HB2 | 1:J:485:TYR:CD2 | 2.35 | 0.62 |
| 1:J:82:ASN:HB2 | 1:J:89:THR:OG1 | 1.98 | 0.62 |
| 1:L:198:GLY:CA | 1:L:328:ASP:HA | 2.29 | 0.62 |
| 1:L:240:VAL:HA | 1:L:243:ALA:HB3 | 1.80 | 0.62 |
| 1:L:37:ASN:H | 1:L:37:ASN:ND2 | 1.96 | 0.62 |
| 1:N:325:ILE:HG13 | 1:N:330:THR:HG23 | 1.80 | 0.62 |
| 2:O:55:LYS:N | 2:O:55:LYS:HE2 | 2.00 | 0.62 |
| 2:O:7:HIS:HB3 | 2:O:45:ASN:HD22 | 1.64 | 0.62 |
| 1:B:310:GLU:O | 1:B:312:ALA:N | 2.32 | 0.62 |
| 1:C:220:ILE:HD12 | 1:C:220:ILE:N | 2.14 | 0.62 |
| 1:C:253:ASP:CG | 1:C:254:VAL:N | 2.53 | 0.62 |
| 1:D:339:GLU:HB3 | 1:D:343:GLN:OE1 | 1.99 | 0.62 |
| 1:D:510:VAL:HG23 | 1:D:511:ALA:H | 1.63 | 0.62 |
| 1:H:223:ALA:HB3 | 1:H:251:ALA:CB | 2.25 | 0.62 |
| 1:I:363:GLU:O | 1:I:367:GLU:HG3 | 2.00 | 0.62 |
| 1:I:180:GLY:HA2 | 1:I:380:LYS:HB3 | 1.80 | 0.62 |
| 1:J:263:VAL:O | 1:J:267:MET:HG2 | 1.99 | 0.62 |
| 1:J:320:ALA:HA | 1:J:334:ASP:O | 1.98 | 0.62 |
| 1:N:194:GLN:HG2 | 1:N:195:PHE:N | 2.13 | 0.62 |
| 2:T:55:LYS:HE2 | 2:T:55:LYS:N | 2.11 | 0.62 |
| 1:A:200:LEU:N | 1:A:200:LEU:HD12 | 2.15 | 0.62 |
| 1:A:372:LEU:O | 1:A:373:ALA:HB2 | 2.00 | 0.62 |
| 1:B:135:SER:HB2 | 1:B:497:THR:HG21 | 1.81 | 0.62 |
| 1:D:239:ALA:HB1 | 1:D:314:LEU:HD23 | 1.79 | 0.62 |
| 1:D:266:THR:HA | 1:D:271:VAL:O | 1.99 | 0.62 |
| 1:D:44:PHE:HD1 | 1:D:44:PHE:H | 1.43 | 0.62 |
| 1:E:472:GLY:HA3 | 1:E:476:TYR:HD2 | 1.64 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:310:GLU:O | 1:F:312:ALA:N | 2.32 | 0.62 |
| 1:G:214:GLU:CB | 1:G:322:ARG:HD3 | 2.20 | 0.62 |
| 1:G:72:GLN:NE2 | 1:G:72:GLN:HA | 2.15 | 0.62 |
| 1:H:16:MET:HG3 | 1:H:520:MET:SD | 2.38 | 0.62 |
| 1:K:147:VAL:HA | 1:K:150:ILE:HD12 | 1.81 | 0.62 |
| 2:O:37:ARG:HG2 | 2:O:37:ARG:HH11 | 1.64 | 0.62 |
| 1:A:207:LYS:CB | 1:A:208:PRO:HD3 | 2.26 | 0.62 |
| 1:B:218:PRO:HA | 1:B:246:PRO:HG2 | 1.81 | 0.62 |
| 1:C:25:ASP:HA | 1:C:28:LYS:HE2 | 1.79 | 0.62 |
| 1:C:411:VAL:HA | 1:C:497:THR:H | 1.64 | 0.62 |
| 1:D:247:LEU:O | 1:D:273:VAL:HG13 | 1.99 | 0.62 |
| 1:D:450:PRO:O | 1:D:454:ILE:HG13 | 1.99 | 0.62 |
| 1:E:234:LEU:H | 1:E:234:LEU:CD1 | 2.12 | 0.62 |
| 1:E:291:ASP:HB3 | 1:E:345:ARG:NH2 | 2.14 | 0.62 |
| 1:J:10:ASN:O | 1:J:11:ASP:C | 2.38 | 0.62 |
| 1:K:290:GLN:O | 1:K:293:ALA:HB3 | 1.99 | 0.62 |
| 1:M:239:ALA:CB | 1:M:314:LEU:HD11 | 2.22 | 0.62 |
| 1:N:363:GLU:O | 1:N:367:GLU:HG3 | 1.99 | 0.62 |
| 2:O:22:ALA:O | 2:O:26:VAL:HB | 1.99 | 0.62 |
| 2:R:18:GLU:CD | 2:R:33:ALA:HB3 | 2.19 | 0.62 |
| 1:A:41:ASP:HB2 | 1:G:69:MET:SD | 2.40 | 0.62 |
| 1:B:35:GLY:HA3 | 1:B:51:LYS:HE2 | 1.81 | 0.62 |
| 1:E:131:LEU:HD21 | 1:E:422:VAL:HG11 | 1.78 | 0.62 |
| 1:F:219:PHE:HB2 | 1:F:247:LEU:CD2 | 2.28 | 0.62 |
| 1:H:31:LEU:HG | 1:H:454:ILE:HD11 | 1.81 | 0.62 |
| 1:I:157:THR:O | 1:I:161:LEU:HD13 | 1.99 | 0.62 |
| 1:K:403:THR:O | 1:K:407:VAL:HG23 | 1.99 | 0.62 |
| 1:M:66:PHE:H | 1:M:69:MET:HG3 | 1.65 | 0.62 |
| 1:N:263:VAL:O | 1:N:267:MET:HG2 | 1.99 | 0.62 |
| 1:N:325:ILE:HD12 | 1:N:325:ILE:N | 2.14 | 0.62 |
| 2:P:17:VAL:HG13 | 2:P:34:LYS:HA | 1.80 | 0.62 |
| 2:Q:50:GLU:O | 2:Q:52:GLY:N | 2.32 | 0.62 |
| 1:B:218:PRO:CA | 1:B:246:PRO:HG2 | 2.30 | 0.62 |
| 1:B:350:ARG:HD3 | 1:B:353:ILE:HD12 | 1.82 | 0.62 |
| 1:C:322:ARG:HB3 | 1:C:333:ILE:CD1 | 2.22 | 0.62 |
| 1:F:134:LEU:N | 1:F:134:LEU:HD12 | 2.15 | 0.62 |
| 1:F:221:LEU:HD13 | 1:F:317:LEU:CD2 | 2.29 | 0.62 |
| 1:G:241:ALA:HA | 1:G:271:VAL:HG12 | 1.79 | 0.62 |
| 1:I:266:THR:O | 1:I:268:ARG:N | 2.31 | 0.62 |
| 1:M:302:SER:HB2 | 1:M:305:ILE:HG13 | 1.82 | 0.62 |
| 1:M:32:GLY:HA2 | 1:M:454:ILE:HD12 | 1.81 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:70:GLY:O | 1:B:74:VAL:HG22 | 2.00 | 0.62 |
| 1:C:281:PHE:H | 1:C:284:ARG:CD | 2.13 | 0.62 |
| 1:D:218:PRO:CA | 1:D:246:PRO:HG2 | 2.30 | 0.62 |
| 1:D:77:VAL:HG12 | 1:D:510:VAL:HG21 | 1.82 | 0.62 |
| 1:E:218:PRO:CA | 1:E:246:PRO:HG2 | 2.29 | 0.62 |
| 1:E:252:GLU:O | 1:E:253:ASP:HB2 | 1.98 | 0.62 |
| 1:E:512:GLY:O | 1:E:515:ILE:HG12 | 1.98 | 0.62 |
| 1:F:18:ARG:HB2 | 1:F:67:GLU:HG2 | 1.80 | 0.62 |
| 1:G:313:THR:N | 1:G:316:ASP:OD2 | 2.33 | 0.62 |
| 1:G:44:PHE:H | 1:G:44:PHE:HD1 | 1.39 | 0.62 |
| 1:I:205:ILE:HA | 1:I:213:VAL:HG22 | 1.82 | 0.62 |
| 1:I:404:ARG:O | 1:I:408:GLU:HG3 | 1.99 | 0.62 |
| 1:K:122:LYS:HE2 | 1:K:429:LEU:HD11 | 1.81 | 0.62 |
| 1:K:308:GLU:HG2 | 1:K:309:LEU:N | 2.13 | 0.62 |
| 1:K:363:GLU:O | 1:K:367:GLU:HG3 | 2.00 | 0.62 |
| 1:M:149:THR:CG2 | 1:M:159:GLY:HA3 | 2.30 | 0.62 |
| 1:M:287:ALA:HB1 | 1:M:368:ARG:CZ | 2.30 | 0.62 |
| 1:N:386:GLU:HG2 | 1:N:390:LYS:HE2 | 1.81 | 0.62 |
| 2:O:40:VAL:CG1 | 2:O:61:VAL:HA | 2.30 | 0.62 |
| 2:P:48:ILE:HG12 | 2:P:54:VAL:HG13 | 1.82 | 0.62 |
| 1:A:277:LYS:HD3 | 1:A:285:ARG:NH2 | 2.13 | 0.62 |
| 1:B:381:VAL:HG21 | 1:B:393:LYS:HA | 1.82 | 0.62 |
| 1:C:219:PHE:HD1 | 1:C:319:GLN:HE21 | 1.48 | 0.62 |
| 1:C:223:ALA:HB3 | 1:C:251:ALA:HB2 | 1.80 | 0.62 |
| 1:C:193:MET:SD | 1:C:371:LYS:HB3 | 2.40 | 0.62 |
| 1:D:259:LEU:O | 1:D:263:VAL:HG23 | 1.98 | 0.62 |
| 1:D:283:ASP:O | 1:D:287:ALA:HB2 | 1.98 | 0.62 |
| 1:E:414:GLY:HA2 | 1:E:495:ASP:OD2 | 2.00 | 0.62 |
| 1:F:257:GLU:O | 1:F:261:THR:HG22 | 2.00 | 0.62 |
| 1:G:450:PRO:O | 1:G:454:ILE:HG13 | 1.99 | 0.62 |
| 1:H:302:SER:HB2 | 1:H:305:ILE:HD12 | 1.82 | 0.62 |
| 1:H:345:ARG:HA | 1:H:348:GLN:NE2 | 2.14 | 0.62 |
| 1:I:385:THR:O | 1:I:389:MET:HB2 | 1.99 | 0.62 |
| 1:K:413:ALA:CB | 1:K:417:VAL:HB | 2.30 | 0.62 |
| 1:L:472:GLY:HA3 | 1:L:476:TYR:HD2 | 1.63 | 0.62 |
| 1:M:164:GLU:O | 1:M:167:ASP:HB3 | 1.99 | 0.62 |
| 2:O:6:LEU:O | 2:O:7:HIS:O | 2.16 | 0.62 |
| 1:A:342:ILE:O | 1:A:346:VAL:HG23 | 1.98 | 0.62 |
| 1:A:360:TYR:O | 1:A:364:LYS:HE2 | 1.99 | 0.62 |
| 1:B:214:GLU:CB | 1:B:322:ARG:HD3 | 2.21 | 0.62 |
| 1:E:94:VAL:HG12 | 1:E:449:ALA:HB1 | 1.81 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:18:ARG:O | 1:F:22:VAL:HG23 | 2.00 | 0.62 |
| 1:F:202:PRO:O | 1:F:205:ILE:HG13 | 2.00 | 0.62 |
| 1:H:200:LEU:CD1 | 1:H:276:VAL:HA | 2.29 | 0.62 |
| 1:H:32:GLY:CA | 1:H:454:ILE:HG23 | 2.30 | 0.62 |
| 1:K:277:LYS:NZ | 1:K:277:LYS:HB2 | 2.15 | 0.62 |
| 1:L:194:GLN:HG2 | 1:L:195:PHE:N | 2.13 | 0.62 |
| 1:M:270:ILE:HG22 | 1:M:271:VAL:N | 2.15 | 0.62 |
| 1:M:314:LEU:H | 1:M:314:LEU:CD1 | 2.10 | 0.62 |
| 1:N:264:VAL:HA | 1:N:267:MET:CG | 2.29 | 0.62 |
| 2:U:78:ILE:HD13 | 2:U:83:VAL:CG2 | 2.27 | 0.62 |
| 1:B:201:SER:HB3 | 1:B:259:LEU:HD22 | 1.82 | 0.61 |
| 1:B:177:VAL:HG11 | 1:B:397:GLU:HG2 | 1.80 | 0.61 |
| 1:B:5:ASP:HB2 | 1:B:524:LEU:HD23 | 1.82 | 0.61 |
| 1:D:44:PHE:HD1 | 1:D:44:PHE:N | 1.97 | 0.61 |
| 1:D:65:LYS:O | 1:D:69:MET:HG3 | 2.00 | 0.61 |
| 1:F:472:GLY:HA3 | 1:F:476:TYR:CD2 | 2.35 | 0.61 |
| 1:J:301:ILE:N | 1:J:301:ILE:HD12 | 2.15 | 0.61 |
| 1:K:135:SER:HA | 1:K:412:VAL:HG12 | 1.82 | 0.61 |
| 1:K:194:GLN:HG3 | 1:K:331:THR:HB | 1.81 | 0.61 |
| 1:L:413:ALA:HB1 | 1:L:417:VAL:HB | 1.81 | 0.61 |
| 1:M:247:LEU:O | 1:M:273:VAL:HB | 1.98 | 0.61 |
| 2:P:77:LYS:C | 2:P:78:ILE:HD12 | 2.20 | 0.61 |
| 1:B:249:ILE:HB | 1:B:275:ALA:CB | 2.31 | 0.61 |
| 1:B:504:LEU:C | 1:B:504:LEU:HD13 | 2.21 | 0.61 |
| 1:C:76:GLU:OE1 | 1:D:387:VAL:HG13 | 2.00 | 0.61 |
| 1:D:266:THR:CG2 | 1:D:273:VAL:H | 2.12 | 0.61 |
| 1:D:33:PRO:HA | 1:D:153:ASN:ND2 | 2.15 | 0.61 |
| 1:F:219:PHE:HB3 | 1:F:317:LEU:HD13 | 1.80 | 0.61 |
| 1:F:25:ASP:HA | 1:F:28:LYS:HE2 | 1.82 | 0.61 |
| 1:F:448:GLU:O | 1:F:452:ARG:HG2 | 2.00 | 0.61 |
| 1:H:270:ILE:HG23 | 1:I:229:ASN:ND2 | 2.15 | 0.61 |
| 1:I:314:LEU:CA | 1:I:317:LEU:HD13 | 2.24 | 0.61 |
| 1:J:219:PHE:CB | 1:J:317:LEU:HD23 | 2.31 | 0.61 |
| 1:N:219:PHE:CE1 | 1:N:245:LYS:HB2 | 2.33 | 0.61 |
| 2:S:37:ARG:HH11 | 2:S:37:ARG:HG2 | 1.66 | 0.61 |
| 1:A:222:LEU:N | 1:A:222:LEU:HD12 | 2.15 | 0.61 |
| 1:A:259:LEU:O | 1:A:263:VAL:HG23 | 2.00 | 0.61 |
| 1:B:52:ASP:OD1 | 1:B:54:VAL:HG12 | 2.00 | 0.61 |
| 1:C:322:ARG:HG2 | 1:C:323:VAL:N | 2.13 | 0.61 |
| 1:C:194:GLN:HB2 | 1:C:331:THR:HG23 | 1.83 | 0.61 |
| 1:D:496:PRO:HG2 | 1:D:499:VAL:HG13 | 1.81 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:285:ARG:HG3 | 1:E:286:LYS:H | 1.64 | 0.61 |
| 1:E:295:LEU:HD23 | 1:E:295:LEU:C | 2.21 | 0.61 |
| 1:G:273:VAL:CG1 | 1:G:274:ALA:N | 2.64 | 0.61 |
| 1:G:299:THR:HB | 1:G:316:ASP:HB3 | 1.82 | 0.61 |
| 1:G:339:GLU:HB3 | 1:G:343:GLN:OE1 | 1.99 | 0.61 |
| 1:H:155:ASP:CG | 1:H:158:VAL:HG23 | 2.20 | 0.61 |
| 1:J:450:PRO:O | 1:J:454:ILE:HG12 | 2.01 | 0.61 |
| 1:L:223:ALA:HB3 | 1:L:251:ALA:CB | 2.25 | 0.61 |
| 1:L:385:THR:O | 1:L:389:MET:HB2 | 2.00 | 0.61 |
| 1:M:248:LEU:HD13 | 1:M:249:ILE:N | 2.15 | 0.61 |
| 1:N:319:GLN:O | 1:N:336:VAL:HG23 | 2.00 | 0.61 |
| 1:B:229:ASN:C | 1:B:231:ARG:H | 2.03 | 0.61 |
| 1:B:510:VAL:HG23 | 1:B:511:ALA:N | 2.16 | 0.61 |
| 1:D:169:VAL:HB | 1:D:173:GLY:HA3 | 1.81 | 0.61 |
| 1:G:227:ILE:N | 1:G:227:ILE:HD12 | 2.15 | 0.61 |
| 1:J:266:THR:HG22 | 1:J:272:LYS:HA | 1.82 | 0.61 |
| 1:K:235:PRO:HG2 | 1:K:236:VAL:H | 1.66 | 0.61 |
| 1:J:270:ILE:HA | 1:K:257:GLU:OE2 | 2.00 | 0.61 |
| 1:L:123:ALA:HB2 | 1:L:440:ILE:HG23 | 1.82 | 0.61 |
| 1:M:426:LEU:H | 1:M:426:LEU:CD2 | 2.10 | 0.61 |
| 2:P:97:ALA:O | 2:Q:1:MET:HA | 2.01 | 0.61 |
| 1:B:247:LEU:HD12 | 1:B:249:ILE:CD1 | 2.30 | 0.61 |
| 1:B:325:ILE:HG13 | 1:B:330:THR:HG23 | 1.82 | 0.61 |
| 1:B:475:ASN:HD22 | 1:B:475:ASN:N | 1.97 | 0.61 |
| 1:D:30:THR:HB | 1:D:51:LYS:HG3 | 1.82 | 0.61 |
| 1:E:278:ALA:HB1 | 1:E:279:PRO:CD | 2.30 | 0.61 |
| 1:E:313:THR:N | 1:E:316:ASP:OD2 | 2.33 | 0.61 |
| 1:E:69:MET:SD | 1:F:41:ASP:HB2 | 2.41 | 0.61 |
| 1:F:127:ALA:O | 1:F:130:GLU:HB2 | 1.99 | 0.61 |
| 1:F:200:LEU:N | 1:F:200:LEU:HD12 | 2.15 | 0.61 |
| 1:F:233:MET:HE3 | 1:F:236:VAL:HB | 1.80 | 0.61 |
| 1:G:417:VAL:HA | 1:G:420:ILE:HG22 | 1.82 | 0.61 |
| 1:G:448:GLU:O | 1:G:452:ARG:HG2 | 2.00 | 0.61 |
| 1:H:247:LEU:H | 1:H:273:VAL:HG12 | 1.64 | 0.61 |
| 1:J:236:VAL:HG23 | 1:J:237:LEU:N | 2.16 | 0.61 |
| 1:M:359:ASP:CA | 1:M:362:ARG:HH12 | 2.12 | 0.61 |
| 1:M:400:LEU:C | 1:M:400:LEU:HD23 | 2.21 | 0.61 |
| 2:P:7:HIS:HB3 | 2:P:45:ASN:ND2 | 2.14 | 0.61 |
| 2:T:43:VAL:HG23 | 2:T:61:VAL:HG22 | 1.82 | 0.61 |
| 1:A:360:TYR:HA | 1:A:363:GLU:CD | 2.19 | 0.61 |
| 1:B:199:TYR:CA | 1:B:276:VAL:HG12 | 2.27 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:146:GLN:NE2 | 1:F:494:LEU:HD11 | 2.15 | 0.61 |
| 1:G:291:ASP:OD1 | 1:G:292:ILE:HG13 | 2.01 | 0.61 |
| 1:G:5:ASP:HB2 | 1:G:524:LEU:HD23 | 1.83 | 0.61 |
| 1:I:270:ILE:HA | 1:J:257:GLU:OE2 | 1.99 | 0.61 |
| 1:N:107:VAL:HG23 | 1:N:108:ALA:N | 2.15 | 0.61 |
| 1:N:191:GLU:HB3 | 1:N:295:LEU:HD11 | 1.82 | 0.61 |
| 1:N:448:GLU:HB3 | 1:N:452:ARG:HD2 | 1.82 | 0.61 |
| 1:B:413:ALA:HB1 | 1:B:417:VAL:HG11 | 1.83 | 0.61 |
| 1:C:291:ASP:OD1 | 1:C:292:ILE:HG13 | 2.00 | 0.61 |
| 1:D:116:LEU:O | 1:D:120:ILE:HG13 | 1.99 | 0.61 |
| 1:D:299:THR:HB | 1:D:316:ASP:HB3 | 1.81 | 0.61 |
| 1:D:84:ALA:HB2 | 1:D:506:TYR:HE2 | 1.66 | 0.61 |
| 1:E:207:LYS:CB | 1:E:208:PRO:HD3 | 2.24 | 0.61 |
| 1:F:265:ASN:HA | 1:F:270:ILE:HD12 | 1.81 | 0.61 |
| 1:G:472:GLY:HA3 | 1:G:476:TYR:CD2 | 2.36 | 0.61 |
| 1:H:217:SER:HB3 | 1:H:321:LYS:HA | 1.82 | 0.61 |
| 1:K:320:ALA:HA | 1:K:334:ASP:O | 2.00 | 0.61 |
| 1:L:161:LEU:HD12 | 1:L:161:LEU:N | 2.16 | 0.61 |
| 1:L:266:THR:HG22 | 1:L:273:VAL:H | 1.65 | 0.61 |
| 1:L:25:ASP:HA | 1:L:28:LYS:HE2 | 1.81 | 0.61 |
| 1:N:191:GLU:HB3 | 1:N:295:LEU:CD1 | 2.29 | 0.61 |
| 2:S:17:VAL:CG2 | 2:S:34:LYS:HD2 | 2.28 | 0.61 |
| 2:T:68:ASN:ND2 | 2:U:74:LYS:HE3 | 2.16 | 0.61 |
| 1:A:227:ILE:HD12 | 1:A:227:ILE:N | 2.15 | 0.61 |
| 1:A:34:LYS:HD2 | 1:A:458:CYS:SG | 2.41 | 0.61 |
| 1:B:266:THR:CG2 | 1:B:273:VAL:H | 2.12 | 0.61 |
| 1:C:368:ARG:CD | 1:C:372:LEU:HD11 | 2.31 | 0.61 |
| 1:D:142:LYS:HE2 | 1:D:146:GLN:OE1 | 2.00 | 0.61 |
| 1:E:234:LEU:N | 1:E:234:LEU:HD12 | 2.14 | 0.61 |
| 1:F:223:ALA:HB3 | 1:F:251:ALA:CB | 2.31 | 0.61 |
| 1:F:259:LEU:O | 1:F:262:LEU:HB3 | 1.99 | 0.61 |
| 1:H:219:PHE:HB3 | 1:H:317:LEU:HD23 | 1.82 | 0.61 |
| 1:J:248:LEU:HD13 | 1:J:249:ILE:N | 2.16 | 0.61 |
| 1:J:232:GLU:HA | 1:J:310:GLU:HG2 | 1.82 | 0.61 |
| 1:L:202:PRO:C | 1:L:204:PHE:H | 2.03 | 0.61 |
| 1:L:221:LEU:HD13 | 1:L:221:LEU:C | 2.21 | 0.61 |
| 1:N:186:GLU:HB2 | 1:N:380:LYS:HB2 | 1.83 | 0.61 |
| 2:Q:18:GLU:CD | 2:Q:33:ALA:HB3 | 2.21 | 0.61 |
| 1:A:146:GLN:HE21 | 1:A:494:LEU:HD11 | 1.65 | 0.61 |
| 1:B:25:ASP:HA | 1:B:28:LYS:HE2 | 1.82 | 0.61 |
| 1:B:247:LEU:O | 1:B:273:VAL:HG13 | 2.01 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:131:LEU:HD21 | 1:B:422:VAL:HG11 | 1.83 | 0.61 |
| 1:C:248:LEU:HD13 | 1:C:249:ILE:N | 2.16 | 0.61 |
| 1:D:339:GLU:H | 1:D:339:GLU:CD | 2.04 | 0.61 |
| 1:E:264:VAL:HA | 1:E:267:MET:HB2 | 1.82 | 0.61 |
| 1:E:239:ALA:HB1 | 1:E:314:LEU:HD23 | 1.83 | 0.61 |
| 1:I:455:VAL:HG13 | 1:I:460:GLU:HB2 | 1.83 | 0.61 |
| 1:K:226:LYS:HG3 | 1:K:252:GLU:HB3 | 1.83 | 0.61 |
| 1:K:267:MET:HG3 | 1:K:267:MET:O | 2.00 | 0.61 |
| 1:L:363:GLU:O | 1:L:367:GLU:HG3 | 2.01 | 0.61 |
| 1:M:219:PHE:HB2 | 1:M:247:LEU:HD23 | 1.82 | 0.61 |
| 1:M:219:PHE:HB3 | 1:M:317:LEU:HD23 | 1.82 | 0.61 |
| 1:M:411:VAL:HG21 | 1:M:494:LEU:CD1 | 2.31 | 0.61 |
| 1:M:135:SER:HA | 1:M:412:VAL:HG12 | 1.82 | 0.61 |
| 1:N:313:THR:HB | 1:N:315:GLU:HG2 | 1.82 | 0.61 |
| 1:N:179:ASP:OD2 | 1:N:390:LYS:HG2 | 2.01 | 0.61 |
| 2:O:20:LYS:N | 2:O:20:LYS:HD2 | 2.16 | 0.61 |
| 2:O:27:LEU:HD23 | 2:O:27:LEU:O | 2.01 | 0.61 |
| 2:R:6:LEU:O | 2:R:7:HIS:O | 2.19 | 0.61 |
| 1:C:475:ASN:HD22 | 1:C:475:ASN:N | 1.97 | 0.61 |
| 1:D:339:GLU:N | 1:D:339:GLU:CD | 2.55 | 0.61 |
| 1:E:222:LEU:HD12 | 1:E:222:LEU:N | 2.15 | 0.61 |
| 1:F:234:LEU:CD1 | 1:F:234:LEU:H | 2.12 | 0.61 |
| 1:F:247:LEU:O | 1:F:273:VAL:HG13 | 2.01 | 0.61 |
| 1:F:381:VAL:CG1 | 1:F:392:LYS:CG | 2.79 | 0.61 |
| 1:H:221:LEU:HD13 | 1:H:221:LEU:C | 2.22 | 0.61 |
| 1:H:257:GLU:O | 1:H:261:THR:HG23 | 2.01 | 0.61 |
| 1:I:178:GLU:O | 1:I:380:LYS:HA | 2.00 | 0.61 |
| 1:L:266:THR:HG21 | 1:L:273:VAL:O | 2.01 | 0.61 |
| 1:L:350:ARG:HE | 1:L:369:VAL:HG11 | 1.66 | 0.61 |
| 1:M:124:VAL:HG13 | 1:M:504:LEU:CD1 | 2.31 | 0.61 |
| 1:M:180:GLY:HA2 | 1:M:380:LYS:HB3 | 1.83 | 0.61 |
| 1:M:499:VAL:HG23 | 1:M:500:THR:N | 2.15 | 0.61 |
| 1:M:69:MET:HE1 | 1:M:522:THR:HB | 1.80 | 0.61 |
| 1:N:247:LEU:HD22 | 1:N:248:LEU:H | 1.65 | 0.61 |
| 2:P:14:ARG:HD3 | 2:P:35:SER:HB3 | 1.81 | 0.61 |
| 2:Q:34:LYS:HG3 | 2:Q:35:SER:H | 1.63 | 0.61 |
| 2:Q:77:LYS:C | 2:Q:78:ILE:HD12 | 2.21 | 0.61 |
| 2:T:77:LYS:HG3 | 2:T:80:ASN:HA | 1.82 | 0.61 |
| 1:A:134:LEU:N | 1:A:134:LEU:HD12 | 2.15 | 0.60 |
| 1:B:273:VAL:CG1 | 1:B:274:ALA:H | 2.12 | 0.60 |
| 1:C:256:GLY:O | 1:C:260:ALA:N | 2.31 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:235:PRO:HG3 | 1:E:310:GLU:HB3 | 1.83 | 0.60 |
| 1:F:194:GLN:HB2 | 1:F:331:THR:HG23 | 1.83 | 0.60 |
| 1:G:272:LYS:NZ | 1:G:272:LYS:HB2 | 2.16 | 0.60 |
| 1:G:399:ALA:O | 1:G:403:THR:HG23 | 1.99 | 0.60 |
| 1:I:228:SER:O | 1:I:257:GLU:HB3 | 2.01 | 0.60 |
| 1:I:284:ARG:HH11 | 1:I:284:ARG:CB | 2.11 | 0.60 |
| 1:J:17:LEU:O | 1:J:20:VAL:HG13 | 2.01 | 0.60 |
| 1:K:191:GLU:HB3 | 1:K:295:LEU:CD1 | 2.30 | 0.60 |
| 1:L:232:GLU:HA | 1:L:310:GLU:CG | 2.31 | 0.60 |
| 1:N:155:ASP:CG | 1:N:158:VAL:HG23 | 2.21 | 0.60 |
| 1:A:291:ASP:HB3 | 1:A:345:ARG:HH21 | 1.66 | 0.60 |
| 1:C:310:GLU:CD | 1:C:310:GLU:H | 2.04 | 0.60 |
| 1:E:413:ALA:HB1 | 1:E:417:VAL:HG11 | 1.83 | 0.60 |
| 1:G:224:ASP:HB2 | 1:G:303:GLU:HB3 | 1.81 | 0.60 |
| 1:K:359:ASP:CA | 1:K:362:ARG:HH12 | 2.05 | 0.60 |
| 1:M:124:VAL:HG13 | 1:M:504:LEU:HD13 | 1.82 | 0.60 |
| 1:M:353:ILE:HD11 | 1:M:369:VAL:HG21 | 1.82 | 0.60 |
| 1:N:221:LEU:HD13 | 1:N:222:LEU:N | 2.15 | 0.60 |
| 2:R:68:ASN:HD22 | 2:S:74:LYS:HE3 | 1.66 | 0.60 |
| 2:U:17:VAL:CG2 | 2:U:34:LYS:HD2 | 2.32 | 0.60 |
| 1:A:124:VAL:HG22 | 1:A:504:LEU:HD11 | 1.83 | 0.60 |
| 1:A:10:ASN:O | 1:A:14:VAL:HG23 | 2.01 | 0.60 |
| 1:B:28:LYS:O | 1:B:30:THR:N | 2.34 | 0.60 |
| 1:D:271:VAL:O | 1:D:271:VAL:HG23 | 2.02 | 0.60 |
| 1:G:194:GLN:HB2 | 1:G:331:THR:HG23 | 1.82 | 0.60 |
| 1:G:433:ASN:HD21 | 1:G:435:ASP:HB2 | 1.65 | 0.60 |
| 1:I:343:GLN:O | 1:I:346:VAL:HB | 2.01 | 0.60 |
| 1:J:216:GLU:HA | 1:J:216:GLU:OE1 | 2.00 | 0.60 |
| 1:J:277:LYS:NZ | 1:J:277:LYS:HB2 | 2.16 | 0.60 |
| 1:J:325:ILE:HG13 | 1:J:330:THR:HG23 | 1.84 | 0.60 |
| 1:K:392:LYS:O | 1:K:396:VAL:HG23 | 2.02 | 0.60 |
| 1:M:264:VAL:HA | 1:M:267:MET:HG2 | 1.83 | 0.60 |
| 1:N:10:ASN:O | 1:N:11:ASP:C | 2.40 | 0.60 |
| 2:U:84:LEU:HD12 | 2:U:84:LEU:N | 2.16 | 0.60 |
| 1:A:160:LYS:HE3 | 1:A:164:GLU:OE2 | 2.01 | 0.60 |
| 1:A:228:SER:HA | 1:A:255:GLU:CB | 2.19 | 0.60 |
| 1:A:339:GLU:CD | 1:A:339:GLU:N | 2.54 | 0.60 |
| 1:B:10:ASN:O | 1:B:14:VAL:HG23 | 2.01 | 0.60 |
| 1:C:308:GLU:HB2 | 1:C:311:LYS:HB2 | 1.81 | 0.60 |
| 1:C:487:ASN:OD1 | 1:C:489:ILE:N | 2.35 | 0.60 |
| 1:D:346:VAL:HG12 | 1:D:350:ARG:NH2 | 2.15 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:44:PHE:HD1 | 1:E:44:PHE:H | 1.47 | 0.60 |
| 1:G:184:GLN:OE1 | 1:G:184:GLN:N | 2.32 | 0.60 |
| 1:G:285:ARG:HG3 | 1:G:286:LYS:H | 1.67 | 0.60 |
| 1:J:314:LEU:H | 1:J:314:LEU:CD1 | 2.02 | 0.60 |
| 1:M:290:GLN:HA | 1:M:290:GLN:OE1 | 2.00 | 0.60 |
| 1:N:214:GLU:HA | 1:N:324:VAL:HG12 | 1.84 | 0.60 |
| 2:R:48:ILE:HG12 | 2:R:54:VAL:HG13 | 1.82 | 0.60 |
| 1:A:313:THR:HB | 1:A:315:GLU:OE2 | 2.00 | 0.60 |
| 1:B:193:MET:O | 1:B:331:THR:HG23 | 2.01 | 0.60 |
| 1:C:259:LEU:O | 1:C:262:LEU:HB3 | 2.01 | 0.60 |
| 1:C:320:ALA:HA | 1:C:334:ASP:O | 2.02 | 0.60 |
| 1:C:472:GLY:HA3 | 1:C:476:TYR:CD2 | 2.36 | 0.60 |
| 1:D:433:ASN:HD21 | 1:D:435:ASP:HB2 | 1.65 | 0.60 |
| 1:F:206:ASN:HB3 | 1:F:214:GLU:H | 1.65 | 0.60 |
| 1:G:349:ILE:HG21 | 1:G:369:VAL:HG22 | 1.82 | 0.60 |
| 1:G:131:LEU:HD23 | 1:G:422:VAL:HG11 | 1.83 | 0.60 |
| 1:I:161:LEU:N | 1:I:161:LEU:HD12 | 2.17 | 0.60 |
| 1:J:214:GLU:HA | 1:J:324:VAL:HG12 | 1.84 | 0.60 |
| 2:R:49:LEU:O | 2:R:55:LYS:NZ | 2.35 | 0.60 |
| 2:T:20:LYS:HG2 | 2:T:27:LEU:CD2 | 2.32 | 0.60 |
| 1:A:372:LEU:O | 1:A:373:ALA:CB | 2.49 | 0.60 |
| 1:C:228:SER:HA | 1:C:255:GLU:CB | 2.25 | 0.60 |
| 1:C:241:ALA:HA | 1:C:271:VAL:HG12 | 1.83 | 0.60 |
| 1:C:52:ASP:OD1 | 1:C:54:VAL:HG12 | 2.02 | 0.60 |
| 1:D:207:LYS:CB | 1:D:208:PRO:HD3 | 2.24 | 0.60 |
| 1:D:295:LEU:O | 1:D:337:GLY:HA3 | 2.00 | 0.60 |
| 1:E:296:THR:CG2 | 1:E:335:GLY:HA3 | 2.24 | 0.60 |
| 1:E:146:GLN:HE21 | 1:E:494:LEU:HD11 | 1.66 | 0.60 |
| 1:K:124:VAL:HG13 | 1:K:504:LEU:HD11 | 1.83 | 0.60 |
| 1:K:206:ASN:OD1 | 1:K:213:VAL:HA | 2.01 | 0.60 |
| 1:K:66:PHE:HA | 1:K:520:MET:HE1 | 1.84 | 0.60 |
| 1:M:302:SER:HB2 | 1:M:305:ILE:CD1 | 2.31 | 0.60 |
| 2:O:20:LYS:HG3 | 2:O:28:THR:O | 2.02 | 0.60 |
| 2:Q:76:GLU:O | 2:Q:83:VAL:HG22 | 2.00 | 0.60 |
| 2:R:17:VAL:HG22 | 2:R:35:SER:N | 2.16 | 0.60 |
| 1:D:270:ILE:HD13 | 2:R:27:LEU:HB2 | 1.83 | 0.60 |
| 1:B:18:ARG:O | 1:B:22:VAL:HG23 | 2.01 | 0.60 |
| 1:C:213:VAL:HB | 1:C:325:ILE:HD13 | 1.84 | 0.60 |
| 1:C:219:PHE:CE2 | 1:C:245:LYS:HB2 | 2.37 | 0.60 |
| 1:C:252:GLU:N | 1:C:252:GLU:OE1 | 2.35 | 0.60 |
| 1:C:249:ILE:HB | 1:C:275:ALA:HB1 | 1.84 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:122:LYS:HE2 | 1:F:429:LEU:HD11 | 1.83 | 0.60 |
| 1:G:499:VAL:CG2 | 1:G:500:THR:N | 2.65 | 0.60 |
| 1:H:200:LEU:HD13 | 1:H:276:VAL:HA | 1.84 | 0.60 |
| 1:H:385:THR:HG23 | 1:H:388:GLU:HB3 | 1.83 | 0.60 |
| 1:H:400:LEU:C | 1:H:400:LEU:HD23 | 2.22 | 0.60 |
| 1:H:499:VAL:HG23 | 1:H:500:THR:N | 2.17 | 0.60 |
| 1:I:465:VAL:O | 1:I:469:VAL:HG23 | 2.02 | 0.60 |
| 1:J:383:ALA:CB | 1:J:389:MET:HA | 2.31 | 0.60 |
| 1:K:270:ILE:HA | 1:L:257:GLU:OE2 | 2.02 | 0.60 |
| 1:K:426:LEU:H | 1:K:426:LEU:CD2 | 2.09 | 0.60 |
| 1:L:112:ASN:O | 1:L:116:LEU:HG | 2.02 | 0.60 |
| 1:M:219:PHE:CE1 | 1:M:245:LYS:HB2 | 2.34 | 0.60 |
| 1:A:270:ILE:HD13 | 2:O:27:LEU:HB2 | 1.84 | 0.60 |
| 2:R:20:LYS:HD2 | 2:R:20:LYS:N | 2.17 | 0.60 |
| 2:S:77:LYS:HG3 | 2:S:80:ASN:HA | 1.83 | 0.60 |
| 1:A:169:VAL:HB | 1:A:173:GLY:HA3 | 1.84 | 0.60 |
| 1:D:193:MET:O | 1:D:331:THR:HG23 | 2.02 | 0.60 |
| 1:E:355:GLU:O | 1:E:362:ARG:NH2 | 2.35 | 0.60 |
| 1:E:352:GLN:C | 1:E:365:LEU:HD11 | 2.22 | 0.60 |
| 1:E:84:ALA:HB2 | 1:E:506:TYR:HE2 | 1.66 | 0.60 |
| 1:F:499:VAL:CG2 | 1:F:500:THR:N | 2.65 | 0.60 |
| 1:G:247:LEU:HD13 | 1:G:248:LEU:N | 2.16 | 0.60 |
| 1:G:499:VAL:HG23 | 1:G:500:THR:N | 2.17 | 0.60 |
| 1:H:411:VAL:HG21 | 1:H:494:LEU:HD12 | 1.83 | 0.60 |
| 1:I:319:GLN:O | 1:I:336:VAL:HG23 | 2.02 | 0.60 |
| 1:J:101:THR:O | 1:J:105:LYS:HG3 | 2.01 | 0.60 |
| 1:L:236:VAL:HG23 | 1:L:237:LEU:N | 2.16 | 0.60 |
| 1:L:235:PRO:HG2 | 1:L:236:VAL:H | 1.66 | 0.60 |
| 1:N:351:GLN:HG2 | 1:N:354:GLU:OE2 | 2.00 | 0.60 |
| 1:N:398:ASP:O | 1:N:401:HIS:HB2 | 2.02 | 0.60 |
| 2:O:34:LYS:HG3 | 2:O:35:SER:H | 1.66 | 0.60 |
| 2:P:92:LEU:O | 2:Q:6:LEU:HB2 | 2.02 | 0.60 |
| 1:B:245:LYS:HA | 1:B:245:LYS:CE | 2.28 | 0.60 |
| 1:C:199:TYR:CZ | 1:C:202:PRO:HA | 2.36 | 0.60 |
| 1:G:368:ARG:HG2 | 1:G:372:LEU:HG | 1.83 | 0.60 |
| 1:G:82:ASN:HD22 | 1:G:86:GLY:HA2 | 1.67 | 0.60 |
| 1:H:169:VAL:HG22 | 1:H:169:VAL:O | 2.01 | 0.60 |
| 1:J:226:LYS:HA | 1:J:252:GLU:HB2 | 1.84 | 0.60 |
| 1:K:395:ARG:O | 1:K:398:ASP:HB2 | 2.02 | 0.60 |
| 1:L:147:VAL:HA | 1:L:150:ILE:HD12 | 1.84 | 0.60 |
| 1:N:302:SER:HB2 | 1:N:305:ILE:HD12 | 1.84 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:358:SER:O | 1:N:362:ARG:HB2 | 2.02 | 0.60 |
| 2:O:73:VAL:HG22 | 2:O:86:MET:HB3 | 1.84 | 0.60 |
| 1:A:256:GLY:O | 1:A:260:ALA:N | 2.30 | 0.60 |
| 1:A:355:GLU:HG3 | 1:A:357:THR:H | 1.67 | 0.60 |
| 1:B:499:VAL:HG23 | 1:B:500:THR:N | 2.16 | 0.60 |
| 1:D:252:GLU:O | 1:D:253:ASP:HB2 | 2.01 | 0.60 |
| 1:D:195:PHE:O | 1:D:329:THR:HG23 | 2.02 | 0.60 |
| 1:E:18:ARG:HB2 | 1:E:67:GLU:HG2 | 1.83 | 0.60 |
| 1:E:29:VAL:HG23 | 1:E:30:THR:HG23 | 1.84 | 0.60 |
| 1:E:219:PHE:HD1 | 1:E:319:GLN:HE21 | 1.50 | 0.60 |
| 1:H:115:ASP:HB3 | 1:H:436:GLN:HG2 | 1.83 | 0.60 |
| 1:H:219:PHE:HB2 | 1:H:247:LEU:HD23 | 1.83 | 0.60 |
| 1:H:359:ASP:CA | 1:H:362:ARG:HH12 | 2.15 | 0.60 |
| 1:I:55:SER:O | 1:I:58:ARG:HB3 | 2.02 | 0.60 |
| 1:K:155:ASP:CG | 1:K:158:VAL:HG23 | 2.22 | 0.60 |
| 1:L:314:LEU:HD12 | 1:L:314:LEU:N | 2.07 | 0.60 |
| 1:L:5:ASP:HB2 | 1:L:524:LEU:CD2 | 2.31 | 0.60 |
| 1:M:55:SER:HA | 1:M:58:ARG:NH1 | 2.17 | 0.60 |
| 1:N:101:THR:O | 1:N:105:LYS:HG3 | 2.02 | 0.60 |
| 1:N:395:ARG:O | 1:N:398:ASP:HB2 | 2.01 | 0.60 |
| 1:N:426:LEU:H | 1:N:426:LEU:CD2 | 2.09 | 0.60 |
| 1:M:36:ARG:HB3 | 1:N:516:THR:O | 2.02 | 0.60 |
| 1:A:234:LEU:N | 1:A:234:LEU:HD12 | 2.16 | 0.59 |
| 1:A:333:ILE:O | 1:A:334:ASP:HB2 | 2.02 | 0.59 |
| 1:B:242:LYS:HD3 | 1:B:242:LYS:C | 2.23 | 0.59 |
| 1:B:512:GLY:O | 1:B:515:ILE:HG12 | 2.00 | 0.59 |
| 1:C:28:LYS:O | 1:C:30:THR:N | 2.35 | 0.59 |
| 1:C:44:PHE:N | 1:C:44:PHE:HD1 | 1.93 | 0.59 |
| 1:F:350:ARG:HD3 | 1:F:353:ILE:HD12 | 1.84 | 0.59 |
| 1:H:124:VAL:O | 1:H:128:VAL:HG23 | 2.02 | 0.59 |
| 1:H:264:VAL:HA | 1:H:267:MET:HG2 | 1.84 | 0.59 |
| 1:I:233:MET:HA | 1:I:233:MET:HE3 | 1.83 | 0.59 |
| 1:I:264:VAL:HA | 1:I:267:MET:HG2 | 1.84 | 0.59 |
| 1:I:232:GLU:CB | 1:I:309:LEU:HD12 | 2.32 | 0.59 |
| 1:J:23:LEU:O | 1:J:27:VAL:HG12 | 2.02 | 0.59 |
| 1:K:222:LEU:HD11 | 1:K:293:ALA:HA | 1.84 | 0.59 |
| 1:L:233:MET:HE2 | 1:L:233:MET:HA | 1.83 | 0.59 |
| 1:L:287:ALA:HB1 | 1:L:368:ARG:CZ | 2.32 | 0.59 |
| 1:L:37:ASN:H | 1:L:37:ASN:HD22 | 1.50 | 0.59 |
| 1:L:499:VAL:CG2 | 1:L:500:THR:N | 2.65 | 0.59 |
| 1:M:478:TYR:CE1 | 1:M:483:GLU:HA | 2.37 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:25:ASP:HA | 1:N:28:LYS:HE2 | 1.84 | 0.59 |
| 1:N:277:LYS:NZ | 1:N:277:LYS:HB2 | 2.17 | 0.59 |
| 2:R:14:ARG:NH1 | 2:R:14:ARG:HB2 | 2.17 | 0.59 |
| 1:B:208:PRO:HB2 | 1:B:212:ALA:CB | 2.33 | 0.59 |
| 1:B:44:PHE:HD1 | 1:B:44:PHE:N | 1.95 | 0.59 |
| 1:C:266:THR:CG2 | 1:C:273:VAL:H | 2.14 | 0.59 |
| 1:G:140:ASP:OD1 | 1:G:142:LYS:HB3 | 2.02 | 0.59 |
| 1:H:385:THR:O | 1:H:389:MET:HB2 | 2.02 | 0.59 |
| 1:L:228:SER:HA | 1:L:255:GLU:HB2 | 1.84 | 0.59 |
| 1:M:216:GLU:OE1 | 1:M:216:GLU:HA | 2.02 | 0.59 |
| 1:N:270:ILE:HG22 | 1:N:271:VAL:N | 2.17 | 0.59 |
| 2:P:50:GLU:O | 2:P:52:GLY:N | 2.35 | 0.59 |
| 2:S:20:LYS:HG2 | 2:S:27:LEU:CD2 | 2.32 | 0.59 |
| 1:A:234:LEU:H | 1:A:234:LEU:CD1 | 2.14 | 0.59 |
| 1:A:313:THR:N | 1:A:316:ASP:OD2 | 2.35 | 0.59 |
| 1:A:350:ARG:HA | 1:A:353:ILE:HD12 | 1.84 | 0.59 |
| 1:B:327:LYS:HD3 | 1:B:327:LYS:H | 1.67 | 0.59 |
| 1:F:486:GLY:HA3 | 1:F:491:MET:HE2 | 1.83 | 0.59 |
| 1:G:229:ASN:C | 1:G:231:ARG:H | 2.06 | 0.59 |
| 1:H:314:LEU:H | 1:H:314:LEU:CD1 | 2.06 | 0.59 |
| 1:I:504:LEU:O | 1:I:504:LEU:HD22 | 2.02 | 0.59 |
| 1:K:146:GLN:O | 1:K:150:ILE:HG13 | 2.02 | 0.59 |
| 1:L:72:GLN:HE21 | 1:L:72:GLN:HA | 1.68 | 0.59 |
| 1:N:226:LYS:HG3 | 1:N:252:GLU:HB3 | 1.85 | 0.59 |
| 1:N:31:LEU:HG | 1:N:454:ILE:CD1 | 2.32 | 0.59 |
| 2:O:17:VAL:CG1 | 2:O:34:LYS:HA | 2.32 | 0.59 |
| 2:O:40:VAL:HG12 | 2:O:61:VAL:HA | 1.84 | 0.59 |
| 1:A:353:ILE:HG12 | 1:A:366:GLN:HE22 | 1.67 | 0.59 |
| 1:C:205:ILE:CD1 | 1:C:211:GLY:HA2 | 2.32 | 0.59 |
| 1:C:259:LEU:O | 1:C:263:VAL:HG23 | 2.03 | 0.59 |
| 1:C:84:ALA:HB2 | 1:C:506:TYR:HE2 | 1.68 | 0.59 |
| 1:D:218:PRO:HA | 1:D:246:PRO:HG2 | 1.83 | 0.59 |
| 1:F:218:PRO:HA | 1:F:246:PRO:HG2 | 1.82 | 0.59 |
| 1:I:116:LEU:HD23 | 1:I:435:ASP:O | 2.02 | 0.59 |
| 1:I:345:ARG:HA | 1:I:348:GLN:NE2 | 2.18 | 0.59 |
| 1:J:217:SER:N | 1:J:218:PRO:HD3 | 2.17 | 0.59 |
| 1:K:169:VAL:O | 1:K:169:VAL:HG22 | 2.02 | 0.59 |
| 1:K:383:ALA:CB | 1:K:389:MET:HA | 2.31 | 0.59 |
| 1:L:135:SER:HA | 1:L:412:VAL:HG12 | 1.83 | 0.59 |
| 1:N:313:THR:HG22 | 1:N:314:LEU:N | 2.17 | 0.59 |
| 1:B:94:VAL:HG12 | 1:B:449:ALA:HB1 | 1.84 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:281:PHE:O | 1:D:284:ARG:HB3 | 2.01 | 0.59 |
| 1:D:325:ILE:HG13 | 1:D:330:THR:HG23 | 1.82 | 0.59 |
| 1:D:392:LYS:O | 1:D:396:VAL:HG23 | 2.02 | 0.59 |
| 1:D:499:VAL:HG23 | 1:D:500:THR:N | 2.17 | 0.59 |
| 1:E:124:VAL:HG13 | 1:E:504:LEU:CD1 | 2.33 | 0.59 |
| 1:E:247:LEU:O | 1:E:273:VAL:HG13 | 2.02 | 0.59 |
| 1:E:326:ASN:ND2 | 1:E:328:ASP:H | 1.99 | 0.59 |
| 1:F:348:GLN:NE2 | 1:F:352:GLN:NE2 | 2.49 | 0.59 |
| 1:F:84:ALA:HB2 | 1:F:506:TYR:HE2 | 1.67 | 0.59 |
| 1:G:54:VAL:HB | 1:G:89:THR:HG21 | 1.83 | 0.59 |
| 1:I:194:GLN:HG2 | 1:I:195:PHE:N | 2.17 | 0.59 |
| 1:I:358:SER:HB3 | 1:I:361:ASP:OD1 | 2.03 | 0.59 |
| 1:J:175:ILE:HD13 | 1:J:404:ARG:NH2 | 2.18 | 0.59 |
| 1:L:232:GLU:HA | 1:L:310:GLU:HG2 | 1.84 | 0.59 |
| 1:M:313:THR:HG22 | 1:M:314:LEU:N | 2.18 | 0.59 |
| 1:N:324:VAL:C | 1:N:325:ILE:HD12 | 2.22 | 0.59 |
| 2:O:43:VAL:HG23 | 2:O:61:VAL:HG22 | 1.84 | 0.59 |
| 1:A:160:LYS:O | 1:A:164:GLU:HG3 | 2.03 | 0.59 |
| 1:A:219:PHE:HB2 | 1:A:247:LEU:CD2 | 2.32 | 0.59 |
| 1:A:242:LYS:C | 1:A:242:LYS:HD3 | 2.23 | 0.59 |
| 1:A:273:VAL:CG1 | 1:A:274:ALA:H | 2.15 | 0.59 |
| 1:A:310:GLU:O | 1:A:312:ALA:N | 2.35 | 0.59 |
| 1:D:25:ASP:HA | 1:D:28:LYS:HE2 | 1.84 | 0.59 |
| 1:D:305:ILE:N | 1:D:305:ILE:CD1 | 2.66 | 0.59 |
| 1:E:285:ARG:HG3 | 1:E:286:LYS:N | 2.18 | 0.59 |
| 1:E:35:GLY:HA3 | 1:E:51:LYS:HE2 | 1.84 | 0.59 |
| 1:E:381:VAL:HG21 | 1:E:393:LYS:HA | 1.85 | 0.59 |
| 1:F:289:LEU:HD23 | 1:F:292:ILE:HD12 | 1.82 | 0.59 |
| 1:H:31:LEU:HG | 1:H:454:ILE:CD1 | 2.31 | 0.59 |
| 1:I:198:GLY:HA3 | 1:I:328:ASP:HA | 1.85 | 0.59 |
| 1:K:384:ALA:O | 1:L:281:PHE:HZ | 1.85 | 0.59 |
| 1:N:223:ALA:HB3 | 1:N:251:ALA:CB | 2.25 | 0.59 |
| 1:N:365:LEU:O | 1:N:369:VAL:HG23 | 2.02 | 0.59 |
| 1:A:339:GLU:H | 1:A:339:GLU:CD | 2.06 | 0.59 |
| 1:B:346:VAL:HG12 | 1:B:350:ARG:HH22 | 1.66 | 0.59 |
| 1:B:348:GLN:NE2 | 1:B:352:GLN:NE2 | 2.49 | 0.59 |
| 1:E:448:GLU:O | 1:E:452:ARG:HG2 | 2.03 | 0.59 |
| 1:G:214:GLU:HA | 1:G:323:VAL:O | 2.03 | 0.59 |
| 1:G:19:GLY:HA3 | 1:G:67:GLU:O | 2.02 | 0.59 |
| 1:A:387:VAL:HG13 | 1:G:76:GLU:OE1 | 2.03 | 0.59 |
| 1:H:359:ASP:O | 1:H:363:GLU:HB2 | 2.02 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:422:VAL:O | 1:H:425:LYS:HB2 | 2.03 | 0.59 |
| 1:I:161:LEU:H | 1:I:161:LEU:CD1 | 2.16 | 0.59 |
| 1:I:205:ILE:HD13 | 1:I:211:GLY:HA2 | 1.84 | 0.59 |
| 1:I:124:VAL:HG13 | 1:I:504:LEU:HD13 | 1.84 | 0.59 |
| 1:K:101:THR:O | 1:K:105:LYS:HG3 | 2.01 | 0.59 |
| 1:K:422:VAL:O | 1:K:426:LEU:HD23 | 2.02 | 0.59 |
| 1:L:31:LEU:HG | 1:L:454:ILE:HD11 | 1.84 | 0.59 |
| 2:R:17:VAL:HG13 | 2:R:34:LYS:HA | 1.84 | 0.59 |
| 2:S:11:ILE:HB | 2:S:42:ALA:HB3 | 1.85 | 0.59 |
| 1:B:77:VAL:HG12 | 1:B:510:VAL:HG21 | 1.84 | 0.59 |
| 1:C:131:LEU:HD21 | 1:C:422:VAL:HG11 | 1.83 | 0.59 |
| 1:C:349:ILE:HG21 | 1:C:369:VAL:HG22 | 1.84 | 0.59 |
| 1:E:302:SER:HB2 | 1:E:305:ILE:HD13 | 1.85 | 0.59 |
| 1:G:207:LYS:CB | 1:G:208:PRO:HD3 | 2.30 | 0.59 |
| 1:G:322:ARG:CG | 1:G:323:VAL:H | 2.10 | 0.59 |
| 1:J:124:VAL:HG13 | 1:J:504:LEU:HD13 | 1.83 | 0.59 |
| 1:L:10:ASN:O | 1:L:11:ASP:C | 2.41 | 0.59 |
| 1:A:215:LEU:O | 1:A:322:ARG:HG3 | 2.03 | 0.59 |
| 1:B:124:VAL:HG13 | 1:B:504:LEU:HD12 | 1.83 | 0.59 |
| 1:B:278:ALA:HB1 | 1:B:279:PRO:HD3 | 1.84 | 0.59 |
| 1:B:482:THR:OG1 | 1:B:484:GLU:HG2 | 2.02 | 0.59 |
| 1:F:313:THR:N | 1:F:316:ASP:OD2 | 2.32 | 0.59 |
| 1:G:253:ASP:CG | 1:G:254:VAL:H | 2.05 | 0.59 |
| 1:G:348:GLN:HE22 | 1:G:352:GLN:NE2 | 2.01 | 0.59 |
| 1:H:17:LEU:O | 1:H:20:VAL:HG13 | 2.03 | 0.59 |
| 1:H:219:PHE:CE1 | 1:H:245:LYS:HB2 | 2.38 | 0.59 |
| 1:H:232:GLU:HA | 1:H:310:GLU:CG | 2.33 | 0.59 |
| 1:H:266:THR:CG2 | 1:H:273:VAL:H | 2.16 | 0.59 |
| 1:H:266:THR:HB | 1:H:272:LYS:HG3 | 1.84 | 0.59 |
| 1:I:277:LYS:HB2 | 1:I:277:LYS:NZ | 2.17 | 0.59 |
| 1:J:247:LEU:HB3 | 1:J:273:VAL:HG11 | 1.83 | 0.59 |
| 1:J:217:SER:HA | 1:J:320:ALA:O | 2.03 | 0.59 |
| 1:K:149:THR:CG2 | 1:K:159:GLY:HA3 | 2.30 | 0.59 |
| 1:K:31:LEU:HG | 1:K:454:ILE:HD11 | 1.85 | 0.59 |
| 1:M:277:LYS:HB2 | 1:M:277:LYS:HZ2 | 1.67 | 0.59 |
| 1:N:228:SER:HA | 1:N:255:GLU:HB2 | 1.85 | 0.59 |
| 2:U:40:VAL:CG2 | 2:U:63:ASP:HB2 | 2.33 | 0.59 |
| 2:U:64:ILE:O | 2:U:94:ILE:HG23 | 2.03 | 0.59 |
| 1:A:177:VAL:HG11 | 1:A:397:GLU:CG | 2.31 | 0.59 |
| 1:A:305:ILE:CG2 | 1:A:306:GLY:H | 2.10 | 0.59 |
| 1:A:44:PHE:N | 1:A:44:PHE:HD1 | 1.94 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:266:THR:HG22 | 1:B:273:VAL:H | 1.68 | 0.59 |
| 1:B:360:TYR:HA | 1:B:363:GLU:CD | 2.23 | 0.59 |
| 1:D:199:TYR:HE2 | 1:D:205:ILE:HG12 | 1.67 | 0.59 |
| 1:F:16:MET:O | 1:F:20:VAL:HG23 | 2.03 | 0.59 |
| 1:H:111:MET:HG2 | 1:H:435:ASP:OD1 | 2.02 | 0.59 |
| 1:N:206:ASN:OD1 | 1:N:213:VAL:HA | 2.03 | 0.59 |
| 1:N:314:LEU:HD12 | 1:N:314:LEU:N | 2.15 | 0.59 |
| 2:Q:6:LEU:O | 2:Q:7:HIS:O | 2.21 | 0.59 |
| 1:A:219:PHE:CE2 | 1:A:245:LYS:HB2 | 2.38 | 0.58 |
| 1:A:499:VAL:CG2 | 1:A:500:THR:N | 2.66 | 0.58 |
| 1:B:346:VAL:CG1 | 1:B:350:ARG:HH22 | 2.16 | 0.58 |
| 1:C:295:LEU:O | 1:C:337:GLY:HA3 | 2.02 | 0.58 |
| 1:D:266:THR:HG22 | 1:D:273:VAL:H | 1.68 | 0.58 |
| 1:F:455:VAL:HG12 | 1:F:460:GLU:O | 2.03 | 0.58 |
| 1:H:123:ALA:HB2 | 1:H:440:ILE:HG23 | 1.85 | 0.58 |
| 1:K:231:ARG:O | 1:K:234:LEU:HG | 2.03 | 0.58 |
| 1:K:314:LEU:N | 1:K:314:LEU:HD12 | 2.06 | 0.58 |
| 1:L:217:SER:N | 1:L:218:PRO:HD3 | 2.18 | 0.58 |
| 1:M:266:THR:CG2 | 1:M:273:VAL:H | 2.16 | 0.58 |
| 1:A:237:LEU:CD2 | 2:O:26:VAL:HG22 | 2.29 | 0.58 |
| 2:O:77:LYS:HG3 | 2:O:80:ASN:HA | 1.85 | 0.58 |
| 2:R:97:ALA:O | 2:S:1:MET:HA | 2.03 | 0.58 |
| 1:A:84:ALA:HB2 | 1:A:506:TYR:HE2 | 1.68 | 0.58 |
| 1:B:130:GLU:O | 1:B:133:ALA:HB3 | 2.03 | 0.58 |
| 1:B:350:ARG:O | 1:B:354:GLU:HG2 | 2.02 | 0.58 |
| 1:C:266:THR:HG22 | 1:C:273:VAL:H | 1.67 | 0.58 |
| 1:C:177:VAL:HG11 | 1:C:397:GLU:HG2 | 1.84 | 0.58 |
| 1:D:321:LYS:HB2 | 1:D:333:ILE:HB | 1.85 | 0.58 |
| 1:F:288:MET:HA | 1:F:291:ASP:OD2 | 2.03 | 0.58 |
| 1:F:472:GLY:HA3 | 1:F:476:TYR:HD2 | 1.68 | 0.58 |
| 1:G:180:GLY:CA | 1:G:380:LYS:HB3 | 2.33 | 0.58 |
| 1:G:84:ALA:HB2 | 1:G:506:TYR:HE2 | 1.68 | 0.58 |
| 1:H:124:VAL:HG13 | 1:H:504:LEU:CD1 | 2.33 | 0.58 |
| 1:H:270:ILE:HG22 | 1:H:271:VAL:N | 2.17 | 0.58 |
| 1:H:282:GLY:O | 1:H:285:ARG:HG2 | 2.02 | 0.58 |
| 1:I:270:ILE:HG22 | 1:I:271:VAL:N | 2.18 | 0.58 |
| 1:J:314:LEU:HD12 | 1:J:314:LEU:N | 2.05 | 0.58 |
| 1:K:221:LEU:HD13 | 1:K:222:LEU:N | 2.18 | 0.58 |
| 1:K:499:VAL:HG23 | 1:K:500:THR:N | 2.18 | 0.58 |
| 1:L:222:LEU:HD22 | 1:L:289:LEU:CD1 | 2.32 | 0.58 |
| 1:L:232:GLU:HB3 | 1:L:309:LEU:CB | 2.17 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:S:14:ARG:CG | 2:S:15:LYS:H | 2.15 | 0.58 |
| 2:T:7:HIS:O | 2:T:8:ASP:HB3 | 2.02 | 0.58 |
| 1:A:281:PHE:O | 1:A:285:ARG:HG2 | 2.03 | 0.58 |
| 1:A:28:LYS:O | 1:A:30:THR:N | 2.36 | 0.58 |
| 1:B:16:MET:O | 1:B:20:VAL:HG23 | 2.04 | 0.58 |
| 1:B:434:GLU:OE2 | 1:B:438:VAL:HG23 | 2.03 | 0.58 |
| 1:C:177:VAL:HG11 | 1:C:397:GLU:CG | 2.33 | 0.58 |
| 1:E:247:LEU:HD13 | 1:E:248:LEU:N | 2.17 | 0.58 |
| 1:E:339:GLU:N | 1:E:339:GLU:CD | 2.57 | 0.58 |
| 1:F:247:LEU:HD13 | 1:F:248:LEU:N | 2.18 | 0.58 |
| 1:G:357:THR:HB | 1:G:361:ASP:CB | 2.33 | 0.58 |
| 1:H:385:THR:HG23 | 1:H:388:GLU:H | 1.68 | 0.58 |
| 1:I:157:THR:O | 1:I:161:LEU:CD1 | 2.51 | 0.58 |
| 1:J:146:GLN:O | 1:J:150:ILE:HG13 | 2.03 | 0.58 |
| 1:K:219:PHE:HB3 | 1:K:317:LEU:HD23 | 1.85 | 0.58 |
| 1:K:415:GLY:N | 1:K:417:VAL:HG23 | 2.16 | 0.58 |
| 1:G:237:LEU:HD22 | 2:U:26:VAL:CG2 | 2.33 | 0.58 |
| 1:A:475:ASN:N | 1:A:475:ASN:HD22 | 2.01 | 0.58 |
| 1:C:233:MET:HE3 | 1:C:236:VAL:HB | 1.83 | 0.58 |
| 1:D:242:LYS:HD3 | 1:D:242:LYS:C | 2.24 | 0.58 |
| 1:E:434:GLU:O | 1:E:435:ASP:C | 2.42 | 0.58 |
| 1:F:285:ARG:HG3 | 1:F:286:LYS:H | 1.68 | 0.58 |
| 1:H:487:ASN:HB3 | 1:H:490:ASP:HB2 | 1.85 | 0.58 |
| 1:I:263:VAL:O | 1:I:267:MET:HG2 | 2.03 | 0.58 |
| 1:J:161:LEU:H | 1:J:161:LEU:HD12 | 1.68 | 0.58 |
| 1:L:107:VAL:HG23 | 1:L:108:ALA:H | 1.67 | 0.58 |
| 1:L:149:THR:HG23 | 1:L:159:GLY:CA | 2.28 | 0.58 |
| 2:O:84:LEU:N | 2:O:84:LEU:HD12 | 2.18 | 0.58 |
| 2:P:18:GLU:CD | 2:P:33:ALA:HB3 | 2.24 | 0.58 |
| 2:S:50:GLU:OE1 | 2:T:50:GLU:HA | 2.02 | 0.58 |
| 1:A:18:ARG:HH11 | 1:A:18:ARG:CB | 2.04 | 0.58 |
| 1:A:273:VAL:CG1 | 1:A:274:ALA:N | 2.67 | 0.58 |
| 1:C:219:PHE:HB2 | 1:C:247:LEU:CD2 | 2.33 | 0.58 |
| 1:D:229:ASN:C | 1:D:231:ARG:H | 2.07 | 0.58 |
| 1:D:512:GLY:O | 1:D:515:ILE:HG12 | 2.03 | 0.58 |
| 1:E:72:GLN:NE2 | 1:E:72:GLN:HA | 2.18 | 0.58 |
| 1:F:308:GLU:H | 1:F:311:LYS:HB3 | 1.68 | 0.58 |
| 1:G:342:ILE:O | 1:G:346:VAL:HG23 | 2.04 | 0.58 |
| 1:I:303:GLU:C | 1:I:305:ILE:H | 2.05 | 0.58 |
| 1:J:149:THR:HG22 | 1:J:156:GLU:HA | 1.85 | 0.58 |
| 1:L:193:MET:HB3 | 1:L:332:ILE:HD11 | 1.86 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:358:SER:O | 1:M:362:ARG:HB2 | 2.03 | 0.58 |
| 2:T:20:LYS:HG2 | 2:T:27:LEU:HD23 | 1.86 | 0.58 |
| 2:U:7:HIS:O | 2:U:8:ASP:HB3 | 2.02 | 0.58 |
| 1:A:327:LYS:HD3 | 1:A:327:LYS:H | 1.69 | 0.58 |
| 1:A:80:LYS:HD2 | 1:A:506:TYR:CZ | 2.39 | 0.58 |
| 1:C:124:VAL:HG13 | 1:C:504:LEU:CD1 | 2.33 | 0.58 |
| 1:C:299:THR:HB | 1:C:316:ASP:HB3 | 1.85 | 0.58 |
| 1:C:221:LEU:HD13 | 1:C:317:LEU:CD2 | 2.33 | 0.58 |
| 1:D:80:LYS:HD2 | 1:D:506:TYR:CZ | 2.38 | 0.58 |
| 1:E:292:ILE:O | 1:E:295:LEU:HB3 | 2.02 | 0.58 |
| 1:E:434:GLU:OE2 | 1:E:438:VAL:HG23 | 2.03 | 0.58 |
| 1:F:177:VAL:HG11 | 1:F:397:GLU:CG | 2.34 | 0.58 |
| 1:G:264:VAL:HA | 1:G:267:MET:HB2 | 1.85 | 0.58 |
| 1:G:310:GLU:O | 1:G:312:ALA:N | 2.36 | 0.58 |
| 1:I:392:LYS:O | 1:I:396:VAL:HG23 | 2.04 | 0.58 |
| 1:J:221:LEU:HD13 | 1:J:222:LEU:N | 2.18 | 0.58 |
| 1:J:299:THR:HB | 1:J:316:ASP:HB3 | 1.86 | 0.58 |
| 1:J:360:TYR:O | 1:J:364:LYS:HB2 | 2.04 | 0.58 |
| 1:K:219:PHE:CE1 | 1:K:245:LYS:HB2 | 2.39 | 0.58 |
| 1:K:282:GLY:O | 1:K:285:ARG:HG2 | 2.04 | 0.58 |
| 1:L:230:ILE:CD1 | 1:L:257:GLU:HG2 | 2.33 | 0.58 |
| 1:L:195:PHE:CE1 | 1:L:330:THR:HB | 2.38 | 0.58 |
| 2:Q:17:VAL:HG13 | 2:Q:34:LYS:HA | 1.84 | 0.58 |
| 2:S:47:ARG:HG2 | 2:S:49:LEU:H | 1.68 | 0.58 |
| 1:B:253:ASP:CG | 1:B:254:VAL:H | 2.07 | 0.58 |
| 1:D:279:PRO:HD2 | 1:D:285:ARG:HA | 1.85 | 0.58 |
| 1:D:82:ASN:HD22 | 1:D:86:GLY:HA2 | 1.68 | 0.58 |
| 1:E:246:PRO:HA | 1:E:272:LYS:O | 2.04 | 0.58 |
| 1:E:162:ILE:HG21 | 1:E:403:THR:HG21 | 1.86 | 0.58 |
| 1:F:273:VAL:CG1 | 1:F:274:ALA:H | 2.15 | 0.58 |
| 1:G:266:THR:CG2 | 1:G:273:VAL:H | 2.17 | 0.58 |
| 1:G:199:TYR:CA | 1:G:276:VAL:HG12 | 2.29 | 0.58 |
| 1:H:69:MET:HE2 | 1:H:522:THR:HB | 1.84 | 0.58 |
| 1:J:233:MET:CE | 1:J:309:LEU:HD13 | 2.34 | 0.58 |
| 1:J:219:PHE:HB2 | 1:J:247:LEU:HD23 | 1.85 | 0.58 |
| 1:K:191:GLU:O | 1:K:334:ASP:HA | 2.04 | 0.58 |
| 1:L:193:MET:HG2 | 1:L:194:GLN:N | 2.18 | 0.58 |
| 1:L:231:ARG:O | 1:L:234:LEU:HG | 2.04 | 0.58 |
| 1:M:221:LEU:HD13 | 1:M:222:LEU:N | 2.19 | 0.58 |
| 1:M:386:GLU:O | 1:M:389:MET:HB3 | 2.04 | 0.58 |
| 1:N:247:LEU:HD22 | 1:N:248:LEU:N | 2.19 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:206:ASN:H | 1:A:213:VAL:HA | 1.68 | 0.58 |
| 1:A:253:ASP:CG | 1:A:254:VAL:H | 2.07 | 0.58 |
| 1:B:199:TYR:CZ | 1:B:202:PRO:HA | 2.38 | 0.58 |
| 1:C:213:VAL:O | 1:C:324:VAL:HA | 2.04 | 0.58 |
| 1:D:227:ILE:HD12 | 1:D:227:ILE:N | 2.18 | 0.58 |
| 1:D:499:VAL:CG2 | 1:D:500:THR:N | 2.66 | 0.58 |
| 1:F:234:LEU:HD12 | 1:F:234:LEU:N | 2.15 | 0.58 |
| 1:H:228:SER:O | 1:H:257:GLU:HB3 | 2.04 | 0.58 |
| 1:H:367:GLU:O | 1:H:370:ALA:HB3 | 2.04 | 0.58 |
| 1:H:415:GLY:N | 1:H:417:VAL:HG23 | 2.17 | 0.58 |
| 1:J:236:VAL:HG23 | 1:J:237:LEU:H | 1.69 | 0.58 |
| 1:M:17:LEU:O | 1:M:20:VAL:HG13 | 2.04 | 0.58 |
| 2:U:57:LEU:HD22 | 2:U:88:GLU:HB2 | 1.85 | 0.58 |
| 2:U:6:LEU:O | 2:U:7:HIS:O | 2.20 | 0.58 |
| 1:A:206:ASN:HB3 | 1:A:214:GLU:H | 1.69 | 0.58 |
| 1:A:215:LEU:C | 1:A:322:ARG:HG3 | 2.24 | 0.58 |
| 1:A:351:GLN:HG2 | 1:B:210:THR:OG1 | 2.04 | 0.58 |
| 1:B:146:GLN:HE21 | 1:B:494:LEU:HD11 | 1.68 | 0.58 |
| 1:C:147:VAL:O | 1:C:150:ILE:HG22 | 2.04 | 0.58 |
| 1:C:418:ALA:O | 1:C:422:VAL:HG13 | 2.04 | 0.58 |
| 1:D:215:LEU:C | 1:D:322:ARG:HG3 | 2.23 | 0.58 |
| 1:D:232:GLU:O | 1:D:233:MET:HB3 | 2.03 | 0.58 |
| 1:D:304:GLU:HB2 | 1:D:305:ILE:HD12 | 1.84 | 0.58 |
| 1:E:174:VAL:HG21 | 1:E:367:GLU:HA | 1.86 | 0.58 |
| 1:F:147:VAL:O | 1:F:150:ILE:HG22 | 2.04 | 0.58 |
| 1:F:232:GLU:O | 1:F:233:MET:HB3 | 2.02 | 0.58 |
| 1:F:365:LEU:O | 1:F:369:VAL:HG23 | 2.04 | 0.58 |
| 1:G:18:ARG:O | 1:G:22:VAL:HG23 | 2.04 | 0.58 |
| 1:G:266:THR:HG22 | 1:G:271:VAL:O | 2.03 | 0.58 |
| 1:G:293:ALA:HB1 | 1:G:298:GLY:O | 2.04 | 0.58 |
| 1:I:146:GLN:HE21 | 1:I:150:ILE:HD11 | 1.68 | 0.58 |
| 1:K:233:MET:CE | 1:K:309:LEU:HD13 | 2.34 | 0.58 |
| 1:M:247:LEU:C | 1:M:247:LEU:HD13 | 2.24 | 0.58 |
| 2:T:50:GLU:O | 2:T:52:GLY:N | 2.36 | 0.58 |
| 1:A:227:ILE:HG22 | 1:A:227:ILE:O | 2.03 | 0.58 |
| 1:A:285:ARG:HG3 | 1:A:286:LYS:H | 1.69 | 0.58 |
| 1:B:249:ILE:HB | 1:B:275:ALA:HB2 | 1.85 | 0.58 |
| 1:C:18:ARG:HB2 | 1:C:67:GLU:HG2 | 1.86 | 0.58 |
| 1:D:237:LEU:C | 1:D:237:LEU:HD23 | 2.24 | 0.58 |
| 1:E:248:LEU:C | 1:E:249:ILE:HD12 | 2.25 | 0.58 |
| 1:E:351:GLN:HG2 | 1:F:210:THR:OG1 | 2.04 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:177:VAL:HG11 | 1:E:397:GLU:HG2 | 1.86 | 0.58 |
| 1:F:230:ILE:O | 1:F:232:GLU:N | 2.37 | 0.58 |
| 1:G:44:PHE:N | 1:G:44:PHE:HD1 | 1.94 | 0.58 |
| 1:H:226:LYS:HD2 | 1:H:252:GLU:HG3 | 1.86 | 0.58 |
| 1:J:123:ALA:HB2 | 1:J:440:ILE:HG23 | 1.86 | 0.58 |
| 1:L:205:ILE:HD13 | 1:L:211:GLY:CA | 2.34 | 0.58 |
| 1:M:219:PHE:CE1 | 1:M:245:LYS:HD2 | 2.39 | 0.58 |
| 1:M:221:LEU:HD13 | 1:M:223:ALA:H | 1.67 | 0.58 |
| 1:M:230:ILE:H | 1:M:230:ILE:CD1 | 1.97 | 0.58 |
| 1:M:415:GLY:N | 1:M:417:VAL:HG23 | 2.18 | 0.58 |
| 1:N:413:ALA:CB | 1:N:417:VAL:HB | 2.34 | 0.58 |
| 2:Q:86:MET:HB2 | 2:Q:90:ASP:OD2 | 2.04 | 0.58 |
| 1:B:234:LEU:HD12 | 1:B:234:LEU:N | 2.17 | 0.57 |
| 1:C:232:GLU:O | 1:C:233:MET:HB3 | 2.03 | 0.57 |
| 1:D:278:ALA:HB1 | 1:D:279:PRO:HD2 | 1.86 | 0.57 |
| 1:E:366:GLN:O | 1:E:369:VAL:HB | 2.03 | 0.57 |
| 1:F:403:THR:O | 1:F:407:VAL:HG23 | 2.03 | 0.57 |
| 1:G:222:LEU:N | 1:G:222:LEU:HD12 | 2.19 | 0.57 |
| 1:H:161:LEU:H | 1:H:161:LEU:HD12 | 1.69 | 0.57 |
| 1:H:302:SER:HB2 | 1:H:305:ILE:CD1 | 2.34 | 0.57 |
| 1:J:160:LYS:HG2 | 1:J:164:GLU:OE2 | 2.03 | 0.57 |
| 1:J:385:THR:O | 1:J:389:MET:HB2 | 2.04 | 0.57 |
| 1:J:39:VAL:HG22 | 1:J:49:ILE:HG12 | 1.85 | 0.57 |
| 1:J:64:ASP:OD1 | 1:J:65:LYS:O | 2.21 | 0.57 |
| 1:K:434:GLU:HA | 1:K:437:ASN:HD22 | 1.67 | 0.57 |
| 1:M:10:ASN:O | 1:M:11:ASP:C | 2.42 | 0.57 |
| 2:O:50:GLU:HA | 2:U:50:GLU:OE1 | 2.03 | 0.57 |
| 1:B:285:ARG:HG3 | 1:B:286:LYS:H | 1.69 | 0.57 |
| 1:B:418:ALA:O | 1:B:422:VAL:HG13 | 2.04 | 0.57 |
| 1:B:96:ALA:O | 1:B:97:GLN:C | 2.42 | 0.57 |
| 1:C:227:ILE:HD12 | 1:C:227:ILE:N | 2.19 | 0.57 |
| 1:C:29:VAL:HG23 | 1:C:30:THR:HG23 | 1.86 | 0.57 |
| 1:C:414:GLY:HA2 | 1:C:495:ASP:OD2 | 2.04 | 0.57 |
| 1:D:124:VAL:HG13 | 1:D:504:LEU:CD1 | 2.33 | 0.57 |
| 1:D:29:VAL:HG23 | 1:D:30:THR:HG23 | 1.87 | 0.57 |
| 1:E:381:VAL:CG1 | 1:E:392:LYS:CG | 2.81 | 0.57 |
| 1:I:32:GLY:CA | 1:I:454:ILE:HG23 | 2.32 | 0.57 |
| 1:J:166:MET:CE | 1:J:171:LYS:HA | 2.33 | 0.57 |
| 1:J:235:PRO:HG2 | 1:J:236:VAL:H | 1.69 | 0.57 |
| 1:J:221:LEU:HD12 | 1:J:249:ILE:HG23 | 1.86 | 0.57 |
| 1:K:214:GLU:HA | 1:K:324:VAL:HG12 | 1.84 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:291:ASP:O | 1:K:294:THR:HB | 2.04 | 0.57 |
| 1:K:324:VAL:C | 1:K:325:ILE:HD12 | 2.24 | 0.57 |
| 1:L:264:VAL:HA | 1:L:267:MET:CG | 2.33 | 0.57 |
| 1:L:475:ASN:ND2 | 1:L:489:ILE:HD12 | 2.18 | 0.57 |
| 1:L:472:GLY:HA3 | 1:L:476:TYR:CD2 | 2.39 | 0.57 |
| 1:B:287:ALA:O | 1:B:290:GLN:NE2 | 2.36 | 0.57 |
| 1:E:248:LEU:HD13 | 1:E:249:ILE:N | 2.18 | 0.57 |
| 1:E:266:THR:CG2 | 1:E:273:VAL:H | 2.17 | 0.57 |
| 1:E:409:GLU:CD | 1:E:501:ARG:HH21 | 2.08 | 0.57 |
| 1:E:5:ASP:HB2 | 1:E:524:LEU:HD23 | 1.86 | 0.57 |
| 1:F:130:GLU:O | 1:F:134:LEU:HD13 | 2.05 | 0.57 |
| 1:F:199:TYR:CA | 1:F:276:VAL:HG12 | 2.32 | 0.57 |
| 1:F:372:LEU:O | 1:F:373:ALA:HB2 | 2.03 | 0.57 |
| 1:G:326:ASN:ND2 | 1:G:328:ASP:N | 2.52 | 0.57 |
| 1:G:417:VAL:HG13 | 1:G:418:ALA:N | 2.20 | 0.57 |
| 1:G:35:GLY:HA3 | 1:G:51:LYS:HE2 | 1.86 | 0.57 |
| 1:H:27:VAL:HG11 | 1:H:93:THR:HG21 | 1.87 | 0.57 |
| 1:K:281:PHE:O | 1:K:284:ARG:NH1 | 2.37 | 0.57 |
| 1:L:367:GLU:O | 1:L:370:ALA:HB3 | 2.05 | 0.57 |
| 1:M:478:TYR:HB2 | 1:M:485:TYR:CE2 | 2.39 | 0.57 |
| 1:M:66:PHE:HD1 | 1:M:520:MET:HE2 | 1.69 | 0.57 |
| 1:N:400:LEU:HD23 | 1:N:400:LEU:C | 2.24 | 0.57 |
| 1:N:422:VAL:O | 1:N:425:LYS:HB2 | 2.04 | 0.57 |
| 2:S:5:PRO:HD3 | 2:S:42:ALA:CB | 2.34 | 0.57 |
| 1:A:288:MET:HA | 1:A:291:ASP:OD2 | 2.04 | 0.57 |
| 1:A:289:LEU:N | 1:A:290:GLN:OE1 | 2.33 | 0.57 |
| 1:B:259:LEU:O | 1:B:263:VAL:HG23 | 2.04 | 0.57 |
| 1:B:322:ARG:CG | 1:B:323:VAL:H | 2.11 | 0.57 |
| 1:D:224:ASP:HB2 | 1:D:303:GLU:HB3 | 1.87 | 0.57 |
| 1:E:218:PRO:HA | 1:E:246:PRO:HG2 | 1.85 | 0.57 |
| 1:E:265:ASN:HB3 | 1:E:271:VAL:HG22 | 1.87 | 0.57 |
| 1:F:199:TYR:CZ | 1:F:202:PRO:HA | 2.39 | 0.57 |
| 1:F:266:THR:CG2 | 1:F:273:VAL:H | 2.18 | 0.57 |
| 1:F:475:ASN:HD22 | 1:F:475:ASN:N | 2.02 | 0.57 |
| 1:G:219:PHE:CE2 | 1:G:245:LYS:HB2 | 2.39 | 0.57 |
| 1:J:356:ALA:CB | 1:J:362:ARG:HE | 2.07 | 0.57 |
| 1:J:478:TYR:CE1 | 1:J:483:GLU:HA | 2.40 | 0.57 |
| 1:K:218:PRO:HB3 | 1:K:246:PRO:C | 2.25 | 0.57 |
| 1:L:227:ILE:O | 1:L:254:VAL:HA | 2.04 | 0.57 |
| 1:A:229:ASN:C | 1:A:231:ARG:H | 2.06 | 0.57 |
| 1:A:290:GLN:OE1 | 1:A:290:GLN:N | 2.37 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:290:GLN:N | 1:B:290:GLN:OE1 | 2.37 | 0.57 |
| 1:D:228:SER:O | 1:D:257:GLU:HB3 | 2.04 | 0.57 |
| 1:D:285:ARG:HG3 | 1:D:286:LYS:N | 2.20 | 0.57 |
| 1:E:249:ILE:HB | 1:E:275:ALA:HB2 | 1.86 | 0.57 |
| 1:E:308:GLU:HB2 | 1:E:311:LYS:HB2 | 1.87 | 0.57 |
| 1:E:404:ARG:HG3 | 1:E:404:ARG:HH11 | 1.69 | 0.57 |
| 1:F:309:LEU:HD12 | 1:F:309:LEU:H | 1.70 | 0.57 |
| 1:G:472:GLY:HA3 | 1:G:476:TYR:HD2 | 1.68 | 0.57 |
| 1:H:256:GLY:O | 1:H:260:ALA:N | 2.37 | 0.57 |
| 1:K:263:VAL:O | 1:K:267:MET:HG2 | 2.04 | 0.57 |
| 1:L:303:GLU:C | 1:L:305:ILE:H | 2.08 | 0.57 |
| 1:A:289:LEU:O | 1:A:292:ILE:HB | 2.04 | 0.57 |
| 1:A:325:ILE:HG13 | 1:A:330:THR:HG23 | 1.86 | 0.57 |
| 1:C:18:ARG:O | 1:C:22:VAL:HG23 | 2.04 | 0.57 |
| 1:C:365:LEU:O | 1:C:369:VAL:HG23 | 2.04 | 0.57 |
| 1:D:107:VAL:HG13 | 1:D:113:PRO:HG3 | 1.85 | 0.57 |
| 1:D:227:ILE:HG22 | 1:D:227:ILE:O | 2.04 | 0.57 |
| 1:D:259:LEU:O | 1:D:262:LEU:HB3 | 2.05 | 0.57 |
| 1:E:327:LYS:HD3 | 1:E:327:LYS:H | 1.68 | 0.57 |
| 1:G:223:ALA:HB3 | 1:G:251:ALA:HB2 | 1.85 | 0.57 |
| 1:G:280:GLY:HA3 | 1:G:284:ARG:HH11 | 1.69 | 0.57 |
| 1:G:310:GLU:H | 1:G:310:GLU:CD | 2.07 | 0.57 |
| 1:H:494:LEU:HD23 | 1:H:494:LEU:H | 1.67 | 0.57 |
| 1:I:31:LEU:HG | 1:I:454:ILE:CD1 | 2.34 | 0.57 |
| 1:I:96:ALA:O | 1:I:100:ILE:HG13 | 2.05 | 0.57 |
| 1:J:66:PHE:HA | 1:J:520:MET:HE1 | 1.87 | 0.57 |
| 1:K:34:LYS:HB2 | 1:K:458:CYS:SG | 2.44 | 0.57 |
| 1:K:362:ARG:NH1 | 1:K:362:ARG:HB3 | 2.19 | 0.57 |
| 1:K:433:ASN:HD22 | 1:K:434:GLU:N | 2.02 | 0.57 |
| 1:L:284:ARG:HH11 | 1:L:284:ARG:CB | 2.15 | 0.57 |
| 1:L:32:GLY:HA3 | 1:L:454:ILE:HG23 | 1.87 | 0.57 |
| 1:M:160:LYS:HG2 | 1:M:164:GLU:OE2 | 2.04 | 0.57 |
| 1:M:235:PRO:HG2 | 1:M:236:VAL:H | 1.70 | 0.57 |
| 2:R:47:ARG:HB3 | 2:R:55:LYS:HG2 | 1.87 | 0.57 |
| 2:U:20:LYS:HG2 | 2:U:27:LEU:CD2 | 2.34 | 0.57 |
| 1:B:299:THR:HB | 1:B:316:ASP:HB3 | 1.86 | 0.57 |
| 1:C:207:LYS:HB2 | 1:C:207:LYS:NZ | 2.20 | 0.57 |
| 1:C:288:MET:O | 1:C:289:LEU:HG | 2.04 | 0.57 |
| 1:C:233:MET:CA | 1:C:310:GLU:HG3 | 2.21 | 0.57 |
| 1:C:346:VAL:HG12 | 1:C:350:ARG:NH2 | 2.18 | 0.57 |
| 1:C:472:GLY:HA3 | 1:C:476:TYR:HD2 | 1.70 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:194:GLN:NE2 | 1:D:329:THR:HG21 | 2.20 | 0.57 |
| 1:D:350:ARG:O | 1:D:353:ILE:HB | 2.05 | 0.57 |
| 1:E:52:ASP:OD1 | 1:E:54:VAL:HG12 | 2.04 | 0.57 |
| 1:H:138:CYS:SG | 1:H:144:ILE:HD13 | 2.45 | 0.57 |
| 1:J:34:LYS:HB2 | 1:J:458:CYS:SG | 2.44 | 0.57 |
| 1:K:161:LEU:H | 1:K:161:LEU:CD1 | 2.17 | 0.57 |
| 1:N:478:TYR:HB2 | 1:N:485:TYR:CD2 | 2.40 | 0.57 |
| 1:A:130:GLU:O | 1:A:134:LEU:HD13 | 2.04 | 0.57 |
| 1:B:236:VAL:O | 1:B:239:ALA:HB3 | 2.05 | 0.57 |
| 1:C:144:ILE:O | 1:C:147:VAL:HG22 | 2.05 | 0.57 |
| 1:C:215:LEU:C | 1:C:322:ARG:HG3 | 2.24 | 0.57 |
| 1:E:314:LEU:HD12 | 1:E:314:LEU:C | 2.25 | 0.57 |
| 1:G:281:PHE:O | 1:G:284:ARG:HB3 | 2.05 | 0.57 |
| 1:H:216:GLU:HA | 1:H:216:GLU:OE1 | 2.05 | 0.57 |
| 1:H:215:LEU:CB | 1:H:218:PRO:HG2 | 2.35 | 0.57 |
| 1:H:392:LYS:O | 1:H:396:VAL:HG23 | 2.05 | 0.57 |
| 1:H:499:VAL:CG2 | 1:H:500:THR:N | 2.68 | 0.57 |
| 1:J:386:GLU:HG2 | 1:J:390:LYS:HE2 | 1.86 | 0.57 |
| 1:L:55:SER:HA | 1:L:58:ARG:NH1 | 2.20 | 0.57 |
| 1:M:193:MET:HG2 | 1:M:194:GLN:N | 2.19 | 0.57 |
| 2:O:5:PRO:CD | 2:O:42:ALA:HB1 | 2.33 | 0.57 |
| 1:A:249:ILE:HB | 1:A:275:ALA:HB2 | 1.86 | 0.57 |
| 1:A:357:THR:HB | 1:A:361:ASP:CB | 2.35 | 0.57 |
| 1:B:291:ASP:HB2 | 1:B:372:LEU:HD21 | 1.85 | 0.57 |
| 1:B:450:PRO:O | 1:B:454:ILE:HG13 | 2.05 | 0.57 |
| 1:C:417:VAL:HA | 1:C:420:ILE:HG22 | 1.86 | 0.57 |
| 1:D:245:LYS:HA | 1:D:245:LYS:CE | 2.32 | 0.57 |
| 1:E:123:ALA:CB | 1:E:440:ILE:HG23 | 2.34 | 0.57 |
| 1:E:456:LEU:HD13 | 1:E:462:PRO:CG | 2.34 | 0.57 |
| 1:F:96:ALA:O | 1:F:97:GLN:C | 2.43 | 0.57 |
| 1:G:23:LEU:HD13 | 1:G:23:LEU:C | 2.25 | 0.57 |
| 1:G:247:LEU:HB3 | 1:G:273:VAL:HG13 | 1.87 | 0.57 |
| 1:G:266:THR:HG22 | 1:G:273:VAL:H | 1.69 | 0.57 |
| 1:G:487:ASN:OD1 | 1:G:489:ILE:N | 2.36 | 0.57 |
| 1:H:171:LYS:HD3 | 1:H:407:VAL:CG1 | 2.35 | 0.57 |
| 1:H:124:VAL:HG13 | 1:H:504:LEU:HD11 | 1.87 | 0.57 |
| 1:I:147:VAL:HA | 1:I:150:ILE:HD12 | 1.87 | 0.57 |
| 1:I:406:ALA:O | 1:I:410:GLY:N | 2.36 | 0.57 |
| 1:K:247:LEU:HD22 | 1:K:248:LEU:N | 2.20 | 0.57 |
| 1:K:411:VAL:HG21 | 1:K:494:LEU:HD12 | 1.86 | 0.57 |
| 1:L:336:VAL:O | 1:L:336:VAL:HG12 | 2.05 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:202:PRO:C | 1:M:204:PHE:H | 2.08 | 0.57 |
| 1:M:233:MET:HA | 1:M:233:MET:HE2 | 1.87 | 0.57 |
| 1:M:248:LEU:HD22 | 1:M:249:ILE:N | 2.18 | 0.57 |
| 1:M:203:TYR:HB2 | 1:M:263:VAL:HG13 | 1.85 | 0.57 |
| 1:M:31:LEU:HG | 1:M:454:ILE:CD1 | 2.35 | 0.57 |
| 2:P:6:LEU:O | 2:P:7:HIS:O | 2.23 | 0.57 |
| 1:A:266:THR:CG2 | 1:A:273:VAL:H | 2.17 | 0.57 |
| 1:B:273:VAL:CG1 | 1:B:274:ALA:N | 2.67 | 0.57 |
| 1:C:278:ALA:HB1 | 1:C:279:PRO:HD3 | 1.85 | 0.57 |
| 1:D:240:VAL:O | 1:D:244:GLY:N | 2.35 | 0.57 |
| 1:D:286:LYS:HA | 1:D:289:LEU:HD12 | 1.87 | 0.57 |
| 1:E:200:LEU:N | 1:E:200:LEU:HD12 | 2.20 | 0.57 |
| 1:E:350:ARG:HD3 | 1:E:353:ILE:HD12 | 1.86 | 0.57 |
| 1:F:237:LEU:HD23 | 1:F:237:LEU:C | 2.25 | 0.57 |
| 1:G:456:LEU:HD13 | 1:G:462:PRO:HG2 | 1.87 | 0.57 |
| 1:H:281:PHE:HZ | 1:N:384:ALA:O | 1.88 | 0.57 |
| 1:K:413:ALA:HB1 | 1:K:417:VAL:HB | 1.85 | 0.57 |
| 1:K:64:ASP:OD1 | 1:K:65:LYS:O | 2.22 | 0.57 |
| 1:M:31:LEU:HG | 1:M:454:ILE:HD11 | 1.86 | 0.57 |
| 1:N:138:CYS:SG | 1:N:144:ILE:HD13 | 2.45 | 0.57 |
| 1:N:55:SER:HA | 1:N:58:ARG:NH1 | 2.20 | 0.57 |
| 2:Q:20:LYS:HG2 | 2:Q:27:LEU:CD2 | 2.35 | 0.57 |
| 2:Q:59:VAL:O | 2:Q:59:VAL:HG23 | 2.05 | 0.57 |
| 2:S:17:VAL:HG13 | 2:S:34:LYS:CA | 2.34 | 0.57 |
| 2:S:6:LEU:O | 2:S:7:HIS:O | 2.21 | 0.57 |
| 1:A:206:ASN:HB2 | 1:A:214:GLU:H | 1.70 | 0.56 |
| 1:A:350:ARG:O | 1:A:354:GLU:HG2 | 2.04 | 0.56 |
| 1:A:177:VAL:CG1 | 1:A:397:GLU:HG2 | 2.35 | 0.56 |
| 1:A:510:VAL:CG2 | 1:A:511:ALA:N | 2.68 | 0.56 |
| 1:A:510:VAL:HG23 | 1:A:511:ALA:H | 1.68 | 0.56 |
| 1:B:333:ILE:O | 1:B:334:ASP:HB2 | 2.05 | 0.56 |
| 1:C:247:LEU:HD13 | 1:C:248:LEU:N | 2.19 | 0.56 |
| 1:D:272:LYS:HB2 | 1:D:272:LYS:NZ | 2.20 | 0.56 |
| 1:F:227:ILE:O | 1:F:227:ILE:HG22 | 2.05 | 0.56 |
| 1:F:450:PRO:O | 1:F:454:ILE:HG13 | 2.05 | 0.56 |
| 1:H:351:GLN:O | 1:H:354:GLU:N | 2.34 | 0.56 |
| 1:K:284:ARG:CB | 1:K:284:ARG:HH11 | 2.17 | 0.56 |
| 1:L:27:VAL:HG11 | 1:L:93:THR:HG21 | 1.87 | 0.56 |
| 1:L:55:SER:O | 1:L:58:ARG:HB3 | 2.05 | 0.56 |
| 1:M:226:LYS:HD2 | 1:M:252:GLU:HG3 | 1.86 | 0.56 |
| 1:N:222:LEU:HD22 | 1:N:289:LEU:HD11 | 1.87 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:314:LEU:CD1 | 1:N:314:LEU:H | 2.14 | 0.56 |
| 1:N:339:GLU:O | 1:N:343:GLN:HG2 | 2.04 | 0.56 |
| 2:T:86:MET:HB2 | 2:T:90:ASP:OD2 | 2.05 | 0.56 |
| 1:A:232:GLU:O | 1:A:233:MET:HB3 | 2.05 | 0.56 |
| 1:A:348:GLN:NE2 | 1:A:352:GLN:HE21 | 2.04 | 0.56 |
| 1:B:219:PHE:HD1 | 1:B:319:GLN:NE2 | 2.02 | 0.56 |
| 1:C:252:GLU:O | 1:C:253:ASP:HB2 | 2.04 | 0.56 |
| 1:C:295:LEU:C | 1:C:295:LEU:HD23 | 2.26 | 0.56 |
| 1:C:368:ARG:HD2 | 1:C:372:LEU:HD11 | 1.87 | 0.56 |
| 1:D:475:ASN:HD22 | 1:D:475:ASN:N | 2.03 | 0.56 |
| 1:E:232:GLU:O | 1:E:233:MET:HB3 | 2.05 | 0.56 |
| 1:E:25:ASP:HA | 1:E:28:LYS:HE2 | 1.87 | 0.56 |
| 1:E:308:GLU:H | 1:E:311:LYS:HB3 | 1.70 | 0.56 |
| 1:E:311:LYS:O | 1:E:312:ALA:HB2 | 2.05 | 0.56 |
| 1:G:134:LEU:O | 1:G:136:VAL:HG13 | 2.04 | 0.56 |
| 1:G:266:THR:HA | 1:G:271:VAL:O | 2.05 | 0.56 |
| 1:H:248:LEU:HD22 | 1:H:249:ILE:H | 1.69 | 0.56 |
| 1:H:419:LEU:HD21 | 1:H:500:THR:HG23 | 1.87 | 0.56 |
| 1:I:362:ARG:NH1 | 1:I:362:ARG:HB3 | 2.21 | 0.56 |
| 1:J:434:GLU:HA | 1:J:437:ASN:HD22 | 1.69 | 0.56 |
| 1:K:247:LEU:HD22 | 1:K:248:LEU:H | 1.70 | 0.56 |
| 1:L:146:GLN:O | 1:L:150:ILE:HG13 | 2.04 | 0.56 |
| 1:N:161:LEU:CD1 | 1:N:161:LEU:H | 2.18 | 0.56 |
| 1:N:421:ARG:HD2 | 1:N:474:GLY:O | 2.05 | 0.56 |
| 2:U:77:LYS:HG3 | 2:U:80:ASN:HA | 1.87 | 0.56 |
| 1:D:150:ILE:HD11 | 4:D:1:ADP:N7 | 2.20 | 0.56 |
| 1:D:326:ASN:ND2 | 1:D:328:ASP:H | 2.03 | 0.56 |
| 1:D:342:ILE:O | 1:D:346:VAL:HG23 | 2.05 | 0.56 |
| 1:D:418:ALA:O | 1:D:422:VAL:HG13 | 2.06 | 0.56 |
| 1:E:19:GLY:HA3 | 1:E:67:GLU:O | 2.05 | 0.56 |
| 1:F:266:THR:HG22 | 1:F:273:VAL:H | 1.70 | 0.56 |
| 1:F:368:ARG:HG2 | 1:F:372:LEU:CG | 2.35 | 0.56 |
| 1:I:30:THR:HB | 1:I:51:LYS:O | 2.05 | 0.56 |
| 1:K:219:PHE:HB2 | 1:K:247:LEU:HD23 | 1.85 | 0.56 |
| 1:L:362:ARG:HB3 | 1:L:362:ARG:HH11 | 1.71 | 0.56 |
| 1:N:266:THR:HG22 | 1:N:272:LYS:HA | 1.88 | 0.56 |
| 2:Q:12:VAL:HG12 | 2:Q:40:VAL:HA | 1.86 | 0.56 |
| 2:Q:78:ILE:HD13 | 2:Q:83:VAL:CG2 | 2.34 | 0.56 |
| 2:R:47:ARG:HG2 | 2:R:49:LEU:H | 1.69 | 0.56 |
| 2:U:40:VAL:HG23 | 2:U:63:ASP:O | 2.05 | 0.56 |
| 1:B:327:LYS:N | 1:B:327:LYS:HD3 | 2.21 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:218:PRO:HA | 1:C:246:PRO:HG2 | 1.87 | 0.56 |
| 1:C:304:GLU:HB2 | 1:C:305:ILE:HD12 | 1.86 | 0.56 |
| 1:D:368:ARG:HG2 | 1:D:372:LEU:CG | 2.36 | 0.56 |
| 1:C:517:THR:HG23 | 1:D:39:VAL:HG23 | 1.87 | 0.56 |
| 1:C:4:LYS:HG3 | 1:D:59:GLU:O | 2.05 | 0.56 |
| 1:F:381:VAL:CG1 | 1:F:392:LYS:HG3 | 2.36 | 0.56 |
| 1:I:166:MET:CE | 1:I:171:LYS:HA | 2.35 | 0.56 |
| 1:I:432:GLN:OE1 | 1:I:432:GLN:N | 2.38 | 0.56 |
| 1:J:264:VAL:HA | 1:J:267:MET:CG | 2.36 | 0.56 |
| 1:L:385:THR:HG23 | 1:L:388:GLU:HB3 | 1.85 | 0.56 |
| 1:L:54:VAL:HG22 | 1:L:89:THR:HG21 | 1.88 | 0.56 |
| 1:N:169:VAL:HG22 | 1:N:169:VAL:O | 2.05 | 0.56 |
| 1:N:383:ALA:CB | 1:N:389:MET:HA | 2.35 | 0.56 |
| 1:N:499:VAL:CG2 | 1:N:500:THR:N | 2.67 | 0.56 |
| 1:A:265:ASN:OD1 | 2:O:27:LEU:HB3 | 2.06 | 0.56 |
| 2:T:55:LYS:H | 2:T:55:LYS:HE3 | 1.70 | 0.56 |
| 1:A:219:PHE:O | 1:A:247:LEU:HD22 | 2.05 | 0.56 |
| 1:A:324:VAL:C | 1:A:325:ILE:HD12 | 2.24 | 0.56 |
| 1:B:241:ALA:HA | 1:B:271:VAL:HG12 | 1.88 | 0.56 |
| 1:D:256:GLY:O | 1:D:257:GLU:C | 2.43 | 0.56 |
| 1:G:41:ASP:O | 1:G:42:LYS:HG3 | 2.06 | 0.56 |
| 1:H:248:LEU:HD13 | 1:H:249:ILE:N | 2.21 | 0.56 |
| 1:H:317:LEU:HD12 | 1:H:317:LEU:N | 2.20 | 0.56 |
| 1:I:193:MET:HG2 | 1:I:194:GLN:N | 2.18 | 0.56 |
| 1:I:499:VAL:CG2 | 1:I:500:THR:N | 2.69 | 0.56 |
| 1:J:256:GLY:HA2 | 1:J:259:LEU:HB3 | 1.86 | 0.56 |
| 1:J:350:ARG:HE | 1:J:369:VAL:HG11 | 1.70 | 0.56 |
| 1:J:356:ALA:HB1 | 1:J:362:ARG:NE | 2.08 | 0.56 |
| 1:K:200:LEU:N | 1:K:200:LEU:HD12 | 2.21 | 0.56 |
| 1:L:428:ASP:O | 1:L:429:LEU:C | 2.44 | 0.56 |
| 2:S:48:ILE:HG22 | 2:S:48:ILE:O | 2.05 | 0.56 |
| 1:A:237:LEU:C | 1:A:237:LEU:HD23 | 2.26 | 0.56 |
| 1:A:433:ASN:OD1 | 1:A:436:GLN:HB2 | 2.05 | 0.56 |
| 1:B:289:LEU:N | 1:B:290:GLN:OE1 | 2.37 | 0.56 |
| 1:B:339:GLU:HB3 | 1:B:343:GLN:OE1 | 2.05 | 0.56 |
| 1:C:229:ASN:HA | 1:C:257:GLU:OE2 | 2.06 | 0.56 |
| 1:E:296:THR:HG22 | 1:E:335:GLY:CA | 2.24 | 0.56 |
| 1:E:411:VAL:HA | 1:E:497:THR:H | 1.68 | 0.56 |
| 1:F:404:ARG:HH11 | 1:F:404:ARG:HG3 | 1.71 | 0.56 |
| 1:H:284:ARG:HH11 | 1:H:284:ARG:CB | 2.14 | 0.56 |
| 1:I:197:ARG:HG3 | 1:I:277:LYS:NZ | 2.20 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:317:LEU:HD12 | 1:I:317:LEU:N | 2.20 | 0.56 |
| 1:J:284:ARG:CB | 1:J:284:ARG:HH11 | 2.15 | 0.56 |
| 1:J:400:LEU:C | 1:J:400:LEU:HD23 | 2.25 | 0.56 |
| 1:K:302:SER:HB2 | 1:K:305:ILE:HD12 | 1.87 | 0.56 |
| 1:L:262:LEU:HA | 1:L:265:ASN:HB3 | 1.88 | 0.56 |
| 1:N:124:VAL:HG13 | 1:N:504:LEU:HD11 | 1.84 | 0.56 |
| 1:N:247:LEU:HB3 | 1:N:273:VAL:HG11 | 1.87 | 0.56 |
| 1:A:309:LEU:H | 1:A:309:LEU:HD12 | 1.70 | 0.56 |
| 1:A:52:ASP:OD1 | 1:A:54:VAL:HG12 | 2.05 | 0.56 |
| 1:C:208:PRO:HB2 | 1:C:212:ALA:HB3 | 1.85 | 0.56 |
| 1:C:346:VAL:CG1 | 1:C:350:ARG:HH22 | 2.16 | 0.56 |
| 1:D:327:LYS:HD3 | 1:D:327:LYS:N | 2.21 | 0.56 |
| 1:E:278:ALA:HB1 | 1:E:279:PRO:HD2 | 1.86 | 0.56 |
| 1:E:455:VAL:HG12 | 1:E:460:GLU:O | 2.05 | 0.56 |
| 1:F:272:LYS:HB2 | 1:F:272:LYS:NZ | 2.20 | 0.56 |
| 1:I:155:ASP:OD1 | 1:I:158:VAL:HG23 | 2.05 | 0.56 |
| 1:I:353:ILE:HD11 | 1:I:369:VAL:HG21 | 1.87 | 0.56 |
| 1:J:229:ASN:HD21 | 1:J:231:ARG:HH12 | 1.52 | 0.56 |
| 1:J:264:VAL:HA | 1:J:267:MET:HG2 | 1.87 | 0.56 |
| 1:J:247:LEU:N | 1:J:273:VAL:HG12 | 2.20 | 0.56 |
| 1:L:506:TYR:O | 1:L:509:SER:HB3 | 2.05 | 0.56 |
| 2:P:43:VAL:HG13 | 2:P:57:LEU:HD12 | 1.87 | 0.56 |
| 2:Q:20:LYS:HG3 | 2:Q:28:THR:O | 2.05 | 0.56 |
| 2:Q:97:ALA:O | 2:R:1:MET:HA | 2.04 | 0.56 |
| 2:R:68:ASN:ND2 | 2:S:74:LYS:HE3 | 2.20 | 0.56 |
| 1:A:65:LYS:O | 1:A:69:MET:HG3 | 2.06 | 0.56 |
| 1:D:247:LEU:HD13 | 1:D:248:LEU:N | 2.20 | 0.56 |
| 1:D:489:ILE:HD12 | 1:D:494:LEU:HD22 | 1.86 | 0.56 |
| 1:E:208:PRO:O | 1:E:212:ALA:HB3 | 2.06 | 0.56 |
| 1:E:219:PHE:O | 1:E:247:LEU:HD22 | 2.06 | 0.56 |
| 1:G:232:GLU:O | 1:G:233:MET:HB3 | 2.06 | 0.56 |
| 1:I:169:VAL:CG1 | 1:I:173:GLY:HA3 | 2.34 | 0.56 |
| 1:I:221:LEU:C | 1:I:221:LEU:HD13 | 2.26 | 0.56 |
| 1:J:426:LEU:CD2 | 1:J:426:LEU:H | 2.09 | 0.56 |
| 1:M:264:VAL:HA | 1:M:267:MET:CG | 2.35 | 0.56 |
| 1:N:235:PRO:HG2 | 1:N:236:VAL:H | 1.70 | 0.56 |
| 1:N:134:LEU:HD11 | 1:N:475:ASN:OD1 | 2.06 | 0.56 |
| 2:S:20:LYS:HG3 | 2:S:28:THR:O | 2.06 | 0.56 |
| 1:A:249:ILE:HB | 1:A:275:ALA:CB | 2.36 | 0.56 |
| 1:A:30:THR:HG22 | 1:A:36:ARG:O | 2.05 | 0.56 |
| 1:A:381:VAL:HG21 | 1:A:393:LYS:HA | 1.87 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:134:LEU:CD1 | 1:B:134:LEU:N | 2.68 | 0.56 |
| 1:B:145:ALA:HB2 | 1:B:163:ALA:HB2 | 1.87 | 0.56 |
| 1:B:23:LEU:HD13 | 1:B:23:LEU:C | 2.26 | 0.56 |
| 1:B:338:GLU:O | 1:B:341:ALA:HB3 | 2.06 | 0.56 |
| 1:B:432:GLN:NE2 | 1:B:436:GLN:HE22 | 2.04 | 0.56 |
| 1:C:184:GLN:OE1 | 1:C:184:GLN:N | 2.38 | 0.56 |
| 1:D:279:PRO:HD2 | 1:D:285:ARG:CB | 2.35 | 0.56 |
| 1:D:368:ARG:O | 1:D:372:LEU:HG | 2.04 | 0.56 |
| 1:D:305:ILE:HD11 | 1:E:203:TYR:OH | 2.06 | 0.56 |
| 1:E:227:ILE:HD12 | 1:E:227:ILE:N | 2.20 | 0.56 |
| 1:E:18:ARG:O | 1:E:22:VAL:HG23 | 2.05 | 0.56 |
| 1:H:324:VAL:C | 1:H:325:ILE:HD12 | 2.26 | 0.56 |
| 1:H:428:ASP:O | 1:H:429:LEU:C | 2.43 | 0.56 |
| 1:K:506:TYR:O | 1:K:509:SER:HB3 | 2.05 | 0.56 |
| 1:L:257:GLU:O | 1:L:261:THR:HG23 | 2.06 | 0.56 |
| 1:N:149:THR:HG22 | 1:N:156:GLU:HA | 1.87 | 0.56 |
| 2:P:40:VAL:HB | 2:P:62:GLY:H | 1.71 | 0.56 |
| 2:S:20:LYS:HA | 2:S:28:THR:HG23 | 1.88 | 0.56 |
| 1:B:262:LEU:HD11 | 1:B:273:VAL:HB | 1.88 | 0.56 |
| 1:B:406:ALA:O | 1:B:410:GLY:N | 2.38 | 0.56 |
| 1:C:291:ASP:HB3 | 1:C:345:ARG:NH2 | 2.19 | 0.56 |
| 1:D:194:GLN:HG3 | 1:D:331:THR:OG1 | 2.06 | 0.56 |
| 1:E:237:LEU:C | 1:E:237:LEU:HD23 | 2.26 | 0.56 |
| 1:E:496:PRO:HG2 | 1:E:499:VAL:HG13 | 1.87 | 0.56 |
| 1:F:164:GLU:O | 1:F:167:ASP:HB3 | 2.06 | 0.56 |
| 1:F:351:GLN:HG2 | 1:G:210:THR:OG1 | 2.06 | 0.56 |
| 1:G:205:ILE:HG12 | 1:G:211:GLY:HA2 | 1.86 | 0.56 |
| 1:I:169:VAL:HG22 | 1:I:169:VAL:O | 2.06 | 0.56 |
| 1:J:359:ASP:O | 1:J:363:GLU:HB2 | 2.05 | 0.56 |
| 1:J:499:VAL:CG2 | 1:J:500:THR:N | 2.69 | 0.56 |
| 1:M:6:VAL:HG22 | 1:M:521:VAL:HG22 | 1.86 | 0.56 |
| 2:O:86:MET:HB2 | 2:O:90:ASP:OD2 | 2.06 | 0.56 |
| 2:O:57:LEU:HD22 | 2:O:88:GLU:HB2 | 1.88 | 0.56 |
| 2:P:65:VAL:CG1 | 2:P:94:ILE:HG12 | 2.30 | 0.56 |
| 1:A:261:THR:O | 1:A:265:ASN:ND2 | 2.39 | 0.56 |
| 1:A:266:THR:HG22 | 1:A:273:VAL:H | 1.71 | 0.56 |
| 1:B:134:LEU:HD11 | 1:B:425:LYS:NZ | 2.21 | 0.56 |
| 1:C:134:LEU:O | 1:C:136:VAL:HG13 | 2.06 | 0.56 |
| 1:C:448:GLU:O | 1:C:452:ARG:HG2 | 2.06 | 0.56 |
| 1:D:5:ASP:HB2 | 1:D:524:LEU:CD2 | 2.36 | 0.56 |
| 1:E:348:GLN:HE22 | 1:E:352:GLN:NE2 | 2.04 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:358:SER:HA | 1:E:362:ARG:CD | 2.36 | 0.56 |
| 1:E:366:GLN:HA | 1:E:369:VAL:CG2 | 2.36 | 0.56 |
| 1:F:248:LEU:HD13 | 1:F:248:LEU:C | 2.27 | 0.56 |
| 1:H:247:LEU:HD13 | 1:H:247:LEU:C | 2.26 | 0.56 |
| 1:H:351:GLN:HG2 | 1:H:354:GLU:OE2 | 2.06 | 0.56 |
| 1:I:209:GLU:HA | 1:I:209:GLU:OE1 | 2.06 | 0.56 |
| 1:I:248:LEU:HD13 | 1:I:248:LEU:C | 2.26 | 0.56 |
| 1:I:449:ALA:HB3 | 1:I:450:PRO:CD | 2.31 | 0.56 |
| 1:J:287:ALA:HB1 | 1:J:368:ARG:CZ | 2.36 | 0.56 |
| 1:J:398:ASP:O | 1:J:401:HIS:HB2 | 2.06 | 0.56 |
| 1:K:362:ARG:HB3 | 1:K:362:ARG:HH11 | 1.71 | 0.56 |
| 1:K:180:GLY:HA2 | 1:K:380:LYS:HB3 | 1.87 | 0.56 |
| 1:K:179:ASP:OD2 | 1:K:390:LYS:HG2 | 2.06 | 0.56 |
| 1:L:249:ILE:HB | 1:L:275:ALA:HB1 | 1.88 | 0.56 |
| 1:N:129:GLU:O | 1:N:132:LYS:N | 2.39 | 0.56 |
| 1:N:193:MET:CG | 1:N:194:GLN:N | 2.67 | 0.56 |
| 2:P:48:ILE:HG22 | 2:P:48:ILE:O | 2.06 | 0.56 |
| 2:P:84:LEU:N | 2:P:84:LEU:HD12 | 2.20 | 0.56 |
| 2:R:20:LYS:HG2 | 2:R:27:LEU:CD2 | 2.35 | 0.56 |
| 2:R:40:VAL:HG21 | 2:R:63:ASP:HB2 | 1.87 | 0.56 |
| 1:A:237:LEU:HD22 | 2:O:26:VAL:CG2 | 2.29 | 0.55 |
| 1:A:283:ASP:O | 1:A:287:ALA:HB2 | 2.05 | 0.55 |
| 1:A:322:ARG:HG2 | 1:A:323:VAL:N | 2.19 | 0.55 |
| 1:C:240:VAL:HG21 | 1:C:247:LEU:HD23 | 1.88 | 0.55 |
| 1:C:285:ARG:HG3 | 1:C:286:LYS:N | 2.21 | 0.55 |
| 1:F:285:ARG:HG3 | 1:F:286:LYS:N | 2.21 | 0.55 |
| 1:G:324:VAL:C | 1:G:325:ILE:HD12 | 2.26 | 0.55 |
| 1:G:349:ILE:HA | 1:G:352:GLN:CD | 2.26 | 0.55 |
| 1:G:80:LYS:HD2 | 1:G:506:TYR:CZ | 2.41 | 0.55 |
| 1:J:228:SER:O | 1:J:257:GLU:HB3 | 2.07 | 0.55 |
| 1:K:15:LYS:HD2 | 1:K:67:GLU:HG3 | 1.87 | 0.55 |
| 1:K:232:GLU:HB3 | 1:K:309:LEU:CB | 2.27 | 0.55 |
| 1:K:428:ASP:O | 1:K:429:LEU:C | 2.45 | 0.55 |
| 2:O:46:GLY:HA3 | 2:O:55:LYS:O | 2.06 | 0.55 |
| 2:U:48:ILE:HG12 | 2:U:54:VAL:HG13 | 1.88 | 0.55 |
| 1:B:234:LEU:H | 1:B:234:LEU:CD1 | 2.17 | 0.55 |
| 1:C:319:GLN:O | 1:C:335:GLY:HA2 | 2.07 | 0.55 |
| 1:D:202:PRO:HG2 | 1:D:203:TYR:CD1 | 2.41 | 0.55 |
| 1:D:233:MET:CE | 1:D:233:MET:O | 2.54 | 0.55 |
| 1:E:281:PHE:O | 1:E:284:ARG:HB3 | 2.07 | 0.55 |
| 1:E:365:LEU:O | 1:E:369:VAL:HG23 | 2.06 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:236:VAL:O | 1:F:239:ALA:HB3 | 2.06 | 0.55 |
| 1:G:496:PRO:HG2 | 1:G:499:VAL:HG13 | 1.88 | 0.55 |
| 1:G:510:VAL:HG23 | 1:G:511:ALA:H | 1.69 | 0.55 |
| 1:H:254:VAL:O | 1:H:259:LEU:HD12 | 2.06 | 0.55 |
| 1:H:313:THR:HG22 | 1:H:314:LEU:N | 2.21 | 0.55 |
| 1:I:325:ILE:HD12 | 1:I:325:ILE:N | 2.20 | 0.55 |
| 1:I:406:ALA:O | 1:I:410:GLY:CA | 2.54 | 0.55 |
| 1:L:17:LEU:HA | 1:L:20:VAL:CG1 | 2.36 | 0.55 |
| 1:M:218:PRO:HB3 | 1:M:246:PRO:HB2 | 1.88 | 0.55 |
| 1:N:288:MET:HA | 1:N:288:MET:CE | 2.36 | 0.55 |
| 1:N:356:ALA:CB | 1:N:362:ARG:HE | 2.12 | 0.55 |
| 2:P:78:ILE:N | 2:P:78:ILE:HD12 | 2.22 | 0.55 |
| 2:S:50:GLU:O | 2:S:52:GLY:N | 2.39 | 0.55 |
| 1:A:106:ALA:O | 1:A:109:ALA:HB3 | 2.07 | 0.55 |
| 1:A:130:GLU:O | 1:A:133:ALA:HB3 | 2.06 | 0.55 |
| 1:A:295:LEU:C | 1:A:295:LEU:HD23 | 2.26 | 0.55 |
| 1:A:472:GLY:HA3 | 1:A:476:TYR:CD2 | 2.42 | 0.55 |
| 1:D:346:VAL:HA | 1:D:349:ILE:HD12 | 1.88 | 0.55 |
| 1:D:174:VAL:HG21 | 1:D:367:GLU:HA | 1.89 | 0.55 |
| 1:E:130:GLU:O | 1:E:133:ALA:HB3 | 2.06 | 0.55 |
| 1:F:94:VAL:HG12 | 1:F:449:ALA:HB1 | 1.88 | 0.55 |
| 1:I:219:PHE:HB3 | 1:I:317:LEU:HD23 | 1.88 | 0.55 |
| 1:I:318:GLY:O | 1:I:319:GLN:HG3 | 2.05 | 0.55 |
| 1:I:55:SER:HA | 1:I:58:ARG:NH1 | 2.21 | 0.55 |
| 1:J:299:THR:OG1 | 1:J:316:ASP:HA | 2.06 | 0.55 |
| 1:K:236:VAL:HG23 | 1:K:237:LEU:N | 2.22 | 0.55 |
| 1:L:157:THR:O | 1:L:161:LEU:HD13 | 2.06 | 0.55 |
| 1:L:362:ARG:HB3 | 1:L:362:ARG:NH1 | 2.21 | 0.55 |
| 1:M:428:ASP:O | 1:M:429:LEU:C | 2.44 | 0.55 |
| 1:N:217:SER:N | 1:N:218:PRO:HD3 | 2.20 | 0.55 |
| 2:U:37:ARG:HG2 | 2:U:37:ARG:NH1 | 2.20 | 0.55 |
| 1:B:203:TYR:H | 1:B:203:TYR:HD1 | 1.54 | 0.55 |
| 1:C:127:ALA:O | 1:C:130:GLU:HB2 | 2.05 | 0.55 |
| 1:C:357:THR:CG2 | 1:C:361:ASP:HB2 | 2.36 | 0.55 |
| 1:C:353:ILE:HG12 | 1:C:366:GLN:NE2 | 2.21 | 0.55 |
| 1:D:233:MET:C | 1:D:235:PRO:CD | 2.73 | 0.55 |
| 1:D:247:LEU:HB3 | 1:D:273:VAL:HG13 | 1.88 | 0.55 |
| 1:D:28:LYS:O | 1:D:30:THR:N | 2.39 | 0.55 |
| 1:E:221:LEU:C | 1:E:222:LEU:HD12 | 2.26 | 0.55 |
| 1:F:381:VAL:HG13 | 1:F:392:LYS:HG3 | 1.89 | 0.55 |
| 1:F:486:GLY:CA | 1:F:491:MET:CE | 2.84 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:289:LEU:HD23 | 1:G:292:ILE:HD12 | 1.89 | 0.55 |
| 1:G:195:PHE:O | 1:G:329:THR:HG23 | 2.07 | 0.55 |
| 1:G:339:GLU:CD | 1:G:339:GLU:N | 2.60 | 0.55 |
| 1:H:217:SER:N | 1:H:218:PRO:HD3 | 2.20 | 0.55 |
| 1:J:284:ARG:H | 1:J:284:ARG:HH11 | 1.54 | 0.55 |
| 1:J:69:MET:HE2 | 1:J:522:THR:HB | 1.85 | 0.55 |
| 1:M:161:LEU:H | 1:M:161:LEU:CD1 | 2.20 | 0.55 |
| 2:O:20:LYS:HD2 | 2:O:20:LYS:H | 1.71 | 0.55 |
| 2:U:20:LYS:HB3 | 2:U:27:LEU:HG | 1.89 | 0.55 |
| 1:A:285:ARG:HG3 | 1:A:286:LYS:N | 2.21 | 0.55 |
| 1:B:134:LEU:H | 1:B:134:LEU:CD1 | 2.19 | 0.55 |
| 1:B:194:GLN:HB2 | 1:B:331:THR:HG23 | 1.87 | 0.55 |
| 1:C:222:LEU:N | 1:C:222:LEU:HD12 | 2.21 | 0.55 |
| 1:C:381:VAL:HG21 | 1:C:393:LYS:HA | 1.88 | 0.55 |
| 1:D:302:SER:HB2 | 1:D:305:ILE:HD13 | 1.87 | 0.55 |
| 1:E:504:LEU:HD13 | 1:E:504:LEU:C | 2.26 | 0.55 |
| 1:F:290:GLN:OE1 | 1:F:290:GLN:N | 2.39 | 0.55 |
| 1:F:7:LYS:HD2 | 1:F:66:PHE:CE2 | 2.42 | 0.55 |
| 1:G:160:LYS:O | 1:G:164:GLU:HG3 | 2.06 | 0.55 |
| 1:H:363:GLU:O | 1:H:367:GLU:HG3 | 2.06 | 0.55 |
| 1:K:193:MET:HG2 | 1:K:194:GLN:N | 2.21 | 0.55 |
| 1:L:215:LEU:CB | 1:L:218:PRO:HG2 | 2.37 | 0.55 |
| 1:M:345:ARG:HA | 1:M:348:GLN:HE21 | 1.69 | 0.55 |
| 1:M:385:THR:HG23 | 1:M:388:GLU:N | 2.17 | 0.55 |
| 1:N:66:PHE:N | 1:N:69:MET:HG3 | 2.20 | 0.55 |
| 2:R:37:ARG:HH11 | 2:R:37:ARG:HG2 | 1.71 | 0.55 |
| 2:T:40:VAL:HB | 2:T:62:GLY:H | 1.72 | 0.55 |
| 2:U:43:VAL:CG1 | 2:U:57:LEU:HD12 | 2.36 | 0.55 |
| 1:A:25:ASP:HA | 1:A:28:LYS:HE2 | 1.87 | 0.55 |
| 1:B:404:ARG:HG3 | 1:B:404:ARG:HH11 | 1.71 | 0.55 |
| 1:C:16:MET:O | 1:C:20:VAL:HG23 | 2.07 | 0.55 |
| 1:C:248:LEU:C | 1:C:248:LEU:HD13 | 2.26 | 0.55 |
| 1:E:134:LEU:N | 1:E:134:LEU:HD12 | 2.21 | 0.55 |
| 1:G:311:LYS:O | 1:G:312:ALA:HB2 | 2.07 | 0.55 |
| 1:I:345:ARG:O | 1:I:348:GLN:HB2 | 2.07 | 0.55 |
| 1:J:421:ARG:HD2 | 1:J:474:GLY:O | 2.06 | 0.55 |
| 1:K:10:ASN:O | 1:K:11:ASP:C | 2.45 | 0.55 |
| 1:K:149:THR:HG22 | 1:K:156:GLU:HA | 1.89 | 0.55 |
| 1:K:205:ILE:HD13 | 1:K:211:GLY:HA2 | 1.89 | 0.55 |
| 1:K:215:LEU:CB | 1:K:218:PRO:HG2 | 2.33 | 0.55 |
| 1:K:478:TYR:HB2 | 1:K:485:TYR:CE2 | 2.42 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:107:VAL:CG2 | 1:L:108:ALA:N | 2.68 | 0.55 |
| 1:L:226:LYS:HD2 | 1:L:252:GLU:HG3 | 1.88 | 0.55 |
| 1:L:36:ARG:HB3 | 1:M:516:THR:O | 2.06 | 0.55 |
| 1:L:448:GLU:HB3 | 1:L:452:ARG:HD2 | 1.89 | 0.55 |
| 1:M:219:PHE:CB | 1:M:317:LEU:HD23 | 2.37 | 0.55 |
| 1:N:37:ASN:ND2 | 1:N:37:ASN:H | 2.05 | 0.55 |
| 1:N:389:MET:HE1 | 1:N:393:LYS:HB2 | 1.89 | 0.55 |
| 1:A:245:LYS:CE | 1:A:245:LYS:HA | 2.30 | 0.55 |
| 1:B:18:ARG:HB2 | 1:B:67:GLU:HG2 | 1.88 | 0.55 |
| 1:B:205:ILE:CD1 | 1:B:211:GLY:HA2 | 2.37 | 0.55 |
| 1:B:401:HIS:O | 1:B:404:ARG:HB2 | 2.05 | 0.55 |
| 1:D:436:GLN:O | 1:D:440:ILE:HG13 | 2.06 | 0.55 |
| 1:E:220:ILE:HG23 | 1:E:248:LEU:HD12 | 1.89 | 0.55 |
| 1:E:368:ARG:HG2 | 1:E:372:LEU:CG | 2.36 | 0.55 |
| 1:E:42:LYS:HE2 | 1:E:48:THR:HB | 1.88 | 0.55 |
| 1:E:486:GLY:CA | 1:E:491:MET:CE | 2.85 | 0.55 |
| 1:E:65:LYS:O | 1:E:69:MET:HG3 | 2.07 | 0.55 |
| 1:G:29:VAL:HG23 | 1:G:30:THR:HG23 | 1.88 | 0.55 |
| 1:H:303:GLU:C | 1:H:305:ILE:H | 2.07 | 0.55 |
| 1:I:31:LEU:HG | 1:I:454:ILE:HD11 | 1.89 | 0.55 |
| 1:J:494:LEU:CD2 | 1:J:494:LEU:N | 2.66 | 0.55 |
| 1:K:406:ALA:O | 1:K:410:GLY:N | 2.34 | 0.55 |
| 1:K:478:TYR:CE1 | 1:K:483:GLU:HA | 2.42 | 0.55 |
| 1:L:140:ASP:O | 1:L:144:ILE:HG12 | 2.06 | 0.55 |
| 1:L:455:VAL:HG13 | 1:L:460:GLU:HB2 | 1.89 | 0.55 |
| 1:A:220:ILE:N | 1:A:220:ILE:CD1 | 2.70 | 0.55 |
| 1:A:308:GLU:H | 1:A:311:LYS:HB3 | 1.72 | 0.55 |
| 1:A:381:VAL:CG1 | 1:A:392:LYS:CG | 2.84 | 0.55 |
| 1:A:434:GLU:O | 1:A:435:ASP:C | 2.44 | 0.55 |
| 1:C:23:LEU:HD13 | 1:C:23:LEU:C | 2.27 | 0.55 |
| 1:D:305:ILE:CG2 | 1:D:306:GLY:H | 1.93 | 0.55 |
| 1:D:452:ARG:HB2 | 1:D:462:PRO:CB | 2.33 | 0.55 |
| 1:G:271:VAL:O | 1:G:271:VAL:HG23 | 2.07 | 0.55 |
| 1:H:184:GLN:HA | 1:H:184:GLN:OE1 | 2.07 | 0.55 |
| 1:H:213:VAL:O | 1:H:324:VAL:HA | 2.06 | 0.55 |
| 1:H:226:LYS:CA | 1:H:252:GLU:HB2 | 2.36 | 0.55 |
| 1:H:66:PHE:N | 1:H:69:MET:HG3 | 2.21 | 0.55 |
| 1:J:226:LYS:HG3 | 1:J:252:GLU:HB3 | 1.88 | 0.55 |
| 1:J:363:GLU:O | 1:J:367:GLU:HG3 | 2.07 | 0.55 |
| 1:M:112:ASN:O | 1:M:116:LEU:HG | 2.06 | 0.55 |
| 1:M:214:GLU:HA | 1:M:324:VAL:HG12 | 1.88 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:32:GLY:HA3 | 1:N:454:ILE:HG23 | 1.89 | 0.55 |
| 2:O:1:MET:HA | 2:U:97:ALA:O | 2.07 | 0.55 |
| 2:O:48:ILE:HG22 | 2:O:48:ILE:O | 2.06 | 0.55 |
| 2:Q:47:ARG:HG2 | 2:Q:49:LEU:H | 1.71 | 0.55 |
| 2:T:3:ILE:HD12 | 2:T:3:ILE:H | 1.72 | 0.55 |
| 1:B:150:ILE:HD11 | 4:B:1:ADP:N7 | 2.22 | 0.55 |
| 1:C:215:LEU:O | 1:C:322:ARG:HG3 | 2.07 | 0.55 |
| 1:E:242:LYS:HD3 | 1:E:242:LYS:C | 2.26 | 0.55 |
| 1:F:409:GLU:CD | 1:F:501:ARG:HH21 | 2.11 | 0.55 |
| 1:G:25:ASP:HA | 1:G:28:LYS:HE2 | 1.88 | 0.55 |
| 1:A:59:GLU:O | 1:G:4:LYS:HG3 | 2.07 | 0.55 |
| 1:I:236:VAL:HG23 | 1:I:237:LEU:N | 2.22 | 0.55 |
| 1:I:288:MET:CE | 1:I:288:MET:HA | 2.37 | 0.55 |
| 1:J:406:ALA:O | 1:J:410:GLY:N | 2.36 | 0.55 |
| 1:K:305:ILE:HG22 | 1:K:307:MET:HG3 | 1.88 | 0.55 |
| 1:K:325:ILE:HG13 | 1:K:330:THR:HG23 | 1.88 | 0.55 |
| 1:K:39:VAL:HG22 | 1:K:49:ILE:HG12 | 1.87 | 0.55 |
| 1:K:417:VAL:O | 1:K:418:ALA:C | 2.44 | 0.55 |
| 1:L:339:GLU:O | 1:L:343:GLN:HG2 | 2.07 | 0.55 |
| 1:M:230:ILE:CD1 | 1:M:257:GLU:HG2 | 2.37 | 0.55 |
| 1:N:215:LEU:CB | 1:N:218:PRO:HG2 | 2.37 | 0.55 |
| 2:P:47:ARG:O | 2:P:54:VAL:HG13 | 2.07 | 0.55 |
| 1:A:417:VAL:HA | 1:A:420:ILE:CG2 | 2.37 | 0.55 |
| 1:A:512:GLY:O | 1:A:515:ILE:HG12 | 2.06 | 0.55 |
| 1:B:219:PHE:HB2 | 1:B:247:LEU:HD22 | 1.88 | 0.55 |
| 1:C:130:GLU:O | 1:C:133:ALA:HB3 | 2.08 | 0.55 |
| 1:F:207:LYS:NZ | 1:F:207:LYS:HB2 | 2.22 | 0.55 |
| 1:F:235:PRO:HG3 | 1:F:310:GLU:HB3 | 1.87 | 0.55 |
| 1:F:177:VAL:HG11 | 1:F:397:GLU:HG2 | 1.89 | 0.55 |
| 1:G:352:GLN:C | 1:G:365:LEU:HD11 | 2.28 | 0.55 |
| 1:G:510:VAL:CG2 | 1:G:511:ALA:N | 2.69 | 0.55 |
| 1:H:221:LEU:HD22 | 1:H:222:LEU:H | 1.72 | 0.55 |
| 1:H:175:ILE:HD13 | 1:H:404:ARG:NH2 | 2.22 | 0.55 |
| 1:H:7:LYS:HG3 | 1:H:66:PHE:CE2 | 2.41 | 0.55 |
| 1:K:219:PHE:CB | 1:K:317:LEU:HD23 | 2.37 | 0.55 |
| 1:K:433:ASN:HD22 | 1:K:434:GLU:H | 1.54 | 0.55 |
| 1:L:254:VAL:O | 1:L:259:LEU:HD12 | 2.07 | 0.55 |
| 1:L:398:ASP:O | 1:L:401:HIS:HB2 | 2.07 | 0.55 |
| 1:M:40:LEU:N | 1:M:40:LEU:HD22 | 2.22 | 0.55 |
| 1:N:413:ALA:HB1 | 1:N:417:VAL:HB | 1.87 | 0.55 |
| 2:P:14:ARG:HG2 | 2:P:15:LYS:H | 1.69 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:14:ARG:HH11 | 2:R:14:ARG:CB | 2.18 | 0.55 |
| 1:C:206:ASN:CB | 1:C:214:GLU:H | 2.20 | 0.54 |
| 1:C:494:LEU:HD23 | 1:C:494:LEU:N | 2.21 | 0.54 |
| 1:E:119:GLY:O | 1:E:440:ILE:HG12 | 2.06 | 0.54 |
| 1:F:70:GLY:O | 1:F:74:VAL:HG22 | 2.07 | 0.54 |
| 1:G:486:GLY:HA3 | 1:G:491:MET:CE | 2.36 | 0.54 |
| 1:H:112:ASN:O | 1:H:116:LEU:HG | 2.06 | 0.54 |
| 1:I:301:ILE:N | 1:I:301:ILE:CD1 | 2.69 | 0.54 |
| 1:I:415:GLY:H | 1:I:417:VAL:CG2 | 2.17 | 0.54 |
| 1:I:421:ARG:NH2 | 1:I:469:VAL:O | 2.39 | 0.54 |
| 1:J:259:LEU:O | 1:J:263:VAL:HG23 | 2.08 | 0.54 |
| 1:K:229:ASN:ND2 | 1:K:231:ARG:HH12 | 2.05 | 0.54 |
| 1:K:356:ALA:HB1 | 1:K:362:ARG:NE | 2.18 | 0.54 |
| 1:K:465:VAL:O | 1:K:469:VAL:HG23 | 2.08 | 0.54 |
| 1:K:478:TYR:HA | 1:K:485:TYR:HA | 1.89 | 0.54 |
| 1:L:392:LYS:O | 1:L:396:VAL:HG23 | 2.06 | 0.54 |
| 1:M:288:MET:HA | 1:M:288:MET:HE2 | 1.89 | 0.54 |
| 1:M:411:VAL:HA | 1:M:497:THR:H | 1.71 | 0.54 |
| 1:N:186:GLU:O | 1:N:379:ILE:HA | 2.07 | 0.54 |
| 1:N:55:SER:O | 1:N:58:ARG:HB3 | 2.07 | 0.54 |
| 1:A:270:ILE:HD11 | 2:O:27:LEU:CD1 | 2.38 | 0.54 |
| 2:S:20:LYS:HG2 | 2:S:27:LEU:HD23 | 1.89 | 0.54 |
| 1:A:368:ARG:CD | 1:A:372:LEU:HD11 | 2.37 | 0.54 |
| 1:B:232:GLU:O | 1:B:233:MET:HB3 | 2.07 | 0.54 |
| 1:B:322:ARG:HB3 | 1:B:333:ILE:CD1 | 2.26 | 0.54 |
| 1:D:112:ASN:HD21 | 1:D:114:MET:HB3 | 1.71 | 0.54 |
| 1:D:252:GLU:O | 1:D:277:LYS:HE2 | 2.07 | 0.54 |
| 1:D:434:GLU:O | 1:D:435:ASP:C | 2.45 | 0.54 |
| 1:E:161:LEU:O | 1:E:164:GLU:HB2 | 2.08 | 0.54 |
| 1:E:417:VAL:HA | 1:E:420:ILE:HG22 | 1.87 | 0.54 |
| 1:G:193:MET:O | 1:G:331:THR:HG23 | 2.07 | 0.54 |
| 1:G:353:ILE:HG22 | 1:G:354:GLU:N | 2.22 | 0.54 |
| 1:H:345:ARG:HH22 | 1:H:368:ARG:HH22 | 1.53 | 0.54 |
| 1:J:40:LEU:HD23 | 1:J:50:THR:HG22 | 1.88 | 0.54 |
| 1:M:217:SER:N | 1:M:218:PRO:HD3 | 2.21 | 0.54 |
| 1:M:345:ARG:O | 1:M:348:GLN:HB2 | 2.07 | 0.54 |
| 1:M:352:GLN:O | 1:M:355:GLU:OE1 | 2.25 | 0.54 |
| 1:M:175:ILE:HD13 | 1:M:404:ARG:NH2 | 2.21 | 0.54 |
| 2:R:50:GLU:OE1 | 2:S:50:GLU:HA | 2.07 | 0.54 |
| 2:S:50:GLU:O | 2:S:50:GLU:HG2 | 2.06 | 0.54 |
| 2:T:14:ARG:CD | 2:T:35:SER:HB3 | 2.33 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:48:ILE:HG12 | 2:T:54:VAL:HG13 | 1.89 | 0.54 |
| 1:B:44:PHE:HD1 | 1:B:44:PHE:H | 1.40 | 0.54 |
| 1:C:135:SER:HB2 | 1:C:497:THR:HG21 | 1.89 | 0.54 |
| 1:D:258:ALA:O | 1:D:261:THR:HG23 | 2.07 | 0.54 |
| 1:D:357:THR:HB | 1:D:361:ASP:CB | 2.37 | 0.54 |
| 1:D:54:VAL:HB | 1:D:89:THR:HG21 | 1.88 | 0.54 |
| 1:E:134:LEU:O | 1:E:136:VAL:HG13 | 2.08 | 0.54 |
| 1:G:200:LEU:O | 1:G:202:PRO:HD2 | 2.07 | 0.54 |
| 1:G:259:LEU:O | 1:G:263:VAL:HG23 | 2.07 | 0.54 |
| 1:G:326:ASN:OD1 | 1:G:329:THR:N | 2.39 | 0.54 |
| 1:G:357:THR:CG2 | 1:G:361:ASP:HB2 | 2.37 | 0.54 |
| 1:H:214:GLU:HA | 1:H:324:VAL:HG12 | 1.88 | 0.54 |
| 1:I:494:LEU:HD23 | 1:I:494:LEU:H | 1.71 | 0.54 |
| 1:J:428:ASP:O | 1:J:429:LEU:C | 2.45 | 0.54 |
| 1:L:465:VAL:O | 1:L:469:VAL:HG23 | 2.07 | 0.54 |
| 1:M:266:THR:HG22 | 1:M:273:VAL:H | 1.72 | 0.54 |
| 1:M:506:TYR:O | 1:M:509:SER:HB3 | 2.08 | 0.54 |
| 1:N:218:PRO:HB3 | 1:N:246:PRO:C | 2.28 | 0.54 |
| 1:A:199:TYR:CE2 | 1:A:205:ILE:HG12 | 2.41 | 0.54 |
| 1:A:357:THR:CG2 | 1:A:361:ASP:HB2 | 2.37 | 0.54 |
| 1:C:277:LYS:HD3 | 1:C:285:ARG:HH22 | 1.72 | 0.54 |
| 1:C:279:PRO:HB3 | 1:C:288:MET:HE1 | 1.88 | 0.54 |
| 1:C:368:ARG:HG2 | 1:C:372:LEU:CG | 2.37 | 0.54 |
| 1:D:203:TYR:H | 1:D:203:TYR:HD1 | 1.55 | 0.54 |
| 1:D:489:ILE:CD1 | 1:D:494:LEU:HD22 | 2.37 | 0.54 |
| 1:E:349:ILE:HA | 1:E:352:GLN:CD | 2.27 | 0.54 |
| 1:E:475:ASN:N | 1:E:475:ASN:HD22 | 2.05 | 0.54 |
| 1:G:77:VAL:HG12 | 1:G:510:VAL:HG21 | 1.89 | 0.54 |
| 1:H:235:PRO:HG2 | 1:H:236:VAL:H | 1.72 | 0.54 |
| 1:J:206:ASN:OD1 | 1:J:213:VAL:HA | 2.07 | 0.54 |
| 1:J:233:MET:HE2 | 1:J:233:MET:HA | 1.90 | 0.54 |
| 1:K:84:ALA:O | 1:K:498:LYS:HE2 | 2.08 | 0.54 |
| 1:L:219:PHE:O | 1:L:247:LEU:HD22 | 2.07 | 0.54 |
| 1:L:350:ARG:HG3 | 1:L:350:ARG:HH11 | 1.73 | 0.54 |
| 1:M:267:MET:O | 1:M:267:MET:HG3 | 2.07 | 0.54 |
| 1:M:247:LEU:N | 1:M:273:VAL:HG12 | 2.23 | 0.54 |
| 1:N:302:SER:HB2 | 1:N:305:ILE:CD1 | 2.37 | 0.54 |
| 1:N:385:THR:O | 1:N:389:MET:HB2 | 2.08 | 0.54 |
| 1:B:127:ALA:O | 1:B:130:GLU:HB2 | 2.08 | 0.54 |
| 1:B:122:LYS:HE2 | 1:B:429:LEU:HD11 | 1.90 | 0.54 |
| 1:C:227:ILE:O | 1:C:227:ILE:HG22 | 2.06 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:313:THR:HG22 | 1:C:314:LEU:N | 2.22 | 0.54 |
| 1:D:220:ILE:HG23 | 1:D:248:LEU:HD12 | 1.88 | 0.54 |
| 1:D:339:GLU:HA | 1:D:342:ILE:HB | 1.89 | 0.54 |
| 1:D:362:ARG:O | 1:D:366:GLN:OE1 | 2.26 | 0.54 |
| 1:F:311:LYS:O | 1:F:312:ALA:HB2 | 2.07 | 0.54 |
| 1:F:339:GLU:N | 1:F:339:GLU:CD | 2.61 | 0.54 |
| 1:F:347:ALA:O | 1:F:350:ARG:HG2 | 2.06 | 0.54 |
| 1:F:19:GLY:HA3 | 1:F:67:GLU:O | 2.07 | 0.54 |
| 1:G:257:GLU:O | 1:G:261:THR:HG22 | 2.07 | 0.54 |
| 1:G:204:PHE:CB | 1:G:274:ALA:HB2 | 2.37 | 0.54 |
| 1:H:232:GLU:HA | 1:H:310:GLU:HG3 | 1.90 | 0.54 |
| 1:H:222:LEU:CD1 | 1:H:293:ALA:HA | 2.38 | 0.54 |
| 1:H:319:GLN:O | 1:H:336:VAL:HG23 | 2.07 | 0.54 |
| 1:I:10:ASN:O | 1:I:11:ASP:C | 2.46 | 0.54 |
| 1:I:218:PRO:HB3 | 1:I:246:PRO:C | 2.28 | 0.54 |
| 1:J:302:SER:HB2 | 1:J:305:ILE:CD1 | 2.37 | 0.54 |
| 1:J:384:ALA:O | 1:K:281:PHE:HZ | 1.90 | 0.54 |
| 1:E:464:VAL:CG2 | 1:K:464:VAL:HA | 2.38 | 0.54 |
| 1:M:419:LEU:O | 1:M:422:VAL:HG22 | 2.08 | 0.54 |
| 1:M:422:VAL:O | 1:M:425:LYS:HB2 | 2.07 | 0.54 |
| 1:M:422:VAL:O | 1:M:426:LEU:HD23 | 2.08 | 0.54 |
| 1:N:284:ARG:CB | 1:N:284:ARG:HH11 | 2.18 | 0.54 |
| 2:P:43:VAL:CG1 | 2:P:57:LEU:HD12 | 2.37 | 0.54 |
| 2:S:47:ARG:HD2 | 2:S:55:LYS:HD2 | 1.88 | 0.54 |
| 1:A:204:PHE:CB | 1:A:274:ALA:HB2 | 2.37 | 0.54 |
| 1:B:205:ILE:HD13 | 1:B:211:GLY:HA2 | 1.90 | 0.54 |
| 1:B:417:VAL:HG13 | 1:B:418:ALA:N | 2.22 | 0.54 |
| 1:C:278:ALA:HB1 | 1:C:279:PRO:HD2 | 1.89 | 0.54 |
| 1:D:451:LEU:C | 1:D:451:LEU:HD23 | 2.27 | 0.54 |
| 1:F:149:THR:HG23 | 1:F:155:ASP:C | 2.28 | 0.54 |
| 1:G:208:PRO:HB2 | 1:G:212:ALA:CB | 2.37 | 0.54 |
| 1:H:287:ALA:HB1 | 1:H:368:ARG:NH2 | 2.22 | 0.54 |
| 1:I:198:GLY:CA | 1:I:328:ASP:HA | 2.37 | 0.54 |
| 1:J:232:GLU:HA | 1:J:310:GLU:CG | 2.36 | 0.54 |
| 1:K:266:THR:HG22 | 1:K:273:VAL:H | 1.72 | 0.54 |
| 1:K:400:LEU:C | 1:K:400:LEU:HD23 | 2.27 | 0.54 |
| 1:K:31:LEU:HG | 1:K:454:ILE:CD1 | 2.38 | 0.54 |
| 1:L:183:LEU:HD22 | 1:M:360:TYR:CE2 | 2.43 | 0.54 |
| 1:L:190:VAL:HG22 | 1:L:191:GLU:N | 2.23 | 0.54 |
| 1:L:302:SER:HB2 | 1:L:305:ILE:HD12 | 1.89 | 0.54 |
| 2:Q:40:VAL:HB | 2:Q:62:GLY:H | 1.73 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:266:THR:HA | 1:A:271:VAL:O | 2.07 | 0.54 |
| 1:B:417:VAL:HA | 1:B:420:ILE:HG22 | 1.89 | 0.54 |
| 1:C:510:VAL:CG2 | 1:C:511:ALA:N | 2.70 | 0.54 |
| 1:D:208:PRO:HB2 | 1:D:212:ALA:CB | 2.38 | 0.54 |
| 1:D:327:LYS:H | 1:D:327:LYS:HD3 | 1.72 | 0.54 |
| 1:D:94:VAL:HG12 | 1:D:449:ALA:HB1 | 1.89 | 0.54 |
| 1:E:130:GLU:HA | 1:E:130:GLU:OE1 | 2.07 | 0.54 |
| 1:I:219:PHE:CE1 | 1:I:245:LYS:HB2 | 2.40 | 0.54 |
| 1:I:453:GLN:NE2 | 1:I:457:ASN:OD1 | 2.40 | 0.54 |
| 1:J:102:GLU:HB2 | 1:J:442:VAL:HG13 | 1.89 | 0.54 |
| 1:K:161:LEU:N | 1:K:161:LEU:HD12 | 2.23 | 0.54 |
| 1:K:69:MET:O | 1:K:73:MET:HG3 | 2.08 | 0.54 |
| 1:M:287:ALA:O | 1:M:290:GLN:HB3 | 2.07 | 0.54 |
| 1:M:434:GLU:O | 1:M:438:VAL:HG23 | 2.08 | 0.54 |
| 1:N:166:MET:CE | 1:N:171:LYS:HA | 2.36 | 0.54 |
| 2:O:40:VAL:HG21 | 2:O:63:ASP:HB2 | 1.90 | 0.54 |
| 1:A:199:TYR:CE1 | 1:A:327:LYS:HG3 | 2.43 | 0.54 |
| 1:B:372:LEU:O | 1:B:373:ALA:HB2 | 2.07 | 0.54 |
| 1:D:510:VAL:CG2 | 1:D:511:ALA:N | 2.70 | 0.54 |
| 1:E:381:VAL:CG1 | 1:E:392:LYS:HG3 | 2.37 | 0.54 |
| 1:F:161:LEU:O | 1:F:164:GLU:HB2 | 2.08 | 0.54 |
| 1:G:177:VAL:HG11 | 1:G:397:GLU:CG | 2.37 | 0.54 |
| 1:H:221:LEU:HD11 | 1:H:223:ALA:HB2 | 1.90 | 0.54 |
| 1:H:198:GLY:CA | 1:H:328:ASP:HA | 2.38 | 0.54 |
| 1:I:433:ASN:HD22 | 1:I:434:GLU:H | 1.56 | 0.54 |
| 1:K:264:VAL:HA | 1:K:267:MET:HG2 | 1.90 | 0.54 |
| 1:L:107:VAL:CG2 | 1:L:108:ALA:H | 2.21 | 0.54 |
| 1:M:107:VAL:CG2 | 1:M:108:ALA:N | 2.71 | 0.54 |
| 1:M:200:LEU:HD13 | 1:M:276:VAL:HA | 1.89 | 0.54 |
| 1:N:222:LEU:CD1 | 1:N:293:ALA:HA | 2.37 | 0.54 |
| 1:N:222:LEU:HD11 | 1:N:293:ALA:HA | 1.89 | 0.54 |
| 2:S:14:ARG:CG | 2:S:15:LYS:N | 2.70 | 0.54 |
| 2:S:92:LEU:O | 2:T:6:LEU:HB2 | 2.08 | 0.54 |
| 1:A:326:ASN:ND2 | 1:A:328:ASP:H | 2.05 | 0.54 |
| 1:B:180:GLY:CA | 1:B:380:LYS:HB3 | 2.38 | 0.54 |
| 1:B:381:VAL:CG1 | 1:B:392:LYS:CG | 2.86 | 0.54 |
| 1:C:271:VAL:O | 1:C:271:VAL:HG23 | 2.08 | 0.54 |
| 1:C:124:VAL:HG13 | 1:C:504:LEU:HD12 | 1.90 | 0.54 |
| 1:E:249:ILE:HG22 | 1:E:250:ILE:N | 2.23 | 0.54 |
| 1:G:372:LEU:O | 1:G:373:ALA:HB2 | 2.08 | 0.54 |
| 1:G:131:LEU:HD21 | 1:G:422:VAL:HG11 | 1.88 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:357:THR:O | 1:H:357:THR:HG22 | 2.07 | 0.54 |
| 1:I:217:SER:N | 1:I:218:PRO:HD3 | 2.23 | 0.54 |
| 1:J:38:VAL:HG13 | 1:K:519:CYS:HB3 | 1.89 | 0.54 |
| 1:J:420:ILE:HG13 | 1:J:451:LEU:HD22 | 1.90 | 0.54 |
| 1:L:155:ASP:CG | 1:L:158:VAL:HG23 | 2.28 | 0.54 |
| 1:L:16:MET:HG3 | 1:L:520:MET:SD | 2.47 | 0.54 |
| 1:L:342:ILE:O | 1:L:346:VAL:HG23 | 2.08 | 0.54 |
| 1:L:370:ALA:O | 1:L:374:GLY:N | 2.37 | 0.54 |
| 1:M:322:ARG:O | 1:M:323:VAL:HB | 2.08 | 0.54 |
| 2:O:77:LYS:C | 2:O:78:ILE:HD12 | 2.28 | 0.54 |
| 2:P:3:ILE:HD12 | 2:P:3:ILE:H | 1.73 | 0.54 |
| 1:B:124:VAL:HG22 | 1:B:504:LEU:HD11 | 1.90 | 0.54 |
| 1:B:256:GLY:O | 1:B:260:ALA:N | 2.38 | 0.54 |
| 1:B:246:PRO:HA | 1:B:272:LYS:O | 2.07 | 0.54 |
| 1:C:245:LYS:CE | 1:C:245:LYS:HA | 2.31 | 0.54 |
| 1:C:220:ILE:HG23 | 1:C:248:LEU:HD12 | 1.89 | 0.54 |
| 1:C:305:ILE:N | 1:C:305:ILE:CD1 | 2.68 | 0.54 |
| 1:C:475:ASN:ND2 | 1:C:475:ASN:N | 2.56 | 0.54 |
| 1:D:35:GLY:HA3 | 1:D:51:LYS:HE2 | 1.90 | 0.54 |
| 1:F:295:LEU:O | 1:F:337:GLY:HA3 | 2.07 | 0.54 |
| 1:G:346:VAL:HG12 | 1:G:350:ARG:HH22 | 1.73 | 0.54 |
| 1:H:406:ALA:O | 1:H:410:GLY:N | 2.39 | 0.54 |
| 1:I:225:LYS:HE2 | 1:I:309:LEU:HD11 | 1.88 | 0.54 |
| 1:J:112:ASN:O | 1:J:116:LEU:HG | 2.07 | 0.54 |
| 1:K:359:ASP:O | 1:K:363:GLU:HB2 | 2.08 | 0.54 |
| 1:L:40:LEU:N | 1:L:40:LEU:HD22 | 2.23 | 0.54 |
| 1:N:226:LYS:HG3 | 1:N:252:GLU:CB | 2.37 | 0.54 |
| 1:N:478:TYR:CE1 | 1:N:483:GLU:HA | 2.42 | 0.54 |
| 2:R:17:VAL:CG1 | 2:R:34:LYS:HA | 2.38 | 0.54 |
| 2:S:20:LYS:H | 2:S:20:LYS:CD | 2.18 | 0.54 |
| 2:S:77:LYS:C | 2:S:78:ILE:HD12 | 2.28 | 0.54 |
| 2:U:41:LEU:O | 2:U:61:VAL:HG13 | 2.07 | 0.54 |
| 1:A:271:VAL:HG23 | 1:A:271:VAL:O | 2.08 | 0.53 |
| 1:A:381:VAL:CG1 | 1:A:392:LYS:HG2 | 2.38 | 0.53 |
| 1:B:237:LEU:C | 1:B:237:LEU:HD23 | 2.27 | 0.53 |
| 1:B:499:VAL:CG2 | 1:B:500:THR:N | 2.70 | 0.53 |
| 1:C:177:VAL:HG22 | 1:C:393:LYS:HG3 | 1.89 | 0.53 |
| 1:C:302:SER:HB2 | 1:C:305:ILE:HB | 1.90 | 0.53 |
| 1:D:130:GLU:O | 1:D:134:LEU:HD13 | 2.07 | 0.53 |
| 1:D:417:VAL:HA | 1:D:420:ILE:HG22 | 1.88 | 0.53 |
| 1:E:107:VAL:HG13 | 1:E:113:PRO:HG3 | 1.89 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:44:PHE:N | 1:E:44:PHE:HD1 | 1.99 | 0.53 |
| 1:E:468:THR:OG1 | 1:E:485:TYR:CE2 | 2.61 | 0.53 |
| 1:F:277:LYS:HD3 | 1:F:285:ARG:NH2 | 2.22 | 0.53 |
| 1:F:252:GLU:HA | 1:F:285:ARG:NH1 | 2.23 | 0.53 |
| 1:F:362:ARG:O | 1:F:366:GLN:OE1 | 2.27 | 0.53 |
| 1:H:152:ALA:O | 1:H:153:ASN:HB3 | 2.08 | 0.53 |
| 1:H:263:VAL:O | 1:H:267:MET:HG2 | 2.08 | 0.53 |
| 1:I:247:LEU:N | 1:I:273:VAL:HG12 | 2.22 | 0.53 |
| 1:I:395:ARG:O | 1:I:398:ASP:HB2 | 2.07 | 0.53 |
| 1:I:421:ARG:HD2 | 1:I:474:GLY:O | 2.08 | 0.53 |
| 1:I:84:ALA:O | 1:I:498:LYS:HE2 | 2.08 | 0.53 |
| 1:J:395:ARG:O | 1:J:398:ASP:HB2 | 2.08 | 0.53 |
| 1:K:143:ALA:C | 1:K:146:GLN:HB3 | 2.29 | 0.53 |
| 1:K:247:LEU:N | 1:K:273:VAL:HG12 | 2.23 | 0.53 |
| 1:K:479:ASN:O | 1:K:483:GLU:N | 2.41 | 0.53 |
| 1:N:213:VAL:O | 1:N:324:VAL:HA | 2.07 | 0.53 |
| 2:P:77:LYS:HA | 2:P:81:GLU:O | 2.08 | 0.53 |
| 2:R:14:ARG:CG | 2:R:15:LYS:H | 2.21 | 0.53 |
| 2:R:20:LYS:HB3 | 2:R:27:LEU:HG | 1.89 | 0.53 |
| 2:R:27:LEU:O | 2:R:27:LEU:HD23 | 2.07 | 0.53 |
| 1:B:285:ARG:HG3 | 1:B:286:LYS:N | 2.23 | 0.53 |
| 1:D:261:THR:O | 1:D:265:ASN:ND2 | 2.41 | 0.53 |
| 1:D:322:ARG:O | 1:D:333:ILE:HG13 | 2.08 | 0.53 |
| 1:D:510:VAL:CG2 | 1:D:511:ALA:H | 2.21 | 0.53 |
| 1:E:277:LYS:HD3 | 1:E:285:ARG:NH2 | 2.23 | 0.53 |
| 1:E:313:THR:HG22 | 1:E:314:LEU:N | 2.24 | 0.53 |
| 1:F:221:LEU:HD13 | 1:F:317:LEU:HD21 | 1.89 | 0.53 |
| 1:F:194:GLN:NE2 | 1:F:329:THR:HG21 | 2.22 | 0.53 |
| 1:F:357:THR:O | 1:F:359:ASP:N | 2.41 | 0.53 |
| 1:F:368:ARG:O | 1:F:372:LEU:HG | 2.07 | 0.53 |
| 1:F:391:GLU:O | 1:F:394:ALA:HB3 | 2.08 | 0.53 |
| 1:F:6:VAL:HG12 | 1:F:521:VAL:HG22 | 1.89 | 0.53 |
| 1:G:237:LEU:HD23 | 1:G:237:LEU:C | 2.29 | 0.53 |
| 1:I:112:ASN:O | 1:I:116:LEU:HG | 2.08 | 0.53 |
| 1:I:428:ASP:O | 1:I:429:LEU:C | 2.45 | 0.53 |
| 1:J:233:MET:HE1 | 1:J:309:LEU:HD13 | 1.89 | 0.53 |
| 1:J:30:THR:HB | 1:J:51:LYS:O | 2.07 | 0.53 |
| 1:J:465:VAL:O | 1:J:469:VAL:HG23 | 2.08 | 0.53 |
| 1:K:256:GLY:O | 1:K:260:ALA:N | 2.41 | 0.53 |
| 1:L:164:GLU:O | 1:L:167:ASP:HB3 | 2.07 | 0.53 |
| 1:L:256:GLY:O | 1:L:260:ALA:N | 2.41 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:282:GLY:O | 1:M:285:ARG:HG2 | 2.06 | 0.53 |
| 1:N:411:VAL:HA | 1:N:497:THR:H | 1.73 | 0.53 |
| 2:O:14:ARG:CG | 2:O:15:LYS:H | 2.20 | 0.53 |
| 2:O:17:VAL:HG11 | 2:O:33:ALA:O | 2.08 | 0.53 |
| 2:P:68:ASN:HD22 | 2:Q:74:LYS:HE3 | 1.73 | 0.53 |
| 2:T:47:ARG:HG2 | 2:T:49:LEU:H | 1.73 | 0.53 |
| 1:A:288:MET:O | 1:A:289:LEU:HG | 2.08 | 0.53 |
| 1:C:391:GLU:O | 1:C:394:ALA:HB3 | 2.08 | 0.53 |
| 1:D:384:ALA:N | 1:D:388:GLU:OE1 | 2.40 | 0.53 |
| 1:E:206:ASN:HB3 | 1:E:214:GLU:H | 1.72 | 0.53 |
| 1:F:205:ILE:CD1 | 1:F:211:GLY:HA2 | 2.38 | 0.53 |
| 1:G:95:LEU:O | 1:G:98:ALA:HB3 | 2.08 | 0.53 |
| 1:H:227:ILE:O | 1:H:254:VAL:HA | 2.08 | 0.53 |
| 1:H:266:THR:HG22 | 1:H:273:VAL:H | 1.72 | 0.53 |
| 1:I:266:THR:HG22 | 1:I:273:VAL:H | 1.73 | 0.53 |
| 1:I:433:ASN:HD22 | 1:I:434:GLU:N | 2.06 | 0.53 |
| 1:K:17:LEU:O | 1:K:20:VAL:HG13 | 2.08 | 0.53 |
| 1:K:370:ALA:O | 1:K:374:GLY:N | 2.40 | 0.53 |
| 1:L:129:GLU:O | 1:L:132:LYS:N | 2.41 | 0.53 |
| 1:L:230:ILE:HD12 | 1:L:257:GLU:HG2 | 1.90 | 0.53 |
| 1:L:434:GLU:HA | 1:L:437:ASN:HD22 | 1.73 | 0.53 |
| 1:N:385:THR:CG2 | 1:N:388:GLU:HB3 | 2.39 | 0.53 |
| 2:S:73:VAL:O | 2:S:74:LYS:HD3 | 2.07 | 0.53 |
| 1:A:200:LEU:CD1 | 1:A:276:VAL:HA | 2.39 | 0.53 |
| 1:B:296:THR:HG22 | 1:B:335:GLY:CA | 2.32 | 0.53 |
| 1:B:313:THR:N | 1:B:316:ASP:OD2 | 2.42 | 0.53 |
| 1:C:409:GLU:CD | 1:C:501:ARG:HH21 | 2.11 | 0.53 |
| 1:D:302:SER:CB | 1:D:305:ILE:HB | 2.36 | 0.53 |
| 1:E:115:ASP:HB3 | 1:E:436:GLN:HG3 | 1.90 | 0.53 |
| 1:G:278:ALA:HB1 | 1:G:279:PRO:HD2 | 1.89 | 0.53 |
| 1:K:226:LYS:HA | 1:K:252:GLU:HB2 | 1.89 | 0.53 |
| 1:L:158:VAL:O | 1:L:160:LYS:N | 2.42 | 0.53 |
| 1:L:24:ALA:HA | 1:L:27:VAL:HG12 | 1.89 | 0.53 |
| 1:L:259:LEU:HD23 | 1:L:259:LEU:C | 2.28 | 0.53 |
| 1:L:32:GLY:CA | 1:L:454:ILE:HG23 | 2.38 | 0.53 |
| 2:T:92:LEU:O | 2:U:6:LEU:HB2 | 2.08 | 0.53 |
| 1:A:207:LYS:HB3 | 1:A:208:PRO:CD | 2.32 | 0.53 |
| 1:B:147:VAL:HA | 1:B:150:ILE:HG22 | 1.90 | 0.53 |
| 1:C:202:PRO:HG2 | 1:C:203:TYR:CD1 | 2.44 | 0.53 |
| 1:C:208:PRO:C | 1:C:212:ALA:HB3 | 2.29 | 0.53 |
| 1:D:143:ALA:HA | 1:D:146:GLN:NE2 | 2.23 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:349:ILE:HG21 | 1:D:369:VAL:HG22 | 1.90 | 0.53 |
| 1:E:177:VAL:HG11 | 1:E:397:GLU:CG | 2.39 | 0.53 |
| 1:F:346:VAL:O | 1:F:349:ILE:HB | 2.09 | 0.53 |
| 1:F:368:ARG:CD | 1:F:372:LEU:HD11 | 2.39 | 0.53 |
| 1:F:418:ALA:O | 1:F:422:VAL:HG13 | 2.09 | 0.53 |
| 1:G:278:ALA:O | 1:G:279:PRO:O | 2.27 | 0.53 |
| 1:H:222:LEU:HD11 | 1:H:293:ALA:HA | 1.90 | 0.53 |
| 1:I:256:GLY:O | 1:I:260:ALA:N | 2.42 | 0.53 |
| 1:J:180:GLY:HA2 | 1:J:380:LYS:HB3 | 1.89 | 0.53 |
| 1:L:214:GLU:HG2 | 1:L:324:VAL:CG1 | 2.38 | 0.53 |
| 1:L:356:ALA:HB1 | 1:L:362:ARG:NE | 2.19 | 0.53 |
| 1:M:314:LEU:HA | 1:M:317:LEU:HD13 | 1.90 | 0.53 |
| 1:M:499:VAL:CG2 | 1:M:500:THR:N | 2.71 | 0.53 |
| 1:N:219:PHE:HB2 | 1:N:247:LEU:HD23 | 1.90 | 0.53 |
| 2:P:55:LYS:HE3 | 2:P:55:LYS:H | 1.72 | 0.53 |
| 2:T:43:VAL:HG13 | 2:T:57:LEU:HD12 | 1.90 | 0.53 |
| 1:A:313:THR:HG22 | 1:A:314:LEU:N | 2.24 | 0.53 |
| 1:C:257:GLU:O | 1:C:261:THR:HG22 | 2.09 | 0.53 |
| 1:D:235:PRO:HG2 | 1:D:236:VAL:H | 1.73 | 0.53 |
| 1:D:346:VAL:O | 1:D:349:ILE:HB | 2.08 | 0.53 |
| 1:E:10:ASN:O | 1:E:14:VAL:HG23 | 2.08 | 0.53 |
| 1:E:234:LEU:N | 1:E:235:PRO:CD | 2.72 | 0.53 |
| 1:E:299:THR:HB | 1:E:316:ASP:HB3 | 1.90 | 0.53 |
| 1:F:349:ILE:HG22 | 1:F:353:ILE:HG13 | 1.89 | 0.53 |
| 1:G:200:LEU:O | 1:G:202:PRO:CD | 2.56 | 0.53 |
| 1:G:219:PHE:O | 1:G:247:LEU:HD22 | 2.09 | 0.53 |
| 1:I:383:ALA:CB | 1:I:389:MET:HA | 2.38 | 0.53 |
| 1:I:478:TYR:CE1 | 1:I:483:GLU:HA | 2.43 | 0.53 |
| 1:J:222:LEU:HD22 | 1:J:289:LEU:HD11 | 1.89 | 0.53 |
| 1:J:308:GLU:OE2 | 1:J:310:GLU:HG3 | 2.09 | 0.53 |
| 1:L:256:GLY:HA2 | 1:L:260:ALA:H | 1.73 | 0.53 |
| 1:M:320:ALA:HA | 1:M:334:ASP:O | 2.08 | 0.53 |
| 1:N:359:ASP:CA | 1:N:362:ARG:HH12 | 2.16 | 0.53 |
| 1:N:428:ASP:O | 1:N:429:LEU:C | 2.46 | 0.53 |
| 2:U:12:VAL:HG12 | 2:U:40:VAL:HA | 1.91 | 0.53 |
| 1:B:84:ALA:HB2 | 1:B:506:TYR:HE2 | 1.72 | 0.53 |
| 1:C:240:VAL:O | 1:C:244:GLY:N | 2.42 | 0.53 |
| 1:C:381:VAL:CG1 | 1:C:392:LYS:HG2 | 2.38 | 0.53 |
| 1:D:311:LYS:O | 1:D:312:ALA:HB2 | 2.09 | 0.53 |
| 1:D:448:GLU:O | 1:D:452:ARG:HG2 | 2.08 | 0.53 |
| 1:F:253:ASP:CG | 1:F:254:VAL:N | 2.63 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:28:LYS:O | 1:F:30:THR:N | 2.41 | 0.53 |
| 1:F:177:VAL:CG1 | 1:F:397:GLU:HG2 | 2.39 | 0.53 |
| 1:H:314:LEU:N | 1:H:314:LEU:HD12 | 2.11 | 0.53 |
| 1:L:31:LEU:HG | 1:L:454:ILE:CD1 | 2.39 | 0.53 |
| 1:M:230:ILE:HD11 | 1:M:257:GLU:HG2 | 1.91 | 0.53 |
| 1:M:421:ARG:NH2 | 1:M:469:VAL:O | 2.42 | 0.53 |
| 1:M:270:ILE:HA | 1:N:257:GLU:OE2 | 2.08 | 0.53 |
| 2:O:11:ILE:HB | 2:O:42:ALA:HB3 | 1.89 | 0.53 |
| 2:O:74:LYS:HE3 | 2:U:68:ASN:HD22 | 1.74 | 0.53 |
| 2:O:78:ILE:HD12 | 2:O:78:ILE:N | 2.24 | 0.53 |
| 2:P:34:LYS:HG3 | 2:P:35:SER:H | 1.73 | 0.53 |
| 2:Q:14:ARG:CG | 2:Q:15:LYS:H | 2.17 | 0.53 |
| 2:R:55:LYS:HE2 | 2:R:55:LYS:N | 2.12 | 0.53 |
| 2:S:78:ILE:N | 2:S:78:ILE:HD12 | 2.24 | 0.53 |
| 1:C:88:GLY:HA2 | 4:C:1:ADP:O2B | 2.09 | 0.53 |
| 1:C:200:LEU:HD12 | 1:C:200:LEU:N | 2.24 | 0.53 |
| 1:C:230:ILE:O | 1:C:232:GLU:N | 2.42 | 0.53 |
| 1:D:319:GLN:O | 1:D:335:GLY:HA2 | 2.08 | 0.53 |
| 1:D:357:THR:O | 1:D:359:ASP:N | 2.42 | 0.53 |
| 1:E:183:LEU:O | 1:E:382:GLY:HA3 | 2.08 | 0.53 |
| 1:F:256:GLY:O | 1:F:260:ALA:N | 2.40 | 0.53 |
| 1:F:349:ILE:HD13 | 1:F:369:VAL:HG22 | 1.89 | 0.53 |
| 1:F:402:ALA:O | 1:F:405:ALA:HB3 | 2.09 | 0.53 |
| 1:F:417:VAL:HA | 1:F:420:ILE:HG22 | 1.90 | 0.53 |
| 1:H:25:ASP:HA | 1:H:28:LYS:HE2 | 1.91 | 0.53 |
| 1:H:395:ARG:O | 1:H:398:ASP:HB2 | 2.09 | 0.53 |
| 1:H:421:ARG:HD2 | 1:H:474:GLY:O | 2.08 | 0.53 |
| 1:H:504:LEU:C | 1:H:504:LEU:HD13 | 2.29 | 0.53 |
| 1:I:406:ALA:O | 1:I:410:GLY:HA2 | 2.09 | 0.53 |
| 1:J:96:ALA:O | 1:J:100:ILE:HG13 | 2.09 | 0.53 |
| 1:K:305:ILE:O | 1:K:305:ILE:HG22 | 2.09 | 0.53 |
| 1:K:455:VAL:HG13 | 1:K:460:GLU:HB2 | 1.90 | 0.53 |
| 1:L:64:ASP:C | 1:L:65:LYS:O | 2.43 | 0.53 |
| 1:L:15:LYS:HD2 | 1:L:67:GLU:HG3 | 1.90 | 0.53 |
| 1:N:157:THR:O | 1:N:161:LEU:HD13 | 2.08 | 0.53 |
| 1:N:204:PHE:CD2 | 1:N:274:ALA:HB1 | 2.43 | 0.53 |
| 1:N:301:ILE:CD1 | 1:N:301:ILE:N | 2.72 | 0.53 |
| 2:Q:43:VAL:CG1 | 2:Q:57:LEU:HD12 | 2.39 | 0.53 |
| 2:T:14:ARG:HG2 | 2:T:15:LYS:H | 1.74 | 0.53 |
| 1:B:222:LEU:HD22 | 1:B:293:ALA:HB2 | 1.91 | 0.53 |
| 1:C:329:THR:CG2 | 1:C:330:THR:N | 2.71 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:96:ALA:O | 1:C:97:GLN:C | 2.46 | 0.53 |
| 1:E:432:GLN:NE2 | 1:E:436:GLN:HE22 | 2.06 | 0.53 |
| 1:G:381:VAL:HG21 | 1:G:393:LYS:HA | 1.90 | 0.53 |
| 1:G:475:ASN:ND2 | 1:G:475:ASN:N | 2.56 | 0.53 |
| 1:K:494:LEU:HD23 | 1:K:494:LEU:H | 1.73 | 0.53 |
| 1:L:385:THR:CG2 | 1:L:388:GLU:HB3 | 2.39 | 0.53 |
| 1:M:194:GLN:HG3 | 1:M:331:THR:HB | 1.91 | 0.53 |
| 1:N:152:ALA:O | 1:N:153:ASN:HB3 | 2.09 | 0.53 |
| 1:N:406:ALA:O | 1:N:410:GLY:N | 2.35 | 0.53 |
| 1:B:284:ARG:HG2 | 1:B:288:MET:HE2 | 1.91 | 0.53 |
| 1:D:289:LEU:O | 1:D:292:ILE:HB | 2.09 | 0.53 |
| 1:E:486:GLY:HA3 | 1:E:491:MET:HE2 | 1.90 | 0.53 |
| 1:E:54:VAL:HB | 1:E:89:THR:HG21 | 1.90 | 0.53 |
| 1:E:509:SER:CB | 1:F:385:THR:HG23 | 2.40 | 0.53 |
| 1:F:452:ARG:HB2 | 1:F:462:PRO:CB | 2.32 | 0.53 |
| 1:G:346:VAL:HA | 1:G:349:ILE:HD12 | 1.90 | 0.53 |
| 1:G:96:ALA:O | 1:G:97:GLN:C | 2.47 | 0.53 |
| 1:H:107:VAL:CG2 | 1:H:108:ALA:N | 2.72 | 0.53 |
| 1:H:145:ALA:O | 1:H:149:THR:HG23 | 2.08 | 0.53 |
| 1:H:193:MET:CG | 1:H:194:GLN:N | 2.71 | 0.53 |
| 1:H:285:ARG:O | 1:H:288:MET:HB2 | 2.09 | 0.53 |
| 1:I:247:LEU:C | 1:I:247:LEU:HD13 | 2.29 | 0.53 |
| 1:I:381:VAL:HB | 1:I:389:MET:HE3 | 1.91 | 0.53 |
| 1:J:385:THR:HG23 | 1:J:388:GLU:HB3 | 1.91 | 0.53 |
| 1:K:499:VAL:CG2 | 1:K:500:THR:N | 2.71 | 0.53 |
| 1:M:398:ASP:O | 1:M:401:HIS:HB2 | 2.08 | 0.53 |
| 1:M:494:LEU:O | 1:M:495:ASP:OD1 | 2.27 | 0.53 |
| 1:N:101:THR:HG22 | 1:N:105:LYS:HE3 | 1.89 | 0.53 |
| 1:N:262:LEU:HA | 1:N:265:ASN:HB3 | 1.91 | 0.53 |
| 2:O:47:ARG:O | 2:O:54:VAL:HG13 | 2.09 | 0.53 |
| 2:Q:14:ARG:CD | 2:Q:35:SER:HB3 | 2.39 | 0.53 |
| 2:Q:49:LEU:O | 2:Q:55:LYS:NZ | 2.41 | 0.53 |
| 2:T:20:LYS:HB3 | 2:T:27:LEU:HG | 1.91 | 0.53 |
| 1:A:112:ASN:HD21 | 1:A:114:MET:HB3 | 1.73 | 0.52 |
| 1:A:360:TYR:H | 1:A:363:GLU:HG3 | 1.74 | 0.52 |
| 1:C:403:THR:O | 1:C:407:VAL:HG23 | 2.09 | 0.52 |
| 1:C:436:GLN:O | 1:C:440:ILE:HG13 | 2.09 | 0.52 |
| 1:D:400:LEU:O | 1:D:400:LEU:HD13 | 2.09 | 0.52 |
| 1:E:368:ARG:CD | 1:E:372:LEU:HD11 | 2.39 | 0.52 |
| 1:F:273:VAL:CG1 | 1:F:274:ALA:N | 2.68 | 0.52 |
| 1:F:77:VAL:CG1 | 1:F:510:VAL:HG21 | 2.39 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:510:VAL:O | 1:F:511:ALA:C | 2.48 | 0.52 |
| 1:G:202:PRO:HG2 | 1:G:203:TYR:CD1 | 2.44 | 0.52 |
| 1:G:381:VAL:CG1 | 1:G:392:LYS:CG | 2.87 | 0.52 |
| 1:H:219:PHE:CB | 1:H:317:LEU:HD23 | 2.39 | 0.52 |
| 1:I:195:PHE:CE1 | 1:I:330:THR:HB | 2.44 | 0.52 |
| 1:I:422:VAL:O | 1:I:426:LEU:HD23 | 2.08 | 0.52 |
| 1:J:218:PRO:HB3 | 1:J:246:PRO:HB2 | 1.90 | 0.52 |
| 1:K:145:ALA:O | 1:K:149:THR:HG23 | 2.10 | 0.52 |
| 1:K:217:SER:HA | 1:K:320:ALA:O | 2.09 | 0.52 |
| 1:K:230:ILE:HD11 | 1:K:257:GLU:O | 2.09 | 0.52 |
| 1:K:247:LEU:HB3 | 1:K:273:VAL:HG11 | 1.91 | 0.52 |
| 1:K:256:GLY:CA | 1:K:259:LEU:HB3 | 2.38 | 0.52 |
| 1:K:353:ILE:HA | 1:K:365:LEU:HD12 | 1.91 | 0.52 |
| 1:K:404:ARG:O | 1:K:408:GLU:HG3 | 2.09 | 0.52 |
| 1:K:455:VAL:HG11 | 1:K:462:PRO:HA | 1.91 | 0.52 |
| 1:L:248:LEU:HD13 | 1:L:248:LEU:C | 2.28 | 0.52 |
| 1:L:358:SER:HB3 | 1:L:361:ASP:OD1 | 2.09 | 0.52 |
| 1:M:198:GLY:CA | 1:M:328:ASP:HA | 2.38 | 0.52 |
| 1:M:231:ARG:O | 1:M:234:LEU:HG | 2.09 | 0.52 |
| 1:N:164:GLU:O | 1:N:167:ASP:HB3 | 2.08 | 0.52 |
| 1:N:450:PRO:O | 1:N:454:ILE:HG12 | 2.09 | 0.52 |
| 1:N:95:LEU:O | 1:N:98:ALA:HB3 | 2.09 | 0.52 |
| 2:O:47:ARG:HD2 | 2:O:55:LYS:HD2 | 1.90 | 0.52 |
| 2:R:34:LYS:HG3 | 2:R:35:SER:N | 2.21 | 0.52 |
| 2:R:48:ILE:HG22 | 2:R:48:ILE:O | 2.08 | 0.52 |
| 1:B:420:ILE:HD11 | 1:B:470:LYS:CG | 2.39 | 0.52 |
| 1:C:486:GLY:HA3 | 1:C:491:MET:CE | 2.39 | 0.52 |
| 1:D:199:TYR:CE2 | 1:D:205:ILE:HG12 | 2.44 | 0.52 |
| 1:D:19:GLY:HA3 | 1:D:67:GLU:O | 2.09 | 0.52 |
| 1:F:107:VAL:HG13 | 1:F:113:PRO:HG3 | 1.90 | 0.52 |
| 1:F:327:LYS:HD3 | 1:F:327:LYS:H | 1.73 | 0.52 |
| 1:F:417:VAL:HG13 | 1:F:418:ALA:N | 2.24 | 0.52 |
| 1:G:235:PRO:HG2 | 1:G:236:VAL:HG23 | 1.91 | 0.52 |
| 1:G:218:PRO:HA | 1:G:246:PRO:HG2 | 1.91 | 0.52 |
| 1:H:161:LEU:CD1 | 1:H:161:LEU:H | 2.22 | 0.52 |
| 1:H:411:VAL:HA | 1:H:497:THR:H | 1.74 | 0.52 |
| 1:I:77:VAL:HG22 | 1:I:506:TYR:HB3 | 1.91 | 0.52 |
| 1:K:129:GLU:O | 1:K:132:LYS:N | 2.41 | 0.52 |
| 1:K:160:LYS:HG2 | 1:K:164:GLU:OE2 | 2.08 | 0.52 |
| 1:L:226:LYS:HG3 | 1:L:252:GLU:HB3 | 1.91 | 0.52 |
| 1:M:161:LEU:N | 1:M:161:LEU:HD12 | 2.23 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:247:LEU:HB3 | 1:M:273:VAL:HG11 | 1.90 | 0.52 |
| 1:M:325:ILE:HG13 | 1:M:330:THR:HG23 | 1.89 | 0.52 |
| 1:N:404:ARG:O | 1:N:408:GLU:HG3 | 2.10 | 0.52 |
| 2:O:4:ARG:HD2 | 2:O:5:PRO:HD2 | 1.90 | 0.52 |
| 1:A:233:MET:C | 1:A:235:PRO:CD | 2.75 | 0.52 |
| 1:B:283:ASP:O | 1:B:287:ALA:HB2 | 2.09 | 0.52 |
| 1:B:486:GLY:HA3 | 1:B:491:MET:CE | 2.39 | 0.52 |
| 1:D:295:LEU:HD23 | 1:D:295:LEU:C | 2.29 | 0.52 |
| 1:D:56:VAL:O | 1:D:57:ALA:C | 2.48 | 0.52 |
| 1:E:253:ASP:CG | 1:E:254:VAL:N | 2.62 | 0.52 |
| 1:E:265:ASN:OD1 | 2:S:27:LEU:HB3 | 2.10 | 0.52 |
| 1:E:510:VAL:HG23 | 1:E:511:ALA:H | 1.73 | 0.52 |
| 1:F:124:VAL:HG22 | 1:F:504:LEU:HD11 | 1.91 | 0.52 |
| 1:F:143:ALA:O | 1:F:146:GLN:HB2 | 2.10 | 0.52 |
| 1:F:220:ILE:HD12 | 1:F:220:ILE:N | 2.24 | 0.52 |
| 1:F:305:ILE:CG2 | 1:F:306:GLY:H | 2.19 | 0.52 |
| 1:F:479:ASN:HB3 | 1:F:482:THR:OG1 | 2.09 | 0.52 |
| 1:F:5:ASP:HB2 | 1:F:524:LEU:CD2 | 2.39 | 0.52 |
| 1:H:109:ALA:HB3 | 1:H:111:MET:CE | 2.39 | 0.52 |
| 1:H:240:VAL:HA | 1:H:243:ALA:HB3 | 1.90 | 0.52 |
| 1:H:287:ALA:HB1 | 1:H:368:ARG:CZ | 2.39 | 0.52 |
| 1:J:221:LEU:HD11 | 1:J:223:ALA:HB2 | 1.91 | 0.52 |
| 1:K:232:GLU:HB2 | 1:K:233:MET:HE3 | 1.91 | 0.52 |
| 1:L:117:LYS:HG2 | 1:L:121:ASP:OD2 | 2.10 | 0.52 |
| 1:L:313:THR:CG2 | 1:L:314:LEU:N | 2.72 | 0.52 |
| 1:L:359:ASP:CA | 1:L:362:ARG:HH12 | 2.10 | 0.52 |
| 1:L:455:VAL:HG11 | 1:L:462:PRO:HA | 1.91 | 0.52 |
| 1:L:90:THR:O | 1:L:93:THR:HB | 2.09 | 0.52 |
| 1:M:205:ILE:HA | 1:M:213:VAL:CG2 | 2.36 | 0.52 |
| 1:N:221:LEU:HD22 | 1:N:222:LEU:H | 1.75 | 0.52 |
| 1:A:78:ALA:O | 1:A:89:THR:HG22 | 2.10 | 0.52 |
| 1:B:134:LEU:H | 1:B:134:LEU:HD12 | 1.75 | 0.52 |
| 1:B:199:TYR:HE2 | 1:B:205:ILE:HG12 | 1.75 | 0.52 |
| 1:B:280:GLY:HA3 | 1:B:284:ARG:HH11 | 1.73 | 0.52 |
| 1:B:284:ARG:O | 1:B:287:ALA:HB3 | 2.10 | 0.52 |
| 1:B:311:LYS:O | 1:B:312:ALA:HB2 | 2.09 | 0.52 |
| 1:B:329:THR:CG2 | 1:B:330:THR:N | 2.72 | 0.52 |
| 1:C:233:MET:C | 1:C:235:PRO:CD | 2.76 | 0.52 |
| 1:C:352:GLN:C | 1:C:365:LEU:HD11 | 2.30 | 0.52 |
| 1:C:455:VAL:O | 1:C:458:CYS:HB2 | 2.09 | 0.52 |
| 1:C:468:THR:OG1 | 1:C:485:TYR:CE2 | 2.62 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:215:LEU:O | 1:D:322:ARG:HG3 | 2.09 | 0.52 |
| 1:E:412:VAL:HG13 | 1:E:497:THR:OG1 | 2.10 | 0.52 |
| 1:E:7:LYS:HD2 | 1:E:66:PHE:CE2 | 2.45 | 0.52 |
| 1:F:184:GLN:N | 1:F:184:GLN:OE1 | 2.39 | 0.52 |
| 1:F:361:ASP:C | 1:F:363:GLU:H | 2.13 | 0.52 |
| 1:G:206:ASN:HB3 | 1:G:214:GLU:H | 1.73 | 0.52 |
| 1:I:190:VAL:HG21 | 1:I:334:ASP:CG | 2.30 | 0.52 |
| 1:I:258:ALA:O | 1:I:261:THR:OG1 | 2.25 | 0.52 |
| 1:I:302:SER:HB2 | 1:I:305:ILE:CD1 | 2.39 | 0.52 |
| 1:I:479:ASN:O | 1:I:483:GLU:N | 2.42 | 0.52 |
| 1:J:302:SER:HB2 | 1:J:305:ILE:HD12 | 1.91 | 0.52 |
| 1:J:66:PHE:N | 1:J:69:MET:HG3 | 2.21 | 0.52 |
| 1:M:299:THR:HB | 1:M:316:ASP:HB3 | 1.90 | 0.52 |
| 1:M:383:ALA:CB | 1:M:389:MET:HA | 2.39 | 0.52 |
| 1:N:230:ILE:HD11 | 1:N:257:GLU:O | 2.10 | 0.52 |
| 2:P:78:ILE:HD13 | 2:P:83:VAL:CG2 | 2.38 | 0.52 |
| 2:R:8:ASP:O | 2:R:87:SER:HA | 2.09 | 0.52 |
| 2:U:55:LYS:N | 2:U:55:LYS:CE | 2.60 | 0.52 |
| 1:A:124:VAL:HG13 | 1:A:504:LEU:CD1 | 2.39 | 0.52 |
| 1:A:308:GLU:HB2 | 1:A:311:LYS:CB | 2.39 | 0.52 |
| 1:B:232:GLU:O | 1:B:233:MET:CB | 2.57 | 0.52 |
| 1:C:264:VAL:HA | 1:C:267:MET:HB2 | 1.91 | 0.52 |
| 1:C:348:GLN:HE22 | 1:C:352:GLN:NE2 | 2.07 | 0.52 |
| 1:C:54:VAL:HB | 1:C:89:THR:HG21 | 1.91 | 0.52 |
| 1:D:124:VAL:HG13 | 1:D:504:LEU:HD12 | 1.92 | 0.52 |
| 1:D:16:MET:O | 1:D:20:VAL:HG23 | 2.10 | 0.52 |
| 1:E:14:VAL:O | 1:E:18:ARG:HG3 | 2.09 | 0.52 |
| 1:E:305:ILE:N | 1:E:305:ILE:CD1 | 2.69 | 0.52 |
| 1:E:433:ASN:HD21 | 1:E:435:ASP:HB2 | 1.74 | 0.52 |
| 1:E:87:ASP:OD1 | 1:E:88:GLY:N | 2.42 | 0.52 |
| 1:F:433:ASN:OD1 | 1:F:436:GLN:HB2 | 2.09 | 0.52 |
| 1:F:477:GLY:HA3 | 1:F:488:MET:SD | 2.48 | 0.52 |
| 1:F:411:VAL:HA | 1:F:497:THR:H | 1.73 | 0.52 |
| 1:H:147:VAL:HA | 1:H:150:ILE:HD12 | 1.91 | 0.52 |
| 1:H:77:VAL:HG22 | 1:H:506:TYR:HB3 | 1.91 | 0.52 |
| 1:I:149:THR:HG22 | 1:I:156:GLU:HA | 1.90 | 0.52 |
| 1:I:131:LEU:CD1 | 1:I:422:VAL:HG11 | 2.39 | 0.52 |
| 1:K:23:LEU:O | 1:K:27:VAL:HG12 | 2.09 | 0.52 |
| 1:K:284:ARG:H | 1:K:284:ARG:HH11 | 1.57 | 0.52 |
| 1:K:358:SER:HB3 | 1:K:361:ASP:OD1 | 2.10 | 0.52 |
| 1:L:249:ILE:HG22 | 1:L:250:ILE:N | 2.25 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:104:LEU:O | 1:M:107:VAL:HG22 | 2.09 | 0.52 |
| 1:M:392:LYS:O | 1:M:396:VAL:HG23 | 2.08 | 0.52 |
| 1:N:420:ILE:CD1 | 1:N:448:GLU:HA | 2.38 | 0.52 |
| 2:O:50:GLU:O | 2:O:52:GLY:N | 2.43 | 0.52 |
| 2:P:14:ARG:CG | 2:P:15:LYS:N | 2.72 | 0.52 |
| 2:U:20:LYS:HD2 | 2:U:20:LYS:N | 2.23 | 0.52 |
| 1:B:200:LEU:HD12 | 1:B:200:LEU:N | 2.24 | 0.52 |
| 1:B:87:ASP:OD1 | 1:B:88:GLY:N | 2.42 | 0.52 |
| 1:C:451:LEU:HD23 | 1:C:451:LEU:C | 2.30 | 0.52 |
| 1:D:127:ALA:O | 1:D:130:GLU:HB2 | 2.08 | 0.52 |
| 1:E:509:SER:OG | 1:F:385:THR:HG23 | 2.10 | 0.52 |
| 1:G:418:ALA:O | 1:G:422:VAL:HG13 | 2.09 | 0.52 |
| 1:G:510:VAL:CG2 | 1:G:511:ALA:H | 2.23 | 0.52 |
| 1:G:7:LYS:HD2 | 1:G:66:PHE:CE2 | 2.45 | 0.52 |
| 1:H:103:GLY:O | 1:H:107:VAL:HG13 | 2.09 | 0.52 |
| 1:H:129:GLU:O | 1:H:132:LYS:N | 2.42 | 0.52 |
| 1:H:301:ILE:CD1 | 1:H:301:ILE:N | 2.73 | 0.52 |
| 1:H:345:ARG:HH22 | 1:H:368:ARG:NH2 | 2.07 | 0.52 |
| 1:H:350:ARG:HE | 1:H:369:VAL:HG11 | 1.75 | 0.52 |
| 1:H:386:GLU:HG2 | 1:H:390:LYS:HE2 | 1.90 | 0.52 |
| 1:I:349:ILE:O | 1:I:350:ARG:C | 2.48 | 0.52 |
| 1:K:487:ASN:O | 1:K:491:MET:HG3 | 2.09 | 0.52 |
| 1:L:149:THR:HG22 | 1:L:156:GLU:O | 2.09 | 0.52 |
| 1:L:230:ILE:HD11 | 1:L:257:GLU:O | 2.09 | 0.52 |
| 1:M:155:ASP:CG | 1:M:158:VAL:HG23 | 2.30 | 0.52 |
| 1:M:221:LEU:C | 1:M:221:LEU:HD13 | 2.30 | 0.52 |
| 1:M:419:LEU:HD21 | 1:M:500:THR:HG23 | 1.92 | 0.52 |
| 1:N:72:GLN:NE2 | 1:N:72:GLN:HA | 2.24 | 0.52 |
| 2:Q:27:LEU:O | 2:Q:27:LEU:HD23 | 2.09 | 0.52 |
| 1:A:134:LEU:O | 1:A:136:VAL:HG13 | 2.10 | 0.52 |
| 1:A:161:LEU:O | 1:A:164:GLU:HB2 | 2.10 | 0.52 |
| 1:C:229:ASN:C | 1:C:231:ARG:H | 2.13 | 0.52 |
| 1:C:265:ASN:HB3 | 1:C:271:VAL:HG22 | 1.92 | 0.52 |
| 1:D:366:GLN:O | 1:D:369:VAL:HB | 2.09 | 0.52 |
| 1:D:368:ARG:HD2 | 1:D:372:LEU:HD11 | 1.91 | 0.52 |
| 1:D:72:GLN:HA | 1:D:72:GLN:NE2 | 2.25 | 0.52 |
| 1:E:124:VAL:HG13 | 1:E:504:LEU:HD12 | 1.91 | 0.52 |
| 1:E:234:LEU:HD23 | 2:S:23:GLY:HA3 | 1.91 | 0.52 |
| 1:E:281:PHE:O | 1:E:285:ARG:HG2 | 2.10 | 0.52 |
| 1:E:213:VAL:O | 1:E:324:VAL:HA | 2.10 | 0.52 |
| 1:F:338:GLU:O | 1:F:341:ALA:HB3 | 2.08 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:420:ILE:HD11 | 1:F:470:LYS:CG | 2.40 | 0.52 |
| 1:H:193:MET:HG2 | 1:H:194:GLN:H | 1.74 | 0.52 |
| 1:I:232:GLU:CB | 1:I:233:MET:HE1 | 2.39 | 0.52 |
| 1:L:145:ALA:HA | 1:L:159:GLY:O | 2.09 | 0.52 |
| 1:L:214:GLU:HG2 | 1:L:324:VAL:HG12 | 1.91 | 0.52 |
| 1:L:64:ASP:OD1 | 1:L:65:LYS:O | 2.27 | 0.52 |
| 1:M:321:LYS:HD2 | 1:M:334:ASP:OD2 | 2.09 | 0.52 |
| 1:N:40:LEU:HD22 | 1:N:40:LEU:N | 2.25 | 0.52 |
| 1:A:322:ARG:CB | 1:A:333:ILE:HD12 | 2.28 | 0.52 |
| 1:A:417:VAL:CA | 1:A:420:ILE:HG22 | 2.39 | 0.52 |
| 1:A:510:VAL:CG2 | 1:A:511:ALA:H | 2.23 | 0.52 |
| 1:B:278:ALA:CB | 1:B:279:PRO:CD | 2.85 | 0.52 |
| 1:C:7:LYS:HD2 | 1:C:66:PHE:CE2 | 2.44 | 0.52 |
| 1:D:472:GLY:HA3 | 1:D:476:TYR:CD2 | 2.44 | 0.52 |
| 1:E:215:LEU:HB3 | 1:E:246:PRO:CB | 2.35 | 0.52 |
| 1:E:496:PRO:HG2 | 1:E:499:VAL:CG1 | 2.40 | 0.52 |
| 1:E:59:GLU:OE1 | 1:E:59:GLU:HA | 2.10 | 0.52 |
| 1:G:253:ASP:CG | 1:G:254:VAL:N | 2.63 | 0.52 |
| 1:I:200:LEU:HD13 | 1:I:276:VAL:HA | 1.90 | 0.52 |
| 1:I:386:GLU:O | 1:I:389:MET:HB3 | 2.10 | 0.52 |
| 1:J:285:ARG:HG2 | 1:J:285:ARG:HH11 | 1.75 | 0.52 |
| 1:J:287:ALA:O | 1:J:290:GLN:N | 2.43 | 0.52 |
| 1:K:222:LEU:HD22 | 1:K:289:LEU:HD11 | 1.90 | 0.52 |
| 1:L:420:ILE:CD1 | 1:L:448:GLU:HA | 2.40 | 0.52 |
| 1:M:200:LEU:CD1 | 1:M:276:VAL:HA | 2.40 | 0.52 |
| 1:H:229:ASN:HD21 | 1:N:270:ILE:HG23 | 1.74 | 0.52 |
| 1:N:222:LEU:HD13 | 1:N:293:ALA:HB2 | 1.92 | 0.52 |
| 2:Q:20:LYS:HG2 | 2:Q:27:LEU:HD23 | 1.91 | 0.52 |
| 2:R:78:ILE:N | 2:R:78:ILE:HD12 | 2.25 | 0.52 |
| 1:A:262:LEU:HD11 | 1:A:273:VAL:HB | 1.92 | 0.52 |
| 1:A:47:PRO:HD3 | 1:G:72:GLN:HB3 | 1.92 | 0.52 |
| 1:C:281:PHE:H | 1:C:284:ARG:NE | 2.07 | 0.52 |
| 1:C:327:LYS:H | 1:C:327:LYS:HD3 | 1.75 | 0.52 |
| 1:D:122:LYS:HE2 | 1:D:429:LEU:HD11 | 1.92 | 0.52 |
| 1:E:177:VAL:HG22 | 1:E:393:LYS:HG3 | 1.90 | 0.52 |
| 1:F:512:GLY:O | 1:F:515:ILE:HG12 | 2.10 | 0.52 |
| 1:G:41:ASP:O | 1:G:42:LYS:CG | 2.57 | 0.52 |
| 1:H:320:ALA:HA | 1:H:334:ASP:O | 2.10 | 0.52 |
| 1:H:403:THR:O | 1:H:407:VAL:HG23 | 2.10 | 0.52 |
| 1:I:257:GLU:O | 1:I:261:THR:HG23 | 2.09 | 0.52 |
| 1:J:169:VAL:O | 1:J:169:VAL:HG22 | 2.10 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:157:THR:O | 1:K:161:LEU:HD13 | 2.10 | 0.52 |
| 1:L:353:ILE:HA | 1:L:365:LEU:CD1 | 2.40 | 0.52 |
| 1:L:450:PRO:O | 1:L:454:ILE:HG12 | 2.09 | 0.52 |
| 1:M:175:ILE:N | 1:M:175:ILE:CD1 | 2.73 | 0.52 |
| 1:M:351:GLN:O | 1:M:354:GLU:N | 2.36 | 0.52 |
| 1:M:55:SER:O | 1:M:58:ARG:HB3 | 2.10 | 0.52 |
| 1:N:266:THR:HG22 | 1:N:273:VAL:H | 1.75 | 0.52 |
| 1:N:420:ILE:HD13 | 1:N:448:GLU:HA | 1.92 | 0.52 |
| 2:R:77:LYS:C | 2:R:78:ILE:HD12 | 2.30 | 0.52 |
| 2:T:78:ILE:HD12 | 2:T:78:ILE:N | 2.25 | 0.52 |
| 1:C:164:GLU:O | 1:C:167:ASP:HB3 | 2.09 | 0.52 |
| 1:C:381:VAL:CG1 | 1:C:392:LYS:CG | 2.88 | 0.52 |
| 1:C:432:GLN:NE2 | 1:C:436:GLN:HE22 | 2.08 | 0.52 |
| 1:D:200:LEU:HD12 | 1:D:200:LEU:N | 2.25 | 0.52 |
| 1:D:266:THR:HG22 | 1:D:273:VAL:N | 2.24 | 0.52 |
| 1:D:381:VAL:CG1 | 1:D:392:LYS:HG2 | 2.39 | 0.52 |
| 1:E:417:VAL:HG13 | 1:E:418:ALA:N | 2.23 | 0.52 |
| 1:F:177:VAL:HG22 | 1:F:393:LYS:HG3 | 1.91 | 0.52 |
| 1:F:406:ALA:O | 1:F:410:GLY:N | 2.43 | 0.52 |
| 1:G:482:THR:OG1 | 1:G:484:GLU:HG2 | 2.09 | 0.52 |
| 1:H:264:VAL:HA | 1:H:267:MET:CG | 2.39 | 0.52 |
| 1:I:256:GLY:O | 1:I:257:GLU:C | 2.46 | 0.52 |
| 1:I:313:THR:HG22 | 1:I:314:LEU:N | 2.24 | 0.52 |
| 1:I:400:LEU:C | 1:I:400:LEU:HD23 | 2.29 | 0.52 |
| 1:J:385:THR:CG2 | 1:J:388:GLU:HB3 | 2.40 | 0.52 |
| 1:L:219:PHE:HE1 | 1:L:245:LYS:HD2 | 1.73 | 0.52 |
| 1:L:395:ARG:O | 1:L:398:ASP:HB2 | 2.10 | 0.52 |
| 1:L:478:TYR:HB2 | 1:L:485:TYR:CD2 | 2.45 | 0.52 |
| 1:L:124:VAL:HG13 | 1:L:504:LEU:HD13 | 1.90 | 0.52 |
| 1:M:259:LEU:C | 1:M:259:LEU:HD23 | 2.31 | 0.52 |
| 1:M:314:LEU:HD12 | 1:M:314:LEU:N | 2.15 | 0.52 |
| 2:Q:20:LYS:HB3 | 2:Q:27:LEU:HG | 1.92 | 0.52 |
| 2:R:14:ARG:NH1 | 2:R:14:ARG:CB | 2.73 | 0.52 |
| 1:A:403:THR:O | 1:A:407:VAL:HG23 | 2.09 | 0.51 |
| 1:B:308:GLU:HB2 | 1:B:311:LYS:HB2 | 1.92 | 0.51 |
| 1:C:218:PRO:HD2 | 1:C:320:ALA:O | 2.09 | 0.51 |
| 1:C:56:VAL:O | 1:C:57:ALA:C | 2.49 | 0.51 |
| 1:D:14:VAL:O | 1:D:18:ARG:HG3 | 2.09 | 0.51 |
| 1:E:228:SER:HA | 1:E:255:GLU:CB | 2.22 | 0.51 |
| 1:E:338:GLU:O | 1:E:342:ILE:HG13 | 2.10 | 0.51 |
| 1:E:77:VAL:HG12 | 1:E:510:VAL:HG21 | 1.92 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:247:LEU:HB3 | 1:F:273:VAL:CG1 | 2.40 | 0.51 |
| 1:G:127:ALA:O | 1:G:130:GLU:HB2 | 2.10 | 0.51 |
| 1:G:222:LEU:HD21 | 1:G:292:ILE:HB | 1.90 | 0.51 |
| 1:G:232:GLU:O | 1:G:310:GLU:OE2 | 2.28 | 0.51 |
| 1:G:325:ILE:CG1 | 1:G:330:THR:HG23 | 2.40 | 0.51 |
| 1:G:325:ILE:HA | 1:G:329:THR:O | 2.10 | 0.51 |
| 1:G:417:VAL:CA | 1:G:420:ILE:HG22 | 2.40 | 0.51 |
| 1:H:385:THR:CG2 | 1:H:388:GLU:HB3 | 2.39 | 0.51 |
| 1:I:301:ILE:H | 1:I:301:ILE:HD12 | 1.73 | 0.51 |
| 1:I:72:GLN:NE2 | 1:I:72:GLN:HA | 2.26 | 0.51 |
| 1:J:218:PRO:CG | 1:J:246:PRO:HB2 | 2.40 | 0.51 |
| 1:J:27:VAL:HG11 | 1:J:93:THR:HG21 | 1.93 | 0.51 |
| 1:K:190:VAL:HG22 | 1:K:191:GLU:N | 2.25 | 0.51 |
| 1:K:7:LYS:HG3 | 1:K:66:PHE:CE2 | 2.45 | 0.51 |
| 1:L:221:LEU:HD12 | 1:L:249:ILE:HG23 | 1.92 | 0.51 |
| 1:L:288:MET:HA | 1:L:288:MET:CE | 2.40 | 0.51 |
| 1:L:293:ALA:HB1 | 1:L:298:GLY:O | 2.10 | 0.51 |
| 1:M:101:THR:HG22 | 1:M:105:LYS:HE3 | 1.90 | 0.51 |
| 1:N:487:ASN:HB3 | 1:N:490:ASP:HB2 | 1.90 | 0.51 |
| 2:P:5:PRO:CD | 2:P:42:ALA:HB1 | 2.39 | 0.51 |
| 2:R:83:VAL:C | 2:R:84:LEU:HD12 | 2.30 | 0.51 |
| 2:U:20:LYS:HG3 | 2:U:28:THR:O | 2.10 | 0.51 |
| 1:A:289:LEU:HD23 | 1:A:292:ILE:HD12 | 1.92 | 0.51 |
| 1:B:304:GLU:HB2 | 1:B:305:ILE:HD12 | 1.91 | 0.51 |
| 1:C:211:GLY:O | 1:C:325:ILE:O | 2.28 | 0.51 |
| 1:C:366:GLN:HA | 1:C:369:VAL:CG2 | 2.39 | 0.51 |
| 1:C:69:MET:CE | 1:D:39:VAL:HG12 | 2.40 | 0.51 |
| 1:D:289:LEU:HA | 1:D:292:ILE:HD12 | 1.91 | 0.51 |
| 1:D:510:VAL:O | 1:D:511:ALA:C | 2.47 | 0.51 |
| 1:E:200:LEU:CD1 | 1:E:276:VAL:HA | 2.40 | 0.51 |
| 1:F:501:ARG:O | 1:F:505:GLN:HG3 | 2.10 | 0.51 |
| 1:G:233:MET:C | 1:G:235:PRO:CD | 2.77 | 0.51 |
| 1:G:261:THR:O | 1:G:265:ASN:ND2 | 2.43 | 0.51 |
| 1:G:180:GLY:HA3 | 1:G:380:LYS:HB3 | 1.92 | 0.51 |
| 1:G:468:THR:OG1 | 1:G:485:TYR:CE2 | 2.61 | 0.51 |
| 1:H:104:LEU:O | 1:H:107:VAL:HG22 | 2.09 | 0.51 |
| 1:H:10:ASN:O | 1:H:11:ASP:C | 2.49 | 0.51 |
| 1:I:354:GLU:CG | 1:I:355:GLU:N | 2.73 | 0.51 |
| 1:I:37:ASN:ND2 | 1:I:37:ASN:H | 2.08 | 0.51 |
| 1:K:197:ARG:HG2 | 1:K:277:LYS:O | 2.11 | 0.51 |
| 1:K:302:SER:HB2 | 1:K:305:ILE:CD1 | 2.40 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:248:LEU:HD22 | 1:L:249:ILE:N | 2.25 | 0.51 |
| 1:M:147:VAL:HA | 1:M:150:ILE:HD12 | 1.91 | 0.51 |
| 1:M:284:ARG:HH11 | 1:M:284:ARG:H | 1.56 | 0.51 |
| 1:M:354:GLU:CG | 1:M:355:GLU:N | 2.73 | 0.51 |
| 1:N:266:THR:HG21 | 1:N:273:VAL:O | 2.10 | 0.51 |
| 1:N:286:LYS:HA | 1:N:286:LYS:CE | 2.33 | 0.51 |
| 2:Q:37:ARG:HG2 | 2:Q:37:ARG:NH1 | 2.25 | 0.51 |
| 1:A:239:ALA:HB1 | 1:A:314:LEU:HD23 | 1.92 | 0.51 |
| 1:A:292:ILE:O | 1:A:295:LEU:HB3 | 2.11 | 0.51 |
| 1:B:130:GLU:O | 1:B:134:LEU:HD13 | 2.11 | 0.51 |
| 1:B:309:LEU:HD12 | 1:B:309:LEU:H | 1.75 | 0.51 |
| 1:B:131:LEU:HD23 | 1:B:422:VAL:HG11 | 1.90 | 0.51 |
| 1:C:366:GLN:O | 1:C:369:VAL:HB | 2.10 | 0.51 |
| 1:D:147:VAL:HA | 1:D:150:ILE:HG22 | 1.90 | 0.51 |
| 1:D:176:THR:OG1 | 1:D:378:VAL:HG22 | 2.10 | 0.51 |
| 1:D:430:ARG:HG2 | 1:D:430:ARG:HH11 | 1.76 | 0.51 |
| 1:F:320:ALA:HA | 1:F:335:GLY:HA2 | 1.91 | 0.51 |
| 1:F:357:THR:CG2 | 1:F:361:ASP:HB2 | 2.40 | 0.51 |
| 1:G:248:LEU:HD13 | 1:G:249:ILE:N | 2.25 | 0.51 |
| 1:G:177:VAL:HG11 | 1:G:397:GLU:HG2 | 1.92 | 0.51 |
| 1:H:219:PHE:CE1 | 1:H:245:LYS:HD2 | 2.44 | 0.51 |
| 1:H:360:TYR:O | 1:H:364:LYS:HB2 | 2.10 | 0.51 |
| 1:H:30:THR:HB | 1:H:51:LYS:O | 2.10 | 0.51 |
| 1:J:101:THR:HG22 | 1:J:105:LYS:HE3 | 1.92 | 0.51 |
| 1:K:205:ILE:HG23 | 1:K:212:ALA:O | 2.10 | 0.51 |
| 1:K:27:VAL:HG11 | 1:K:93:THR:HG21 | 1.93 | 0.51 |
| 1:L:157:THR:O | 1:L:161:LEU:CD1 | 2.58 | 0.51 |
| 1:L:478:TYR:CE1 | 1:L:483:GLU:HA | 2.46 | 0.51 |
| 1:M:363:GLU:O | 1:M:367:GLU:HG3 | 2.11 | 0.51 |
| 1:M:40:LEU:HD23 | 1:M:50:THR:HG22 | 1.93 | 0.51 |
| 1:N:17:LEU:O | 1:N:20:VAL:HG13 | 2.10 | 0.51 |
| 1:F:261:THR:HB | 2:T:29:GLY:HA3 | 1.92 | 0.51 |
| 2:T:78:ILE:HD13 | 2:T:83:VAL:CG2 | 2.39 | 0.51 |
| 1:A:256:GLY:HA2 | 1:A:259:LEU:HD12 | 1.91 | 0.51 |
| 1:A:313:THR:CG2 | 1:A:315:GLU:HG3 | 2.40 | 0.51 |
| 1:A:321:LYS:HD2 | 1:A:333:ILE:HG22 | 1.92 | 0.51 |
| 1:C:401:HIS:O | 1:C:404:ARG:HB2 | 2.10 | 0.51 |
| 1:D:160:LYS:O | 1:D:164:GLU:HG3 | 2.10 | 0.51 |
| 1:E:16:MET:O | 1:E:20:VAL:HG23 | 2.10 | 0.51 |
| 1:F:111:MET:CE | 1:F:438:VAL:HG21 | 2.41 | 0.51 |
| 1:F:357:THR:HB | 1:F:361:ASP:CB | 2.41 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:256:GLY:O | 1:G:257:GLU:C | 2.49 | 0.51 |
| 1:H:65:LYS:O | 1:H:66:PHE:CB | 2.46 | 0.51 |
| 1:I:351:GLN:O | 1:I:354:GLU:N | 2.32 | 0.51 |
| 1:J:161:LEU:H | 1:J:161:LEU:CD1 | 2.24 | 0.51 |
| 1:K:107:VAL:CG2 | 1:K:108:ALA:N | 2.74 | 0.51 |
| 1:K:200:LEU:HD13 | 1:K:276:VAL:HA | 1.91 | 0.51 |
| 1:L:206:ASN:ND2 | 1:L:207:LYS:HE2 | 2.25 | 0.51 |
| 1:L:230:ILE:H | 1:L:230:ILE:CD1 | 2.16 | 0.51 |
| 1:L:494:LEU:CD2 | 1:L:494:LEU:N | 2.72 | 0.51 |
| 1:M:23:LEU:O | 1:M:27:VAL:HG12 | 2.10 | 0.51 |
| 1:M:302:SER:HB2 | 1:M:305:ILE:CG1 | 2.39 | 0.51 |
| 2:O:20:LYS:HG2 | 2:O:27:LEU:HD23 | 1.91 | 0.51 |
| 2:R:14:ARG:CG | 2:R:35:SER:HB3 | 2.39 | 0.51 |
| 2:T:20:LYS:HG3 | 2:T:28:THR:O | 2.10 | 0.51 |
| 1:B:475:ASN:ND2 | 1:B:475:ASN:N | 2.57 | 0.51 |
| 1:B:65:LYS:O | 1:B:69:MET:HG3 | 2.09 | 0.51 |
| 1:C:272:LYS:HB2 | 1:C:272:LYS:HZ2 | 1.75 | 0.51 |
| 1:C:292:ILE:O | 1:C:295:LEU:HB3 | 2.10 | 0.51 |
| 1:C:434:GLU:OE2 | 1:C:438:VAL:HG23 | 2.11 | 0.51 |
| 1:D:249:ILE:HG22 | 1:D:250:ILE:N | 2.24 | 0.51 |
| 1:D:253:ASP:CG | 1:D:254:VAL:H | 2.13 | 0.51 |
| 1:E:357:THR:HB | 1:E:361:ASP:CB | 2.41 | 0.51 |
| 1:F:229:ASN:C | 1:F:231:ARG:N | 2.64 | 0.51 |
| 1:F:54:VAL:HB | 1:F:89:THR:HG21 | 1.91 | 0.51 |
| 1:H:190:VAL:HG22 | 1:H:191:GLU:N | 2.26 | 0.51 |
| 1:I:218:PRO:HB3 | 1:I:246:PRO:HB2 | 1.91 | 0.51 |
| 1:J:169:VAL:CG1 | 1:J:173:GLY:HA3 | 2.39 | 0.51 |
| 1:J:478:TYR:HB2 | 1:J:485:TYR:CE2 | 2.46 | 0.51 |
| 1:K:232:GLU:HA | 1:K:310:GLU:CG | 2.41 | 0.51 |
| 1:K:222:LEU:CD1 | 1:K:293:ALA:HA | 2.41 | 0.51 |
| 1:L:158:VAL:C | 1:L:160:LYS:N | 2.64 | 0.51 |
| 1:L:285:ARG:HA | 1:L:288:MET:HB2 | 1.92 | 0.51 |
| 1:N:426:LEU:N | 1:N:426:LEU:HD23 | 2.12 | 0.51 |
| 1:H:73:MET:HE3 | 1:N:49:ILE:HD11 | 1.93 | 0.51 |
| 2:T:14:ARG:CG | 2:T:15:LYS:N | 2.74 | 0.51 |
| 2:T:48:ILE:HG22 | 2:T:48:ILE:O | 2.11 | 0.51 |
| 1:B:249:ILE:HG22 | 1:B:250:ILE:N | 2.26 | 0.51 |
| 1:B:278:ALA:HB1 | 1:B:279:PRO:HD2 | 1.89 | 0.51 |
| 1:B:313:THR:HG22 | 1:B:314:LEU:N | 2.25 | 0.51 |
| 1:C:237:LEU:C | 1:C:237:LEU:HD23 | 2.31 | 0.51 |
| 1:C:272:LYS:NZ | 1:C:272:LYS:HB2 | 2.24 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:366:GLN:HA | 1:D:369:VAL:CG2 | 2.41 | 0.51 |
| 1:E:27:VAL:HG13 | 1:E:53:GLY:HA2 | 1.92 | 0.51 |
| 1:F:145:ALA:O | 1:F:159:GLY:HA3 | 2.11 | 0.51 |
| 1:F:262:LEU:HD11 | 1:F:273:VAL:HB | 1.92 | 0.51 |
| 1:F:194:GLN:HG3 | 1:F:330:THR:O | 2.11 | 0.51 |
| 1:F:456:LEU:HD13 | 1:F:462:PRO:HG2 | 1.93 | 0.51 |
| 1:J:302:SER:HB2 | 1:J:305:ILE:HG13 | 1.92 | 0.51 |
| 1:K:248:LEU:HD13 | 1:K:249:ILE:N | 2.25 | 0.51 |
| 1:K:248:LEU:HD22 | 1:K:249:ILE:H | 1.76 | 0.51 |
| 1:K:313:THR:HB | 1:K:315:GLU:HG2 | 1.93 | 0.51 |
| 1:L:109:ALA:HB3 | 1:L:111:MET:HE3 | 1.93 | 0.51 |
| 1:L:138:CYS:SG | 1:L:144:ILE:HD13 | 2.51 | 0.51 |
| 1:N:308:GLU:OE2 | 1:N:310:GLU:HG3 | 2.10 | 0.51 |
| 2:S:17:VAL:HG22 | 2:S:35:SER:N | 2.26 | 0.51 |
| 2:S:47:ARG:HD3 | 2:S:49:LEU:CD1 | 2.37 | 0.51 |
| 1:A:23:LEU:HD13 | 1:A:23:LEU:C | 2.31 | 0.51 |
| 1:A:249:ILE:HG22 | 1:A:250:ILE:N | 2.26 | 0.51 |
| 1:A:131:LEU:HD23 | 1:A:422:VAL:HG11 | 1.91 | 0.51 |
| 1:A:496:PRO:HG2 | 1:A:499:VAL:HG13 | 1.91 | 0.51 |
| 1:B:252:GLU:HA | 1:B:285:ARG:NH1 | 2.26 | 0.51 |
| 1:B:346:VAL:HG12 | 1:B:350:ARG:NH2 | 2.26 | 0.51 |
| 1:C:235:PRO:HG2 | 1:C:236:VAL:HG23 | 1.92 | 0.51 |
| 1:C:333:ILE:O | 1:C:334:ASP:HB2 | 2.11 | 0.51 |
| 1:D:357:THR:CG2 | 1:D:361:ASP:HB2 | 2.40 | 0.51 |
| 1:G:221:LEU:C | 1:G:222:LEU:HD12 | 2.31 | 0.51 |
| 1:G:283:ASP:O | 1:G:287:ALA:HB2 | 2.11 | 0.51 |
| 1:H:180:GLY:HA2 | 1:H:380:LYS:HB3 | 1.93 | 0.51 |
| 1:H:231:ARG:O | 1:H:234:LEU:HG | 2.11 | 0.51 |
| 1:H:256:GLY:CA | 1:H:259:LEU:HB3 | 2.39 | 0.51 |
| 1:H:259:LEU:HD23 | 1:H:259:LEU:C | 2.31 | 0.51 |
| 1:I:321:LYS:HD2 | 1:I:334:ASP:OD2 | 2.11 | 0.51 |
| 1:I:40:LEU:N | 1:I:40:LEU:HD22 | 2.24 | 0.51 |
| 1:K:40:LEU:HD22 | 1:K:40:LEU:N | 2.25 | 0.51 |
| 1:K:16:MET:HG3 | 1:K:520:MET:SD | 2.50 | 0.51 |
| 1:L:320:ALA:HA | 1:L:334:ASP:O | 2.10 | 0.51 |
| 1:M:93:THR:O | 1:M:96:ALA:HB3 | 2.10 | 0.51 |
| 2:R:7:HIS:C | 2:R:9:ARG:H | 2.14 | 0.51 |
| 2:T:14:ARG:HB2 | 2:T:14:ARG:NH1 | 2.26 | 0.51 |
| 2:T:47:ARG:HB3 | 2:T:55:LYS:HG2 | 1.92 | 0.51 |
| 1:A:234:LEU:HA | 1:A:237:LEU:HB3 | 1.93 | 0.51 |
| 1:B:147:VAL:O | 1:B:150:ILE:HG22 | 2.11 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:252:GLU:O | 1:C:277:LYS:HE2 | 2.11 | 0.51 |
| 1:D:267:MET:O | 1:D:269:GLY:N | 2.44 | 0.51 |
| 1:D:78:ALA:O | 1:D:89:THR:HG22 | 2.11 | 0.51 |
| 1:F:279:PRO:HB3 | 1:F:288:MET:HE1 | 1.93 | 0.51 |
| 1:F:436:GLN:O | 1:F:440:ILE:HG13 | 2.10 | 0.51 |
| 1:G:309:LEU:H | 1:G:309:LEU:HD12 | 1.75 | 0.51 |
| 1:H:343:GLN:O | 1:H:346:VAL:HB | 2.10 | 0.51 |
| 1:I:166:MET:HE2 | 1:I:171:LYS:HG2 | 1.92 | 0.51 |
| 1:I:235:PRO:HG2 | 1:I:236:VAL:H | 1.76 | 0.51 |
| 1:J:191:GLU:O | 1:J:334:ASP:HA | 2.11 | 0.51 |
| 1:L:351:GLN:O | 1:L:354:GLU:N | 2.27 | 0.51 |
| 1:M:149:THR:HG22 | 1:M:156:GLU:O | 2.11 | 0.51 |
| 1:M:311:LYS:HD2 | 1:M:311:LYS:N | 2.26 | 0.51 |
| 1:M:178:GLU:O | 1:M:380:LYS:HA | 2.11 | 0.51 |
| 1:M:72:GLN:HA | 1:M:72:GLN:NE2 | 2.24 | 0.51 |
| 1:N:66:PHE:HD1 | 1:N:520:MET:HE2 | 1.73 | 0.51 |
| 2:S:7:HIS:HB2 | 2:S:46:GLY:O | 2.11 | 0.51 |
| 1:A:130:GLU:HA | 1:A:130:GLU:OE1 | 2.11 | 0.51 |
| 1:A:194:GLN:NE2 | 1:A:329:THR:HG21 | 2.26 | 0.51 |
| 1:A:357:THR:HB | 1:A:361:ASP:HB2 | 1.92 | 0.51 |
| 1:B:301:ILE:HG12 | 1:B:307:MET:HE2 | 1.93 | 0.51 |
| 1:C:290:GLN:O | 1:C:294:THR:N | 2.40 | 0.51 |
| 1:C:309:LEU:HD12 | 1:C:309:LEU:H | 1.76 | 0.51 |
| 1:D:279:PRO:HD2 | 1:D:285:ARG:CA | 2.41 | 0.51 |
| 1:D:333:ILE:O | 1:D:334:ASP:HB2 | 2.09 | 0.51 |
| 1:D:482:THR:OG1 | 1:D:484:GLU:HG2 | 2.11 | 0.51 |
| 1:E:160:LYS:HE3 | 1:E:164:GLU:OE2 | 2.10 | 0.51 |
| 1:E:320:ALA:HA | 1:E:335:GLY:HA2 | 1.92 | 0.51 |
| 1:E:357:THR:CG2 | 1:E:361:ASP:HB2 | 2.41 | 0.51 |
| 1:F:80:LYS:HD2 | 1:F:506:TYR:CZ | 2.46 | 0.51 |
| 1:G:207:LYS:HB2 | 1:G:207:LYS:HZ2 | 1.75 | 0.51 |
| 1:G:305:ILE:N | 1:G:305:ILE:CD1 | 2.69 | 0.51 |
| 1:G:434:GLU:OE2 | 1:G:438:VAL:HG23 | 2.10 | 0.51 |
| 1:H:266:THR:HG21 | 1:H:273:VAL:O | 2.10 | 0.51 |
| 1:J:385:THR:HG23 | 1:J:388:GLU:N | 2.24 | 0.51 |
| 1:J:413:ALA:CB | 1:J:417:VAL:HB | 2.41 | 0.51 |
| 1:K:425:LYS:O | 1:K:427:ALA:N | 2.44 | 0.51 |
| 1:K:95:LEU:O | 1:K:98:ALA:HB3 | 2.11 | 0.51 |
| 1:M:247:LEU:HD22 | 1:M:248:LEU:H | 1.76 | 0.51 |
| 1:M:355:GLU:O | 1:M:357:THR:N | 2.44 | 0.51 |
| 1:M:421:ARG:HA | 1:M:421:ARG:HE | 1.75 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:465:VAL:O | 1:N:469:VAL:HG23 | 2.11 | 0.51 |
| 2:O:17:VAL:HG13 | 2:O:34:LYS:CA | 2.39 | 0.51 |
| 2:S:14:ARG:HB2 | 2:S:14:ARG:NH1 | 2.26 | 0.51 |
| 1:A:213:VAL:O | 1:A:324:VAL:HA | 2.11 | 0.51 |
| 1:A:240:VAL:O | 1:A:244:GLY:N | 2.41 | 0.51 |
| 1:A:366:GLN:HA | 1:A:369:VAL:CG2 | 2.41 | 0.51 |
| 1:B:195:PHE:CE1 | 1:B:330:THR:HB | 2.45 | 0.51 |
| 1:B:194:GLN:HG3 | 1:B:330:THR:O | 2.10 | 0.51 |
| 1:B:174:VAL:HG21 | 1:B:367:GLU:HA | 1.91 | 0.51 |
| 1:C:308:GLU:H | 1:C:311:LYS:HB3 | 1.76 | 0.51 |
| 1:D:205:ILE:CD1 | 1:D:211:GLY:HA2 | 2.41 | 0.51 |
| 1:D:291:ASP:O | 1:D:295:LEU:HB2 | 2.10 | 0.51 |
| 1:D:381:VAL:CG1 | 1:D:392:LYS:CG | 2.89 | 0.51 |
| 1:D:403:THR:O | 1:D:407:VAL:HG23 | 2.10 | 0.51 |
| 1:E:279:PRO:HG2 | 1:E:288:MET:HE3 | 1.92 | 0.51 |
| 1:G:242:LYS:HD3 | 1:G:243:ALA:N | 2.26 | 0.51 |
| 1:G:289:LEU:N | 1:G:290:GLN:OE1 | 2.36 | 0.51 |
| 1:G:325:ILE:HG22 | 1:G:326:ASN:O | 2.11 | 0.51 |
| 1:G:353:ILE:O | 1:G:355:GLU:N | 2.44 | 0.51 |
| 1:H:149:THR:HG22 | 1:H:156:GLU:HA | 1.90 | 0.51 |
| 1:I:216:GLU:OE1 | 1:I:216:GLU:HA | 2.10 | 0.51 |
| 1:J:232:GLU:HB3 | 1:J:309:LEU:CB | 2.31 | 0.51 |
| 1:J:313:THR:CG2 | 1:J:314:LEU:N | 2.73 | 0.51 |
| 1:K:313:THR:CG2 | 1:K:314:LEU:N | 2.74 | 0.51 |
| 1:M:109:ALA:HB3 | 1:M:111:MET:HE3 | 1.93 | 0.51 |
| 1:M:169:VAL:CG1 | 1:M:173:GLY:HA3 | 2.37 | 0.51 |
| 1:M:221:LEU:CD1 | 1:M:223:ALA:H | 2.24 | 0.51 |
| 1:M:284:ARG:HH11 | 1:M:284:ARG:CB | 2.19 | 0.51 |
| 1:M:288:MET:HE3 | 1:M:288:MET:HA | 1.93 | 0.51 |
| 1:M:478:TYR:HB2 | 1:M:485:TYR:CD2 | 2.46 | 0.51 |
| 1:N:149:THR:HG22 | 1:N:156:GLU:O | 2.11 | 0.51 |
| 1:N:161:LEU:N | 1:N:161:LEU:HD12 | 2.24 | 0.51 |
| 2:P:7:HIS:HA | 2:P:45:ASN:N | 2.24 | 0.51 |
| 1:A:279:PRO:HD2 | 1:A:285:ARG:HA | 1.94 | 0.50 |
| 1:A:362:ARG:HA | 1:A:365:LEU:CD1 | 2.40 | 0.50 |
| 1:B:194:GLN:NE2 | 1:B:329:THR:HG21 | 2.26 | 0.50 |
| 1:B:215:LEU:C | 1:B:322:ARG:HG3 | 2.31 | 0.50 |
| 1:B:180:GLY:HA2 | 1:B:380:LYS:HB3 | 1.92 | 0.50 |
| 1:B:42:LYS:HE2 | 1:B:48:THR:HB | 1.92 | 0.50 |
| 1:B:510:VAL:O | 1:B:511:ALA:C | 2.49 | 0.50 |
| 1:D:381:VAL:HG21 | 1:D:393:LYS:HA | 1.92 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:443:ALA:O | 1:D:447:MET:HG3 | 2.10 | 0.50 |
| 1:E:142:LYS:HE2 | 1:E:146:GLN:OE1 | 2.11 | 0.50 |
| 1:E:227:ILE:HG22 | 1:E:227:ILE:O | 2.11 | 0.50 |
| 1:E:95:LEU:O | 1:E:99:ILE:HG13 | 2.10 | 0.50 |
| 1:G:391:GLU:O | 1:G:394:ALA:HB3 | 2.11 | 0.50 |
| 1:G:135:SER:HB2 | 1:G:497:THR:HG21 | 1.93 | 0.50 |
| 1:H:425:LYS:O | 1:H:427:ALA:N | 2.43 | 0.50 |
| 1:J:253:ASP:OD1 | 1:J:254:VAL:N | 2.33 | 0.50 |
| 1:J:476:TYR:HA | 1:J:486:GLY:O | 2.11 | 0.50 |
| 1:J:478:TYR:HA | 1:J:485:TYR:HA | 1.92 | 0.50 |
| 1:K:145:ALA:HA | 1:K:159:GLY:O | 2.11 | 0.50 |
| 1:K:233:MET:HE3 | 1:K:309:LEU:HD13 | 1.93 | 0.50 |
| 1:K:236:VAL:O | 1:K:239:ALA:N | 2.43 | 0.50 |
| 1:K:366:GLN:O | 1:K:369:VAL:HB | 2.10 | 0.50 |
| 1:L:37:ASN:N | 1:L:37:ASN:ND2 | 2.56 | 0.50 |
| 1:M:236:VAL:HG23 | 1:M:237:LEU:N | 2.26 | 0.50 |
| 1:M:496:PRO:O | 1:M:497:THR:C | 2.48 | 0.50 |
| 1:N:299:THR:HB | 1:N:316:ASP:HB3 | 1.93 | 0.50 |
| 1:N:464:VAL:O | 1:N:467:ASN:HB3 | 2.11 | 0.50 |
| 2:R:75:SER:OG | 2:R:82:GLU:OE1 | 2.29 | 0.50 |
| 2:U:14:ARG:CG | 2:U:15:LYS:H | 2.22 | 0.50 |
| 1:A:417:VAL:C | 1:A:420:ILE:HG22 | 2.31 | 0.50 |
| 1:A:72:GLN:NE2 | 1:A:72:GLN:HA | 2.26 | 0.50 |
| 1:B:211:GLY:O | 1:B:325:ILE:O | 2.30 | 0.50 |
| 1:B:361:ASP:O | 1:B:365:LEU:HB2 | 2.11 | 0.50 |
| 1:D:200:LEU:CD1 | 1:D:276:VAL:HA | 2.41 | 0.50 |
| 1:E:112:ASN:HD21 | 1:E:114:MET:HB3 | 1.76 | 0.50 |
| 1:F:134:LEU:N | 1:F:134:LEU:CD1 | 2.74 | 0.50 |
| 1:F:230:ILE:C | 1:F:232:GLU:N | 2.64 | 0.50 |
| 1:F:329:THR:CG2 | 1:F:330:THR:N | 2.74 | 0.50 |
| 1:G:350:ARG:HA | 1:G:353:ILE:HD12 | 1.93 | 0.50 |
| 1:G:401:HIS:O | 1:G:404:ARG:HB2 | 2.11 | 0.50 |
| 1:G:5:ASP:HB2 | 1:G:524:LEU:CD2 | 2.40 | 0.50 |
| 1:H:247:LEU:O | 1:H:273:VAL:HB | 2.11 | 0.50 |
| 1:I:140:ASP:O | 1:I:144:ILE:HG12 | 2.11 | 0.50 |
| 1:J:301:ILE:HG21 | 1:J:309:LEU:HD23 | 1.93 | 0.50 |
| 1:L:152:ALA:O | 1:L:153:ASN:HB3 | 2.11 | 0.50 |
| 1:L:169:VAL:HG22 | 1:L:169:VAL:O | 2.11 | 0.50 |
| 1:L:301:ILE:HG21 | 1:L:309:LEU:HD23 | 1.94 | 0.50 |
| 1:M:413:ALA:CB | 1:M:417:VAL:HB | 2.41 | 0.50 |
| 1:M:420:ILE:HG23 | 1:M:470:LYS:HD3 | 1.92 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:140:ASP:O | 1:N:144:ILE:HG12 | 2.11 | 0.50 |
| 1:N:205:ILE:HA | 1:N:213:VAL:HG22 | 1.93 | 0.50 |
| 1:N:200:LEU:HD11 | 1:N:277:LYS:H | 1.76 | 0.50 |
| 1:N:32:GLY:CA | 1:N:454:ILE:HG23 | 2.41 | 0.50 |
| 1:M:41:ASP:HB2 | 1:N:69:MET:CE | 2.41 | 0.50 |
| 2:O:20:LYS:CB | 2:O:27:LEU:HG | 2.40 | 0.50 |
| 2:R:40:VAL:HB | 2:R:62:GLY:H | 1.77 | 0.50 |
| 1:A:311:LYS:O | 1:A:312:ALA:HB2 | 2.11 | 0.50 |
| 1:B:207:LYS:CB | 1:B:208:PRO:HD3 | 2.32 | 0.50 |
| 1:B:501:ARG:O | 1:B:505:GLN:HG3 | 2.11 | 0.50 |
| 1:C:311:LYS:O | 1:C:312:ALA:HB2 | 2.12 | 0.50 |
| 1:C:355:GLU:C | 1:C:357:THR:H | 2.15 | 0.50 |
| 1:D:267:MET:C | 1:D:269:GLY:N | 2.64 | 0.50 |
| 1:D:267:MET:N | 1:D:267:MET:HE3 | 2.27 | 0.50 |
| 1:D:361:ASP:O | 1:D:365:LEU:HB2 | 2.11 | 0.50 |
| 1:F:33:PRO:HG2 | 1:F:34:LYS:H | 1.76 | 0.50 |
| 1:F:510:VAL:HG23 | 1:F:511:ALA:H | 1.75 | 0.50 |
| 1:G:147:VAL:O | 1:G:150:ILE:HG22 | 2.12 | 0.50 |
| 1:G:134:LEU:HD11 | 1:G:425:LYS:NZ | 2.27 | 0.50 |
| 1:G:451:LEU:HD23 | 1:G:451:LEU:C | 2.32 | 0.50 |
| 1:H:362:ARG:O | 1:H:366:GLN:HB2 | 2.12 | 0.50 |
| 1:I:189:VAL:O | 1:I:189:VAL:HG23 | 2.10 | 0.50 |
| 1:I:64:ASP:OD1 | 1:I:65:LYS:O | 2.29 | 0.50 |
| 1:K:55:SER:HA | 1:K:58:ARG:NH1 | 2.26 | 0.50 |
| 1:L:247:LEU:HD22 | 1:L:248:LEU:N | 2.26 | 0.50 |
| 1:L:222:LEU:CD2 | 1:L:289:LEU:HD11 | 2.38 | 0.50 |
| 1:L:219:PHE:HB3 | 1:L:317:LEU:HD23 | 1.92 | 0.50 |
| 1:L:479:ASN:OD1 | 1:L:481:ALA:HB3 | 2.11 | 0.50 |
| 1:M:215:LEU:CB | 1:M:218:PRO:HG2 | 2.40 | 0.50 |
| 1:M:290:GLN:CG | 1:M:345:ARG:HH21 | 2.25 | 0.50 |
| 1:M:47:PRO:HG3 | 1:N:73:MET:HG3 | 1.93 | 0.50 |
| 1:N:194:GLN:HG3 | 1:N:331:THR:HB | 1.92 | 0.50 |
| 1:N:247:LEU:N | 1:N:273:VAL:HG12 | 2.26 | 0.50 |
| 1:N:290:GLN:HA | 1:N:290:GLN:OE1 | 2.11 | 0.50 |
| 1:C:270:ILE:HD13 | 2:Q:27:LEU:HB2 | 1.92 | 0.50 |
| 2:Q:9:ARG:NH1 | 2:Q:86:MET:HA | 2.26 | 0.50 |
| 2:T:18:GLU:CD | 2:T:33:ALA:HB3 | 2.31 | 0.50 |
| 1:A:257:GLU:O | 1:A:261:THR:HG22 | 2.10 | 0.50 |
| 1:A:281:PHE:O | 1:A:284:ARG:HB3 | 2.12 | 0.50 |
| 1:A:290:GLN:O | 1:A:294:THR:N | 2.43 | 0.50 |
| 1:A:327:LYS:HD3 | 1:A:327:LYS:N | 2.25 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:346:VAL:O | 1:A:349:ILE:HB | 2.11 | 0.50 |
| 1:C:450:PRO:O | 1:C:454:ILE:HG13 | 2.11 | 0.50 |
| 1:C:19:GLY:HA3 | 1:C:67:GLU:O | 2.12 | 0.50 |
| 1:E:150:ILE:HD11 | 4:E:1:ADP:N7 | 2.25 | 0.50 |
| 1:E:249:ILE:HB | 1:E:275:ALA:HB1 | 1.93 | 0.50 |
| 1:F:134:LEU:CD1 | 1:F:134:LEU:H | 2.24 | 0.50 |
| 1:F:339:GLU:H | 1:F:339:GLU:CD | 2.15 | 0.50 |
| 1:F:349:ILE:HG21 | 1:F:369:VAL:CG2 | 2.40 | 0.50 |
| 1:G:134:LEU:N | 1:G:134:LEU:HD12 | 2.26 | 0.50 |
| 1:I:256:GLY:HA2 | 1:I:260:ALA:H | 1.75 | 0.50 |
| 1:I:346:VAL:O | 1:I:350:ARG:HG2 | 2.11 | 0.50 |
| 1:J:219:PHE:CE1 | 1:J:245:LYS:HD2 | 2.46 | 0.50 |
| 1:J:222:LEU:CD1 | 1:J:293:ALA:HA | 2.42 | 0.50 |
| 1:J:55:SER:HA | 1:J:58:ARG:NH1 | 2.26 | 0.50 |
| 1:K:383:ALA:HB3 | 1:K:389:MET:HA | 1.94 | 0.50 |
| 1:K:30:THR:HB | 1:K:51:LYS:O | 2.10 | 0.50 |
| 1:L:169:VAL:CG1 | 1:L:173:GLY:HA3 | 2.37 | 0.50 |
| 1:L:383:ALA:CB | 1:L:389:MET:HA | 2.41 | 0.50 |
| 1:L:419:LEU:HD12 | 1:L:447:MET:HB3 | 1.93 | 0.50 |
| 1:M:259:LEU:HD23 | 1:M:260:ALA:N | 2.26 | 0.50 |
| 1:N:385:THR:HG23 | 1:N:388:GLU:N | 2.25 | 0.50 |
| 1:N:64:ASP:OD1 | 1:N:65:LYS:O | 2.30 | 0.50 |
| 2:P:47:ARG:HB3 | 2:P:55:LYS:HG2 | 1.94 | 0.50 |
| 2:P:47:ARG:HD3 | 2:P:49:LEU:CD1 | 2.36 | 0.50 |
| 2:R:12:VAL:HA | 2:R:41:LEU:HG | 1.94 | 0.50 |
| 2:T:14:ARG:CG | 2:T:35:SER:HB3 | 2.42 | 0.50 |
| 1:A:6:VAL:HG12 | 1:A:521:VAL:HG13 | 1.94 | 0.50 |
| 1:D:221:LEU:C | 1:D:222:LEU:HD12 | 2.32 | 0.50 |
| 1:D:486:GLY:HA3 | 1:D:491:MET:CE | 2.42 | 0.50 |
| 1:E:207:LYS:HB3 | 1:E:208:PRO:CD | 2.30 | 0.50 |
| 1:E:305:ILE:CG2 | 1:E:306:GLY:H | 2.12 | 0.50 |
| 1:G:240:VAL:O | 1:G:244:GLY:N | 2.37 | 0.50 |
| 1:H:143:ALA:C | 1:H:146:GLN:HB3 | 2.31 | 0.50 |
| 1:H:262:LEU:HA | 1:H:265:ASN:HB3 | 1.94 | 0.50 |
| 1:H:391:GLU:O | 1:H:394:ALA:HB3 | 2.12 | 0.50 |
| 1:H:419:LEU:HD21 | 1:H:500:THR:CG2 | 2.41 | 0.50 |
| 1:I:240:VAL:HA | 1:I:243:ALA:HB3 | 1.94 | 0.50 |
| 1:I:420:ILE:HG13 | 1:I:451:LEU:HD22 | 1.92 | 0.50 |
| 1:K:301:ILE:CD1 | 1:K:301:ILE:N | 2.73 | 0.50 |
| 1:K:450:PRO:O | 1:K:454:ILE:HG12 | 2.11 | 0.50 |
| 1:M:266:THR:HG21 | 1:M:273:VAL:O | 2.12 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:222:LEU:CD1 | 1:M:293:ALA:HA | 2.41 | 0.50 |
| 1:M:367:GLU:O | 1:M:370:ALA:HB3 | 2.11 | 0.50 |
| 1:M:479:ASN:O | 1:M:483:GLU:N | 2.42 | 0.50 |
| 1:M:494:LEU:HD23 | 1:M:494:LEU:H | 1.72 | 0.50 |
| 1:N:117:LYS:HG2 | 1:N:121:ASP:OD2 | 2.11 | 0.50 |
| 2:T:43:VAL:CG1 | 2:T:57:LEU:HD12 | 2.42 | 0.50 |
| 1:A:302:SER:CB | 1:A:305:ILE:HB | 2.41 | 0.50 |
| 1:A:302:SER:HB2 | 1:A:305:ILE:CD1 | 2.41 | 0.50 |
| 1:A:361:ASP:O | 1:A:365:LEU:HB2 | 2.12 | 0.50 |
| 1:D:220:ILE:CD1 | 1:D:220:ILE:N | 2.74 | 0.50 |
| 1:E:256:GLY:O | 1:E:260:ALA:N | 2.38 | 0.50 |
| 1:E:372:LEU:O | 1:E:373:ALA:HB2 | 2.11 | 0.50 |
| 1:F:10:ASN:O | 1:F:14:VAL:HG23 | 2.11 | 0.50 |
| 1:F:292:ILE:O | 1:F:295:LEU:HB3 | 2.11 | 0.50 |
| 1:F:358:SER:HA | 1:F:362:ARG:CD | 2.42 | 0.50 |
| 1:G:252:GLU:O | 1:G:277:LYS:HE2 | 2.11 | 0.50 |
| 1:I:107:VAL:CG2 | 1:I:108:ALA:N | 2.75 | 0.50 |
| 1:I:233:MET:CE | 1:I:309:LEU:HD13 | 2.42 | 0.50 |
| 1:I:179:ASP:OD2 | 1:I:390:LYS:HG2 | 2.12 | 0.50 |
| 1:I:15:LYS:HD2 | 1:I:67:GLU:HG3 | 1.93 | 0.50 |
| 1:J:107:VAL:CG2 | 1:J:108:ALA:N | 2.75 | 0.50 |
| 1:K:345:ARG:HA | 1:K:348:GLN:HE21 | 1.73 | 0.50 |
| 1:M:256:GLY:CA | 1:M:259:LEU:HB3 | 2.41 | 0.50 |
| 1:N:135:SER:HA | 1:N:412:VAL:HG12 | 1.94 | 0.50 |
| 2:O:60:LYS:HG2 | 2:O:63:ASP:OD2 | 2.12 | 0.50 |
| 1:A:279:PRO:HB3 | 1:A:288:MET:HE3 | 1.93 | 0.50 |
| 1:A:339:GLU:HA | 1:A:342:ILE:HB | 1.93 | 0.50 |
| 1:A:392:LYS:O | 1:A:396:VAL:HG23 | 2.11 | 0.50 |
| 1:A:77:VAL:HG12 | 1:A:510:VAL:HG21 | 1.94 | 0.50 |
| 1:B:225:LYS:C | 1:B:252:GLU:HB2 | 2.31 | 0.50 |
| 1:B:353:ILE:O | 1:B:355:GLU:N | 2.45 | 0.50 |
| 1:C:510:VAL:HG23 | 1:C:511:ALA:H | 1.75 | 0.50 |
| 1:E:200:LEU:O | 1:E:202:PRO:HD2 | 2.12 | 0.50 |
| 1:E:233:MET:C | 1:E:235:PRO:CD | 2.76 | 0.50 |
| 1:E:461:GLU:OE2 | 1:K:452:ARG:NH2 | 2.45 | 0.50 |
| 1:G:199:TYR:HE1 | 1:G:327:LYS:HG3 | 1.76 | 0.50 |
| 1:G:199:TYR:CZ | 1:G:202:PRO:HA | 2.47 | 0.50 |
| 1:G:247:LEU:HB3 | 1:G:273:VAL:CG1 | 2.42 | 0.50 |
| 1:H:218:PRO:HB3 | 1:H:246:PRO:HB2 | 1.92 | 0.50 |
| 1:H:236:VAL:HG23 | 1:H:237:LEU:N | 2.26 | 0.50 |
| 1:H:288:MET:CE | 1:H:288:MET:HA | 2.41 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:353:ILE:HG12 | 1:H:365:LEU:CB | 2.41 | 0.50 |
| 1:H:74:VAL:O | 1:H:75:LYS:C | 2.50 | 0.50 |
| 1:J:323:VAL:CG2 | 1:J:332:ILE:HG22 | 2.41 | 0.50 |
| 1:J:190:VAL:HG21 | 1:J:334:ASP:CG | 2.31 | 0.50 |
| 1:K:112:ASN:O | 1:K:116:LEU:HG | 2.12 | 0.50 |
| 1:L:109:ALA:HB3 | 1:L:111:MET:CE | 2.42 | 0.50 |
| 1:L:302:SER:HB2 | 1:L:305:ILE:CD1 | 2.42 | 0.50 |
| 1:L:314:LEU:CA | 1:L:317:LEU:HD13 | 2.40 | 0.50 |
| 1:L:354:GLU:CG | 1:L:355:GLU:N | 2.75 | 0.50 |
| 1:M:129:GLU:O | 1:M:132:LYS:N | 2.44 | 0.50 |
| 1:M:487:ASN:HB3 | 1:M:490:ASP:HB2 | 1.94 | 0.50 |
| 1:M:16:MET:HG3 | 1:M:520:MET:SD | 2.51 | 0.50 |
| 1:N:193:MET:CG | 1:N:194:GLN:H | 2.24 | 0.50 |
| 1:N:198:GLY:CA | 1:N:328:ASP:HA | 2.41 | 0.50 |
| 1:A:270:ILE:HD11 | 2:O:27:LEU:HD13 | 1.94 | 0.50 |
| 1:A:234:LEU:N | 1:A:235:PRO:CD | 2.73 | 0.50 |
| 1:B:149:THR:OG1 | 1:B:156:GLU:HA | 2.11 | 0.50 |
| 1:B:199:TYR:O | 1:B:199:TYR:HD1 | 1.95 | 0.50 |
| 1:B:202:PRO:HG2 | 1:B:203:TYR:CD1 | 2.47 | 0.50 |
| 1:B:349:ILE:HA | 1:B:352:GLN:CD | 2.32 | 0.50 |
| 1:B:434:GLU:O | 1:B:437:ASN:N | 2.45 | 0.50 |
| 1:C:35:GLY:HA3 | 1:C:51:LYS:HE2 | 1.93 | 0.50 |
| 1:D:234:LEU:HA | 1:D:237:LEU:HB3 | 1.94 | 0.50 |
| 1:D:404:ARG:HG3 | 1:D:404:ARG:NH1 | 2.26 | 0.50 |
| 1:F:315:GLU:OE1 | 1:F:316:ASP:N | 2.45 | 0.50 |
| 1:F:59:GLU:OE1 | 1:F:59:GLU:HA | 2.11 | 0.50 |
| 1:G:262:LEU:HD11 | 1:G:273:VAL:HB | 1.92 | 0.50 |
| 1:G:313:THR:HB | 1:G:315:GLU:OE2 | 2.12 | 0.50 |
| 1:H:353:ILE:HG12 | 1:H:365:LEU:HB3 | 1.94 | 0.50 |
| 1:H:448:GLU:HB3 | 1:H:452:ARG:HD2 | 1.93 | 0.50 |
| 1:I:286:LYS:HA | 1:I:286:LYS:CE | 2.36 | 0.50 |
| 1:I:434:GLU:HA | 1:I:437:ASN:HD22 | 1.75 | 0.50 |
| 1:I:476:TYR:HA | 1:I:486:GLY:O | 2.12 | 0.50 |
| 1:J:124:VAL:O | 1:J:128:VAL:HG23 | 2.11 | 0.50 |
| 1:J:149:THR:CG2 | 1:J:159:GLY:HA3 | 2.41 | 0.50 |
| 1:J:422:VAL:O | 1:J:426:LEU:CD2 | 2.59 | 0.50 |
| 1:L:23:LEU:O | 1:L:27:VAL:HG12 | 2.11 | 0.50 |
| 1:M:232:GLU:HB2 | 1:M:233:MET:HE3 | 1.93 | 0.50 |
| 2:R:58:ASP:N | 2:R:88:GLU:OE2 | 2.40 | 0.50 |
| 2:S:40:VAL:HB | 2:S:62:GLY:N | 2.26 | 0.50 |
| 2:T:6:LEU:O | 2:T:7:HIS:O | 2.29 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:302:SER:HB2 | 1:C:305:ILE:CD1 | 2.36 | 0.50 |
| 1:D:267:MET:C | 1:D:269:GLY:H | 2.15 | 0.50 |
| 1:D:290:GLN:OE1 | 1:D:290:GLN:N | 2.40 | 0.50 |
| 1:E:279:PRO:HB2 | 1:E:285:ARG:HA | 1.94 | 0.50 |
| 1:E:291:ASP:O | 1:E:295:LEU:HB2 | 2.12 | 0.50 |
| 1:F:329:THR:HG22 | 1:F:330:THR:N | 2.27 | 0.50 |
| 1:F:451:LEU:C | 1:F:451:LEU:HD23 | 2.32 | 0.50 |
| 1:G:346:VAL:O | 1:G:349:ILE:HB | 2.12 | 0.50 |
| 1:G:351:GLN:O | 1:G:351:GLN:NE2 | 2.45 | 0.50 |
| 1:G:417:VAL:C | 1:G:420:ILE:HG22 | 2.32 | 0.50 |
| 1:G:432:GLN:NE2 | 1:G:436:GLN:HE22 | 2.10 | 0.50 |
| 1:H:230:ILE:HD11 | 1:H:257:GLU:O | 2.11 | 0.50 |
| 1:I:202:PRO:C | 1:I:204:PHE:H | 2.15 | 0.50 |
| 1:J:7:LYS:HG3 | 1:J:66:PHE:CE2 | 2.47 | 0.50 |
| 1:L:266:THR:O | 1:L:268:ARG:N | 2.45 | 0.50 |
| 1:M:69:MET:O | 1:M:73:MET:HG3 | 2.12 | 0.50 |
| 2:S:14:ARG:CD | 2:S:35:SER:HB3 | 2.36 | 0.50 |
| 1:A:232:GLU:O | 1:A:233:MET:CB | 2.60 | 0.49 |
| 1:B:452:ARG:HB2 | 1:B:462:PRO:CB | 2.33 | 0.49 |
| 1:B:77:VAL:HG22 | 1:B:78:ALA:N | 2.27 | 0.49 |
| 1:C:143:ALA:O | 1:C:146:GLN:HB2 | 2.12 | 0.49 |
| 1:C:246:PRO:HA | 1:C:272:LYS:O | 2.12 | 0.49 |
| 1:D:134:LEU:O | 1:D:136:VAL:HG13 | 2.11 | 0.49 |
| 1:D:211:GLY:O | 1:D:325:ILE:O | 2.30 | 0.49 |
| 1:F:130:GLU:O | 1:F:133:ALA:HB3 | 2.11 | 0.49 |
| 1:F:14:VAL:O | 1:F:18:ARG:HG3 | 2.11 | 0.49 |
| 1:F:210:THR:O | 1:F:210:THR:HG22 | 2.12 | 0.49 |
| 1:F:325:ILE:HG22 | 1:F:326:ASN:N | 2.26 | 0.49 |
| 1:E:509:SER:HB3 | 1:F:385:THR:HG23 | 1.94 | 0.49 |
| 1:F:443:ALA:O | 1:F:447:MET:HG3 | 2.12 | 0.49 |
| 1:G:203:TYR:HD1 | 1:G:203:TYR:H | 1.59 | 0.49 |
| 1:G:218:PRO:CA | 1:G:246:PRO:HG2 | 2.42 | 0.49 |
| 1:G:279:PRO:CB | 1:G:288:MET:HE3 | 2.41 | 0.49 |
| 1:G:326:ASN:HD21 | 1:G:328:ASP:HB2 | 1.77 | 0.49 |
| 1:G:352:GLN:O | 1:G:355:GLU:HB2 | 2.12 | 0.49 |
| 1:H:109:ALA:HB3 | 1:H:111:MET:HE3 | 1.93 | 0.49 |
| 1:H:232:GLU:HA | 1:H:310:GLU:HG2 | 1.94 | 0.49 |
| 1:H:93:THR:O | 1:H:96:ALA:HB3 | 2.11 | 0.49 |
| 1:I:370:ALA:O | 1:I:371:LYS:C | 2.50 | 0.49 |
| 1:J:32:GLY:HA3 | 1:J:454:ILE:HG23 | 1.94 | 0.49 |
| 1:K:288:MET:CE | 1:K:288:MET:HA | 2.41 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:186:GLU:HB2 | 1:M:380:LYS:HB2 | 1.94 | 0.49 |
| 1:M:186:GLU:O | 1:M:379:ILE:HA | 2.11 | 0.49 |
| 1:M:299:THR:OG1 | 1:M:316:ASP:HA | 2.12 | 0.49 |
| 1:M:343:GLN:O | 1:M:346:VAL:HB | 2.12 | 0.49 |
| 1:N:15:LYS:HD2 | 1:N:67:GLU:HG3 | 1.94 | 0.49 |
| 2:P:14:ARG:HB2 | 2:P:14:ARG:NH1 | 2.26 | 0.49 |
| 1:A:234:LEU:O | 1:A:238:GLU:N | 2.38 | 0.49 |
| 1:A:409:GLU:CD | 1:A:501:ARG:HH21 | 2.14 | 0.49 |
| 1:B:19:GLY:HA3 | 1:B:67:GLU:O | 2.12 | 0.49 |
| 1:D:207:LYS:HB3 | 1:D:208:PRO:CD | 2.29 | 0.49 |
| 1:D:352:GLN:O | 1:D:355:GLU:HB2 | 2.12 | 0.49 |
| 1:D:406:ALA:O | 1:D:410:GLY:N | 2.44 | 0.49 |
| 1:E:360:TYR:H | 1:E:363:GLU:HG3 | 1.77 | 0.49 |
| 1:F:23:LEU:C | 1:F:23:LEU:HD13 | 2.32 | 0.49 |
| 1:F:381:VAL:CG1 | 1:F:392:LYS:HG2 | 2.42 | 0.49 |
| 1:F:468:THR:OG1 | 1:F:485:TYR:CE2 | 2.65 | 0.49 |
| 1:H:256:GLY:O | 1:H:257:GLU:C | 2.50 | 0.49 |
| 1:H:434:GLU:O | 1:H:438:VAL:HG23 | 2.11 | 0.49 |
| 1:I:266:THR:HG21 | 1:I:273:VAL:O | 2.11 | 0.49 |
| 1:H:36:ARG:HB3 | 1:I:516:THR:O | 2.12 | 0.49 |
| 1:J:200:LEU:HD13 | 1:J:275:ALA:O | 2.12 | 0.49 |
| 1:J:256:GLY:O | 1:J:260:ALA:N | 2.44 | 0.49 |
| 1:J:40:LEU:N | 1:J:40:LEU:CD2 | 2.74 | 0.49 |
| 1:K:381:VAL:HB | 1:K:389:MET:HE3 | 1.93 | 0.49 |
| 1:L:270:ILE:HG23 | 1:M:229:ASN:HD21 | 1.77 | 0.49 |
| 1:M:107:VAL:HG23 | 1:M:108:ALA:H | 1.77 | 0.49 |
| 1:M:95:LEU:O | 1:M:98:ALA:HB3 | 2.12 | 0.49 |
| 2:P:68:ASN:ND2 | 2:Q:74:LYS:HE3 | 2.26 | 0.49 |
| 1:A:352:GLN:O | 1:A:355:GLU:HB2 | 2.11 | 0.49 |
| 1:A:353:ILE:O | 1:A:355:GLU:N | 2.46 | 0.49 |
| 1:A:385:THR:OG1 | 1:A:388:GLU:HB2 | 2.12 | 0.49 |
| 1:B:247:LEU:HB3 | 1:B:273:VAL:HG13 | 1.93 | 0.49 |
| 1:D:305:ILE:CG2 | 1:D:306:GLY:N | 2.61 | 0.49 |
| 1:E:160:LYS:O | 1:E:164:GLU:HG3 | 2.12 | 0.49 |
| 1:E:208:PRO:HB2 | 1:E:212:ALA:CB | 2.42 | 0.49 |
| 1:F:232:GLU:O | 1:F:233:MET:CB | 2.60 | 0.49 |
| 1:G:164:GLU:O | 1:G:167:ASP:HB3 | 2.12 | 0.49 |
| 1:G:285:ARG:HG3 | 1:G:286:LYS:N | 2.27 | 0.49 |
| 1:H:233:MET:HE1 | 1:H:309:LEU:HD13 | 1.94 | 0.49 |
| 1:H:399:ALA:O | 1:H:400:LEU:C | 2.51 | 0.49 |
| 1:I:217:SER:HB3 | 1:I:321:LYS:HA | 1.94 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:129:GLU:O | 1:J:132:LYS:N | 2.46 | 0.49 |
| 1:J:189:VAL:HG23 | 1:J:189:VAL:O | 2.12 | 0.49 |
| 1:J:31:LEU:HG | 1:J:454:ILE:HD11 | 1.94 | 0.49 |
| 1:K:385:THR:HG23 | 1:K:388:GLU:N | 2.27 | 0.49 |
| 1:K:6:VAL:HG22 | 1:K:521:VAL:HG22 | 1.93 | 0.49 |
| 1:L:152:ALA:HB2 | 1:L:158:VAL:HG11 | 1.93 | 0.49 |
| 1:L:225:LYS:HG3 | 1:L:227:ILE:HD13 | 1.94 | 0.49 |
| 1:L:288:MET:HA | 1:L:288:MET:HE3 | 1.94 | 0.49 |
| 1:L:301:ILE:CD1 | 1:L:301:ILE:N | 2.76 | 0.49 |
| 1:L:305:ILE:HG22 | 1:L:307:MET:HG3 | 1.93 | 0.49 |
| 1:L:357:THR:O | 1:L:357:THR:HG22 | 2.11 | 0.49 |
| 1:L:362:ARG:O | 1:L:366:GLN:HB2 | 2.12 | 0.49 |
| 1:L:95:LEU:O | 1:L:98:ALA:HB3 | 2.12 | 0.49 |
| 1:M:197:ARG:HG3 | 1:M:277:LYS:NZ | 2.28 | 0.49 |
| 1:N:422:VAL:O | 1:N:426:LEU:HD23 | 2.13 | 0.49 |
| 1:N:433:ASN:HD22 | 1:N:434:GLU:N | 2.10 | 0.49 |
| 1:N:484:GLU:O | 1:N:491:MET:HE1 | 2.12 | 0.49 |
| 2:P:37:ARG:HG2 | 2:P:37:ARG:NH1 | 2.27 | 0.49 |
| 2:Q:57:LEU:HD22 | 2:Q:88:GLU:HB2 | 1.95 | 0.49 |
| 2:T:83:VAL:C | 2:T:84:LEU:HD12 | 2.32 | 0.49 |
| 1:A:177:VAL:HG22 | 1:A:393:LYS:HG3 | 1.93 | 0.49 |
| 1:A:233:MET:HE3 | 1:A:236:VAL:HB | 1.95 | 0.49 |
| 1:A:293:ALA:O | 1:A:294:THR:C | 2.51 | 0.49 |
| 1:A:434:GLU:OE2 | 1:A:438:VAL:HG23 | 2.11 | 0.49 |
| 1:A:456:LEU:HD13 | 1:A:462:PRO:HG3 | 1.93 | 0.49 |
| 1:B:177:VAL:CG1 | 1:B:397:GLU:HG2 | 2.43 | 0.49 |
| 1:C:266:THR:HG22 | 1:C:273:VAL:N | 2.27 | 0.49 |
| 1:D:277:LYS:HG2 | 1:D:278:ALA:N | 2.27 | 0.49 |
| 1:E:237:LEU:HD22 | 2:S:26:VAL:CG2 | 2.42 | 0.49 |
| 1:E:219:PHE:CE2 | 1:E:245:LYS:HB2 | 2.48 | 0.49 |
| 1:E:247:LEU:HB3 | 1:E:273:VAL:CG1 | 2.42 | 0.49 |
| 1:E:28:LYS:O | 1:E:30:THR:N | 2.45 | 0.49 |
| 1:E:309:LEU:H | 1:E:309:LEU:CD1 | 2.25 | 0.49 |
| 1:E:309:LEU:N | 1:E:309:LEU:HD12 | 2.25 | 0.49 |
| 1:F:112:ASN:HD22 | 1:F:115:ASP:CG | 2.15 | 0.49 |
| 1:F:265:ASN:HB3 | 1:F:271:VAL:HG22 | 1.92 | 0.49 |
| 1:G:272:LYS:CB | 1:G:272:LYS:NZ | 2.75 | 0.49 |
| 1:G:357:THR:HB | 1:G:361:ASP:HB2 | 1.94 | 0.49 |
| 1:G:496:PRO:HG2 | 1:G:499:VAL:CG1 | 2.43 | 0.49 |
| 1:G:56:VAL:O | 1:G:57:ALA:C | 2.50 | 0.49 |
| 1:G:27:VAL:HG12 | 1:G:90:THR:HG23 | 1.93 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:233:MET:HB3 | 1:H:237:LEU:HB2 | 1.94 | 0.49 |
| 1:H:349:ILE:HA | 1:H:352:GLN:NE2 | 2.27 | 0.49 |
| 1:H:455:VAL:HG13 | 1:H:460:GLU:HB2 | 1.94 | 0.49 |
| 1:I:370:ALA:O | 1:I:374:GLY:N | 2.36 | 0.49 |
| 1:J:381:VAL:HB | 1:J:389:MET:HE3 | 1.94 | 0.49 |
| 1:K:203:TYR:HB2 | 1:K:263:VAL:HG13 | 1.95 | 0.49 |
| 1:K:19:GLY:HA3 | 1:K:67:GLU:O | 2.12 | 0.49 |
| 1:M:174:VAL:C | 1:M:175:ILE:HD12 | 2.32 | 0.49 |
| 1:N:112:ASN:O | 1:N:116:LEU:HG | 2.11 | 0.49 |
| 1:N:367:GLU:O | 1:N:370:ALA:HB3 | 2.12 | 0.49 |
| 2:U:17:VAL:HG13 | 2:U:34:LYS:CA | 2.41 | 0.49 |
| 1:A:115:ASP:HB3 | 1:A:436:GLN:HG3 | 1.93 | 0.49 |
| 1:B:234:LEU:N | 1:B:235:PRO:CD | 2.73 | 0.49 |
| 1:B:249:ILE:N | 1:B:249:ILE:CD1 | 2.76 | 0.49 |
| 1:C:153:ASN:O | 1:C:154:SER:HB2 | 2.13 | 0.49 |
| 1:D:353:ILE:O | 1:D:355:GLU:N | 2.45 | 0.49 |
| 1:E:247:LEU:HD13 | 1:E:248:LEU:O | 2.12 | 0.49 |
| 1:E:413:ALA:HB1 | 1:E:417:VAL:CG1 | 2.42 | 0.49 |
| 1:F:207:LYS:HB2 | 1:F:207:LYS:HZ2 | 1.77 | 0.49 |
| 1:F:320:ALA:HA | 1:F:334:ASP:O | 2.13 | 0.49 |
| 1:H:232:GLU:OE1 | 1:H:232:GLU:N | 2.33 | 0.49 |
| 1:H:314:LEU:C | 1:H:316:ASP:H | 2.16 | 0.49 |
| 1:H:381:VAL:HB | 1:H:389:MET:CE | 2.41 | 0.49 |
| 1:I:131:LEU:HD12 | 1:I:422:VAL:HG11 | 1.95 | 0.49 |
| 1:I:149:THR:HG21 | 1:I:156:GLU:HA | 1.93 | 0.49 |
| 1:I:413:ALA:CB | 1:I:417:VAL:HB | 2.42 | 0.49 |
| 1:I:506:TYR:O | 1:I:509:SER:HB3 | 2.13 | 0.49 |
| 1:J:290:GLN:OE1 | 1:J:293:ALA:HB3 | 2.12 | 0.49 |
| 1:K:434:GLU:O | 1:K:438:VAL:HG23 | 2.12 | 0.49 |
| 1:K:441:LYS:O | 1:K:442:VAL:C | 2.49 | 0.49 |
| 1:L:106:ALA:HA | 1:L:111:MET:HE1 | 1.94 | 0.49 |
| 1:L:411:VAL:HA | 1:L:497:THR:H | 1.76 | 0.49 |
| 1:M:420:ILE:HG13 | 1:M:451:LEU:HD22 | 1.94 | 0.49 |
| 1:N:190:VAL:HG21 | 1:N:334:ASP:CG | 2.33 | 0.49 |
| 2:O:17:VAL:HG22 | 2:O:35:SER:N | 2.27 | 0.49 |
| 2:Q:5:PRO:HD3 | 2:Q:42:ALA:CB | 2.39 | 0.49 |
| 1:A:278:ALA:HB1 | 1:A:279:PRO:HD2 | 1.93 | 0.49 |
| 1:A:418:ALA:O | 1:A:422:VAL:HG13 | 2.11 | 0.49 |
| 1:B:429:LEU:HG | 1:B:440:ILE:HD13 | 1.95 | 0.49 |
| 1:C:200:LEU:CD1 | 1:C:276:VAL:HA | 2.42 | 0.49 |
| 1:C:252:GLU:HG3 | 1:C:285:ARG:HH11 | 1.78 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:87:ASP:OD1 | 1:C:88:GLY:N | 2.46 | 0.49 |
| 1:E:232:GLU:O | 1:E:233:MET:CB | 2.60 | 0.49 |
| 1:E:241:ALA:HA | 1:E:271:VAL:HG12 | 1.93 | 0.49 |
| 1:E:409:GLU:OE1 | 1:E:501:ARG:NH2 | 2.46 | 0.49 |
| 1:F:228:SER:O | 1:F:257:GLU:HB3 | 2.12 | 0.49 |
| 1:F:434:GLU:O | 1:F:435:ASP:C | 2.49 | 0.49 |
| 1:G:319:GLN:O | 1:G:335:GLY:HA2 | 2.12 | 0.49 |
| 1:G:383:ALA:HB3 | 1:G:389:MET:CE | 2.43 | 0.49 |
| 1:H:221:LEU:HD13 | 1:H:223:ALA:N | 2.28 | 0.49 |
| 1:I:301:ILE:HG21 | 1:I:309:LEU:HD23 | 1.93 | 0.49 |
| 1:I:449:ALA:CB | 1:I:450:PRO:HD3 | 2.31 | 0.49 |
| 1:J:354:GLU:CG | 1:J:355:GLU:N | 2.76 | 0.49 |
| 1:J:409:GLU:O | 1:J:497:THR:HB | 2.12 | 0.49 |
| 1:J:510:VAL:HG13 | 1:J:511:ALA:N | 2.28 | 0.49 |
| 1:M:146:GLN:HE21 | 1:M:150:ILE:HD11 | 1.77 | 0.49 |
| 1:M:223:ALA:HB3 | 1:M:251:ALA:HB2 | 1.94 | 0.49 |
| 1:M:441:LYS:O | 1:M:442:VAL:C | 2.50 | 0.49 |
| 1:N:37:ASN:HB3 | 1:N:51:LYS:CG | 2.43 | 0.49 |
| 2:Q:43:VAL:HG12 | 2:Q:57:LEU:HD12 | 1.94 | 0.49 |
| 2:R:50:GLU:O | 2:R:52:GLY:N | 2.46 | 0.49 |
| 2:T:12:VAL:HG12 | 2:T:40:VAL:HA | 1.93 | 0.49 |
| 1:A:242:LYS:HD3 | 1:A:243:ALA:N | 2.28 | 0.49 |
| 1:A:501:ARG:O | 1:A:505:GLN:HG3 | 2.12 | 0.49 |
| 1:B:256:GLY:HA2 | 1:B:259:LEU:HB2 | 1.94 | 0.49 |
| 1:D:233:MET:HE2 | 1:D:233:MET:O | 2.13 | 0.49 |
| 1:D:434:GLU:OE2 | 1:D:438:VAL:HG23 | 2.12 | 0.49 |
| 1:E:357:THR:HB | 1:E:361:ASP:HB2 | 1.94 | 0.49 |
| 1:E:358:SER:HA | 1:E:362:ARG:HD2 | 1.94 | 0.49 |
| 1:F:147:VAL:HA | 1:F:150:ILE:HG22 | 1.95 | 0.49 |
| 1:G:281:PHE:H | 1:G:284:ARG:HD2 | 1.78 | 0.49 |
| 1:G:358:SER:HA | 1:G:362:ARG:HD2 | 1.94 | 0.49 |
| 1:G:404:ARG:HG3 | 1:G:404:ARG:NH1 | 2.26 | 0.49 |
| 1:H:130:GLU:HG3 | 1:H:426:LEU:HD22 | 1.95 | 0.49 |
| 1:H:149:THR:CG2 | 1:H:159:GLY:HA3 | 2.37 | 0.49 |
| 1:H:221:LEU:O | 1:H:222:LEU:HD23 | 2.12 | 0.49 |
| 1:H:233:MET:HA | 1:H:233:MET:CE | 2.40 | 0.49 |
| 1:H:247:LEU:N | 1:H:273:VAL:HG12 | 2.28 | 0.49 |
| 1:H:472:GLY:HA3 | 1:H:476:TYR:CD2 | 2.47 | 0.49 |
| 1:H:472:GLY:HA3 | 1:H:476:TYR:HD2 | 1.77 | 0.49 |
| 1:I:72:GLN:NE2 | 1:I:75:LYS:HD3 | 2.28 | 0.49 |
| 1:J:93:THR:O | 1:J:96:ALA:HB3 | 2.13 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:191:GLU:O | 1:M:334:ASP:HA | 2.13 | 0.49 |
| 1:M:422:VAL:HG23 | 1:M:423:ALA:N | 2.26 | 0.49 |
| 1:N:494:LEU:CD2 | 1:N:494:LEU:N | 2.73 | 0.49 |
| 2:Q:48:ILE:HG22 | 2:Q:48:ILE:O | 2.12 | 0.49 |
| 1:A:240:VAL:C | 1:A:242:LYS:N | 2.64 | 0.49 |
| 1:A:329:THR:CG2 | 1:A:330:THR:N | 2.76 | 0.49 |
| 1:A:346:VAL:HA | 1:A:349:ILE:HD12 | 1.94 | 0.49 |
| 1:A:400:LEU:HD13 | 1:A:400:LEU:O | 2.12 | 0.49 |
| 1:B:272:LYS:NZ | 1:B:272:LYS:HB2 | 2.28 | 0.49 |
| 1:B:496:PRO:O | 1:B:499:VAL:HG22 | 2.13 | 0.49 |
| 1:B:54:VAL:HB | 1:B:89:THR:HG21 | 1.93 | 0.49 |
| 1:C:345:ARG:O | 1:C:349:ILE:HG13 | 2.11 | 0.49 |
| 1:C:397:GLU:O | 1:C:400:LEU:HB3 | 2.13 | 0.49 |
| 1:D:199:TYR:OH | 1:D:211:GLY:HA3 | 2.13 | 0.49 |
| 1:D:23:LEU:HD22 | 1:D:60:ILE:HG13 | 1.95 | 0.49 |
| 1:D:249:ILE:C | 1:D:250:ILE:HG13 | 2.32 | 0.49 |
| 1:D:270:ILE:CD1 | 2:R:27:LEU:HB2 | 2.42 | 0.49 |
| 1:D:288:MET:HA | 1:D:291:ASP:OD2 | 2.12 | 0.49 |
| 1:D:309:LEU:HD12 | 1:D:309:LEU:N | 2.27 | 0.49 |
| 1:E:355:GLU:HG3 | 1:E:357:THR:H | 1.78 | 0.49 |
| 1:E:417:VAL:O | 1:E:420:ILE:CG2 | 2.57 | 0.49 |
| 1:E:511:ALA:O | 1:E:515:ILE:HG23 | 2.12 | 0.49 |
| 1:F:256:GLY:HA2 | 1:F:259:LEU:HB2 | 1.94 | 0.49 |
| 1:F:287:ALA:O | 1:F:290:GLN:NE2 | 2.39 | 0.49 |
| 1:F:31:LEU:HD12 | 4:F:1:ADP:O1A | 2.12 | 0.49 |
| 1:G:234:LEU:N | 1:G:235:PRO:CD | 2.76 | 0.49 |
| 1:G:417:VAL:HA | 1:G:420:ILE:CG2 | 2.41 | 0.49 |
| 1:H:285:ARG:HA | 1:H:288:MET:HB2 | 1.95 | 0.49 |
| 1:I:152:ALA:O | 1:I:153:ASN:HB3 | 2.13 | 0.49 |
| 1:I:164:GLU:O | 1:I:167:ASP:HB3 | 2.13 | 0.49 |
| 1:J:448:GLU:HB3 | 1:J:452:ARG:HD2 | 1.95 | 0.49 |
| 1:J:487:ASN:HB3 | 1:J:490:ASP:HB2 | 1.95 | 0.49 |
| 1:K:247:LEU:C | 1:K:247:LEU:HD13 | 2.32 | 0.49 |
| 1:K:357:THR:HG22 | 1:K:357:THR:O | 2.13 | 0.49 |
| 1:L:219:PHE:HE1 | 1:L:245:LYS:HB2 | 1.76 | 0.49 |
| 1:M:96:ALA:O | 1:M:100:ILE:HG13 | 2.13 | 0.49 |
| 1:M:346:VAL:O | 1:M:350:ARG:HG2 | 2.13 | 0.49 |
| 1:A:127:ALA:O | 1:A:130:GLU:HB2 | 2.12 | 0.49 |
| 1:A:284:ARG:HG2 | 1:A:288:MET:HE1 | 1.94 | 0.49 |
| 1:A:433:ASN:HD21 | 1:A:435:ASP:HB2 | 1.78 | 0.49 |
| 1:A:96:ALA:O | 1:A:97:GLN:C | 2.49 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:106:ALA:O | 1:B:109:ALA:HB3 | 2.13 | 0.49 |
| 1:C:199:TYR:CA | 1:C:276:VAL:HG12 | 2.39 | 0.49 |
| 1:C:285:ARG:O | 1:C:288:MET:N | 2.43 | 0.49 |
| 1:D:265:ASN:HB3 | 1:D:271:VAL:HG22 | 1.95 | 0.49 |
| 1:D:44:PHE:HB2 | 1:D:45:GLY:H | 1.49 | 0.49 |
| 1:E:443:ALA:O | 1:E:447:MET:HG3 | 2.12 | 0.49 |
| 1:F:220:ILE:HG23 | 1:F:248:LEU:HD12 | 1.93 | 0.49 |
| 1:F:357:THR:HB | 1:F:361:ASP:HB2 | 1.94 | 0.49 |
| 1:G:205:ILE:CG1 | 1:G:211:GLY:HA2 | 2.43 | 0.49 |
| 1:G:381:VAL:CG1 | 1:G:392:LYS:HG2 | 2.43 | 0.49 |
| 1:H:179:ASP:OD2 | 1:H:390:LYS:HG2 | 2.13 | 0.49 |
| 1:I:419:LEU:HD21 | 1:I:500:THR:HG23 | 1.95 | 0.49 |
| 1:J:145:ALA:O | 1:J:149:THR:HG23 | 2.12 | 0.49 |
| 1:J:354:GLU:HG2 | 1:J:355:GLU:H | 1.77 | 0.49 |
| 1:K:287:ALA:O | 1:K:288:MET:C | 2.51 | 0.49 |
| 1:L:184:GLN:OE1 | 1:L:184:GLN:HA | 2.12 | 0.49 |
| 1:L:415:GLY:H | 1:L:417:VAL:CG2 | 2.23 | 0.49 |
| 1:N:226:LYS:HA | 1:N:252:GLU:HB2 | 1.93 | 0.49 |
| 2:R:14:ARG:CG | 2:R:15:LYS:N | 2.76 | 0.49 |
| 2:R:5:PRO:HB2 | 2:R:9:ARG:O | 2.12 | 0.49 |
| 2:U:11:ILE:HB | 2:U:42:ALA:HB3 | 1.95 | 0.49 |
| 1:A:206:ASN:HB3 | 1:A:214:GLU:N | 2.26 | 0.49 |
| 1:A:448:GLU:O | 1:A:452:ARG:HG2 | 2.13 | 0.49 |
| 1:B:353:ILE:HG12 | 1:B:366:GLN:HE22 | 1.78 | 0.49 |
| 1:C:107:VAL:HG13 | 1:C:113:PRO:HG3 | 1.94 | 0.49 |
| 1:C:134:LEU:N | 1:C:134:LEU:HD12 | 2.28 | 0.49 |
| 1:C:496:PRO:HG2 | 1:C:499:VAL:HG13 | 1.93 | 0.49 |
| 1:D:146:GLN:NE2 | 1:D:494:LEU:HD11 | 2.28 | 0.49 |
| 1:E:249:ILE:HD13 | 1:E:274:ALA:O | 2.13 | 0.49 |
| 1:E:383:ALA:HB3 | 1:E:389:MET:HE2 | 1.94 | 0.49 |
| 1:F:195:PHE:CE1 | 1:F:330:THR:HB | 2.48 | 0.49 |
| 1:F:305:ILE:N | 1:F:305:ILE:CD1 | 2.74 | 0.49 |
| 1:G:199:TYR:CE1 | 1:G:327:LYS:HG3 | 2.48 | 0.49 |
| 1:G:77:VAL:HG22 | 1:G:78:ALA:N | 2.28 | 0.49 |
| 1:H:353:ILE:O | 1:H:353:ILE:HG22 | 2.13 | 0.49 |
| 1:H:426:LEU:H | 1:H:426:LEU:CD2 | 2.22 | 0.49 |
| 1:H:433:ASN:HD22 | 1:H:434:GLU:N | 2.11 | 0.49 |
| 1:H:64:ASP:OD1 | 1:H:65:LYS:O | 2.30 | 0.49 |
| 1:I:448:GLU:HB3 | 1:I:452:ARG:HD2 | 1.95 | 0.49 |
| 1:J:157:THR:O | 1:J:161:LEU:HD13 | 2.12 | 0.49 |
| 1:J:175:ILE:CD1 | 1:J:175:ILE:N | 2.73 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:186:GLU:HB2 | 1:J:380:LYS:HB2 | 1.95 | 0.49 |
| 1:K:311:LYS:HD2 | 1:K:311:LYS:N | 2.28 | 0.49 |
| 1:L:199:TYR:CZ | 1:L:327:LYS:HA | 2.48 | 0.49 |
| 1:M:215:LEU:HB3 | 1:M:218:PRO:CG | 2.42 | 0.49 |
| 1:M:214:GLU:HG2 | 1:M:324:VAL:HG12 | 1.94 | 0.49 |
| 1:M:350:ARG:HE | 1:M:369:VAL:CG1 | 2.26 | 0.49 |
| 1:N:259:LEU:O | 1:N:263:VAL:HG23 | 2.13 | 0.49 |
| 1:N:392:LYS:O | 1:N:396:VAL:HG23 | 2.11 | 0.49 |
| 2:O:59:VAL:HG23 | 2:O:59:VAL:O | 2.13 | 0.49 |
| 1:B:468:THR:OG1 | 1:B:485:TYR:CE2 | 2.64 | 0.48 |
| 1:C:77:VAL:HG12 | 1:C:510:VAL:HG21 | 1.93 | 0.48 |
| 1:E:261:THR:O | 1:E:265:ASN:ND2 | 2.46 | 0.48 |
| 1:E:199:TYR:HE1 | 1:E:327:LYS:HG3 | 1.78 | 0.48 |
| 1:F:245:LYS:CE | 1:F:245:LYS:HA | 2.34 | 0.48 |
| 1:F:200:LEU:CD1 | 1:F:276:VAL:HA | 2.43 | 0.48 |
| 1:G:220:ILE:CD1 | 1:G:220:ILE:N | 2.76 | 0.48 |
| 1:G:279:PRO:HB2 | 1:G:285:ARG:CA | 2.42 | 0.48 |
| 1:G:327:LYS:H | 1:G:327:LYS:HD3 | 1.78 | 0.48 |
| 1:H:449:ALA:HB3 | 1:H:450:PRO:CD | 2.34 | 0.48 |
| 1:H:90:THR:O | 1:H:93:THR:HB | 2.12 | 0.48 |
| 1:I:228:SER:O | 1:I:258:ALA:N | 2.46 | 0.48 |
| 1:J:132:LYS:O | 1:J:135:SER:HB3 | 2.13 | 0.48 |
| 1:J:267:MET:O | 1:J:267:MET:HG3 | 2.12 | 0.48 |
| 1:J:353:ILE:O | 1:J:353:ILE:HG22 | 2.13 | 0.48 |
| 1:K:314:LEU:C | 1:K:316:ASP:H | 2.16 | 0.48 |
| 1:L:119:GLY:O | 1:L:440:ILE:HG12 | 2.13 | 0.48 |
| 1:L:411:VAL:HG21 | 1:L:494:LEU:HD12 | 1.95 | 0.48 |
| 1:L:413:ALA:HB3 | 1:L:417:VAL:HB | 1.95 | 0.48 |
| 1:L:422:VAL:O | 1:L:426:LEU:HD23 | 2.12 | 0.48 |
| 1:N:232:GLU:HA | 1:N:310:GLU:HG2 | 1.94 | 0.48 |
| 1:A:194:GLN:O | 1:A:371:LYS:NZ | 2.40 | 0.48 |
| 1:A:391:GLU:O | 1:A:394:ALA:HB3 | 2.12 | 0.48 |
| 1:A:486:GLY:HA3 | 1:A:491:MET:HE2 | 1.95 | 0.48 |
| 1:B:183:LEU:O | 1:B:382:GLY:HA3 | 2.12 | 0.48 |
| 1:B:301:ILE:HG12 | 1:B:307:MET:CE | 2.43 | 0.48 |
| 1:B:362:ARG:O | 1:B:366:GLN:OE1 | 2.30 | 0.48 |
| 1:B:413:ALA:HB1 | 1:B:417:VAL:CG1 | 2.42 | 0.48 |
| 1:C:180:GLY:CA | 1:C:380:LYS:HB3 | 2.43 | 0.48 |
| 1:C:247:LEU:HB3 | 1:C:273:VAL:HG13 | 1.94 | 0.48 |
| 1:D:219:PHE:HB3 | 1:D:317:LEU:CD1 | 2.42 | 0.48 |
| 1:D:215:LEU:O | 1:D:322:ARG:HA | 2.13 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:390:LYS:O | 1:D:391:GLU:C | 2.52 | 0.48 |
| 1:D:96:ALA:O | 1:D:97:GLN:C | 2.52 | 0.48 |
| 1:D:9:GLY:HA2 | 1:D:13:ARG:NH1 | 2.27 | 0.48 |
| 1:E:168:LYS:O | 1:E:170:GLY:N | 2.45 | 0.48 |
| 1:F:252:GLU:N | 1:F:252:GLU:OE1 | 2.47 | 0.48 |
| 1:G:174:VAL:HG23 | 1:G:370:ALA:HB2 | 1.95 | 0.48 |
| 1:G:194:GLN:NE2 | 1:G:329:THR:HG21 | 2.27 | 0.48 |
| 1:H:207:LYS:HG3 | 1:H:214:GLU:OE2 | 2.13 | 0.48 |
| 1:I:266:THR:HG21 | 1:I:273:VAL:H | 1.77 | 0.48 |
| 1:J:238:GLU:O | 1:J:241:ALA:HB3 | 2.13 | 0.48 |
| 1:J:319:GLN:O | 1:J:336:VAL:HG23 | 2.13 | 0.48 |
| 1:K:344:GLY:O | 1:K:347:ALA:HB3 | 2.13 | 0.48 |
| 1:L:289:LEU:O | 1:L:292:ILE:HB | 2.13 | 0.48 |
| 1:L:386:GLU:O | 1:L:389:MET:HB3 | 2.13 | 0.48 |
| 1:L:77:VAL:HG11 | 1:L:510:VAL:HB | 1.94 | 0.48 |
| 1:M:494:LEU:N | 1:M:494:LEU:CD2 | 2.76 | 0.48 |
| 1:N:496:PRO:O | 1:N:497:THR:C | 2.51 | 0.48 |
| 2:P:20:LYS:CG | 2:P:27:LEU:HD23 | 2.44 | 0.48 |
| 2:T:57:LEU:HD22 | 2:T:88:GLU:HB2 | 1.95 | 0.48 |
| 1:A:308:GLU:O | 1:A:309:LEU:O | 2.31 | 0.48 |
| 1:A:466:ALA:O | 1:A:470:LYS:HG3 | 2.13 | 0.48 |
| 1:B:200:LEU:O | 1:B:202:PRO:HD2 | 2.13 | 0.48 |
| 1:B:233:MET:C | 1:B:235:PRO:CD | 2.76 | 0.48 |
| 1:B:305:ILE:N | 1:B:305:ILE:CD1 | 2.76 | 0.48 |
| 1:B:434:GLU:O | 1:B:435:ASP:C | 2.50 | 0.48 |
| 1:C:115:ASP:HB3 | 1:C:436:GLN:HG3 | 1.95 | 0.48 |
| 1:C:417:VAL:HG13 | 1:C:418:ALA:N | 2.28 | 0.48 |
| 1:D:131:LEU:HD21 | 1:D:422:VAL:HG11 | 1.92 | 0.48 |
| 1:D:455:VAL:O | 1:D:458:CYS:HB2 | 2.13 | 0.48 |
| 1:E:420:ILE:HD11 | 1:E:470:LYS:CG | 2.44 | 0.48 |
| 1:F:217:SER:N | 1:F:218:PRO:CD | 2.76 | 0.48 |
| 1:H:102:GLU:HB2 | 1:H:442:VAL:HG13 | 1.94 | 0.48 |
| 1:H:501:ARG:O | 1:H:502:SER:C | 2.52 | 0.48 |
| 1:H:72:GLN:NE2 | 1:H:72:GLN:HA | 2.29 | 0.48 |
| 1:I:129:GLU:O | 1:I:132:LYS:N | 2.46 | 0.48 |
| 1:I:230:ILE:CD1 | 1:I:257:GLU:HG2 | 2.44 | 0.48 |
| 1:J:290:GLN:O | 1:J:293:ALA:HB3 | 2.13 | 0.48 |
| 1:J:217:SER:HB3 | 1:J:321:LYS:HA | 1.95 | 0.48 |
| 1:J:353:ILE:HD11 | 1:J:369:VAL:HG21 | 1.95 | 0.48 |
| 1:K:432:GLN:N | 1:K:432:GLN:OE1 | 2.47 | 0.48 |
| 1:M:413:ALA:HB1 | 1:M:417:VAL:HB | 1.93 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:81:ALA:HA | 1:M:506:TYR:CD2 | 2.48 | 0.48 |
| 1:N:294:THR:HG21 | 1:N:345:ARG:HB2 | 1.94 | 0.48 |
| 2:Q:48:ILE:HG12 | 2:Q:54:VAL:CG1 | 2.38 | 0.48 |
| 2:Q:7:HIS:O | 2:Q:7:HIS:ND1 | 2.46 | 0.48 |
| 1:A:360:TYR:N | 1:A:363:GLU:HG3 | 2.28 | 0.48 |
| 1:A:37:ASN:OD1 | 1:A:51:LYS:HB2 | 2.13 | 0.48 |
| 1:B:208:PRO:HB2 | 1:B:212:ALA:HB3 | 1.94 | 0.48 |
| 1:C:272:LYS:CB | 1:C:272:LYS:NZ | 2.76 | 0.48 |
| 1:C:27:VAL:HG12 | 1:C:90:THR:HG23 | 1.94 | 0.48 |
| 1:E:78:ALA:O | 1:E:89:THR:HG22 | 2.12 | 0.48 |
| 1:G:333:ILE:O | 1:G:334:ASP:HB2 | 2.14 | 0.48 |
| 1:H:225:LYS:HG3 | 1:H:227:ILE:HD13 | 1.94 | 0.48 |
| 1:H:455:VAL:HG11 | 1:H:461:GLU:O | 2.13 | 0.48 |
| 1:I:352:GLN:O | 1:I:355:GLU:OE1 | 2.31 | 0.48 |
| 1:J:229:ASN:ND2 | 1:J:231:ARG:NH1 | 2.55 | 0.48 |
| 1:J:90:THR:O | 1:J:93:THR:HB | 2.14 | 0.48 |
| 1:K:422:VAL:O | 1:K:426:LEU:CD2 | 2.61 | 0.48 |
| 1:L:285:ARG:O | 1:L:288:MET:HB2 | 2.14 | 0.48 |
| 1:M:266:THR:HB | 1:M:272:LYS:HG3 | 1.95 | 0.48 |
| 1:M:302:SER:HB2 | 1:M:305:ILE:HD12 | 1.96 | 0.48 |
| 1:M:366:GLN:O | 1:M:369:VAL:HB | 2.13 | 0.48 |
| 1:N:221:LEU:HD11 | 1:N:223:ALA:HB2 | 1.96 | 0.48 |
| 1:N:441:LYS:O | 1:N:442:VAL:C | 2.51 | 0.48 |
| 2:R:6:LEU:H | 2:R:9:ARG:HB2 | 1.78 | 0.48 |
| 1:B:200:LEU:CD1 | 1:B:276:VAL:HA | 2.44 | 0.48 |
| 1:B:295:LEU:C | 1:B:295:LEU:HD23 | 2.34 | 0.48 |
| 1:B:448:GLU:O | 1:B:452:ARG:HG2 | 2.13 | 0.48 |
| 1:C:305:ILE:CG2 | 1:C:306:GLY:H | 2.07 | 0.48 |
| 1:C:409:GLU:OE1 | 1:C:501:ARG:NH2 | 2.47 | 0.48 |
| 1:C:417:VAL:O | 1:C:421:ARG:HB2 | 2.13 | 0.48 |
| 1:D:291:ASP:HB3 | 1:D:345:ARG:NH2 | 2.25 | 0.48 |
| 1:E:271:VAL:O | 1:E:271:VAL:HG23 | 2.13 | 0.48 |
| 1:E:283:ASP:O | 1:E:287:ALA:HB2 | 2.14 | 0.48 |
| 1:E:465:VAL:O | 1:E:466:ALA:C | 2.52 | 0.48 |
| 1:F:381:VAL:HG13 | 1:F:392:LYS:CG | 2.43 | 0.48 |
| 1:F:504:LEU:HD13 | 1:F:504:LEU:C | 2.33 | 0.48 |
| 1:G:252:GLU:HA | 1:G:285:ARG:NH1 | 2.28 | 0.48 |
| 1:G:465:VAL:O | 1:G:466:ALA:C | 2.52 | 0.48 |
| 1:G:510:VAL:O | 1:G:511:ALA:C | 2.51 | 0.48 |
| 1:H:7:LYS:HG3 | 1:H:66:PHE:CZ | 2.49 | 0.48 |
| 1:J:97:GLN:O | 1:J:98:ALA:C | 2.52 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:221:LEU:HD11 | 1:K:223:ALA:HB2 | 1.96 | 0.48 |
| 1:K:302:SER:HB2 | 1:K:305:ILE:CG1 | 2.43 | 0.48 |
| 1:K:472:GLY:HA3 | 1:K:476:TYR:HD2 | 1.78 | 0.48 |
| 1:L:256:GLY:O | 1:L:257:GLU:C | 2.52 | 0.48 |
| 1:L:267:MET:O | 1:L:267:MET:HG3 | 2.14 | 0.48 |
| 1:L:66:PHE:N | 1:L:69:MET:HG3 | 2.27 | 0.48 |
| 1:L:80:LYS:O | 1:L:83:ASP:HB2 | 2.13 | 0.48 |
| 1:M:179:ASP:OD2 | 1:M:390:LYS:HG2 | 2.14 | 0.48 |
| 1:M:404:ARG:O | 1:M:408:GLU:HG3 | 2.13 | 0.48 |
| 1:M:421:ARG:HD2 | 1:M:474:GLY:O | 2.12 | 0.48 |
| 2:P:14:ARG:NH2 | 2:P:84:LEU:HD21 | 2.28 | 0.48 |
| 2:S:83:VAL:C | 2:S:84:LEU:HD12 | 2.33 | 0.48 |
| 2:T:94:ILE:N | 2:U:4:ARG:O | 2.45 | 0.48 |
| 1:A:326:ASN:OD1 | 1:A:329:THR:N | 2.43 | 0.48 |
| 1:A:413:ALA:HB1 | 1:A:417:VAL:HG11 | 1.96 | 0.48 |
| 1:B:285:ARG:HG3 | 1:B:286:LYS:HG3 | 1.96 | 0.48 |
| 1:B:365:LEU:O | 1:B:369:VAL:HG23 | 2.13 | 0.48 |
| 1:C:124:VAL:HG22 | 1:C:504:LEU:HD11 | 1.95 | 0.48 |
| 1:C:174:VAL:HG12 | 1:C:175:ILE:N | 2.29 | 0.48 |
| 1:C:234:LEU:N | 1:C:235:PRO:CD | 2.75 | 0.48 |
| 1:D:208:PRO:HB2 | 1:D:212:ALA:HB3 | 1.96 | 0.48 |
| 1:D:23:LEU:C | 1:D:23:LEU:HD13 | 2.34 | 0.48 |
| 1:D:302:SER:C | 1:D:304:GLU:N | 2.66 | 0.48 |
| 1:D:360:TYR:HA | 1:D:363:GLU:CD | 2.33 | 0.48 |
| 1:E:208:PRO:C | 1:E:212:ALA:HB3 | 2.34 | 0.48 |
| 1:E:290:GLN:N | 1:E:290:GLN:OE1 | 2.42 | 0.48 |
| 1:E:295:LEU:HD23 | 1:E:335:GLY:O | 2.13 | 0.48 |
| 1:E:383:ALA:HB3 | 1:E:389:MET:CE | 2.43 | 0.48 |
| 1:F:249:ILE:CD1 | 1:F:249:ILE:N | 2.77 | 0.48 |
| 1:G:232:GLU:O | 1:G:233:MET:CB | 2.61 | 0.48 |
| 1:G:279:PRO:HD2 | 1:G:285:ARG:HB2 | 1.95 | 0.48 |
| 1:G:320:ALA:HA | 1:G:334:ASP:O | 2.13 | 0.48 |
| 1:G:325:ILE:HG13 | 1:G:330:THR:HA | 1.95 | 0.48 |
| 1:G:400:LEU:O | 1:G:400:LEU:HD13 | 2.14 | 0.48 |
| 1:G:512:GLY:O | 1:G:515:ILE:HG12 | 2.13 | 0.48 |
| 1:H:101:THR:O | 1:H:105:LYS:HG3 | 2.12 | 0.48 |
| 1:H:122:LYS:O | 1:H:125:THR:HB | 2.13 | 0.48 |
| 1:I:426:LEU:H | 1:I:426:LEU:CD2 | 2.14 | 0.48 |
| 1:J:417:VAL:O | 1:J:418:ALA:C | 2.51 | 0.48 |
| 1:L:93:THR:O | 1:L:96:ALA:HB3 | 2.13 | 0.48 |
| 1:M:266:THR:O | 1:M:268:ARG:N | 2.46 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:102:GLU:HB2 | 1:M:442:VAL:HG13 | 1.94 | 0.48 |
| 1:L:37:ASN:O | 1:M:517:THR:HA | 2.14 | 0.48 |
| 1:N:190:VAL:HG22 | 1:N:191:GLU:N | 2.28 | 0.48 |
| 2:P:48:ILE:HG23 | 2:P:54:VAL:HG22 | 1.94 | 0.48 |
| 2:R:44:GLY:O | 2:R:45:ASN:C | 2.51 | 0.48 |
| 2:R:84:LEU:N | 2:R:84:LEU:CD1 | 2.77 | 0.48 |
| 2:S:14:ARG:CB | 2:S:14:ARG:HH11 | 2.26 | 0.48 |
| 2:U:83:VAL:C | 2:U:84:LEU:HD12 | 2.33 | 0.48 |
| 1:A:147:VAL:HG23 | 1:A:148:GLY:N | 2.29 | 0.48 |
| 1:A:153:ASN:O | 1:A:154:SER:HB2 | 2.14 | 0.48 |
| 1:B:160:LYS:O | 1:B:164:GLU:HG3 | 2.13 | 0.48 |
| 1:B:248:LEU:HD13 | 1:B:248:LEU:C | 2.33 | 0.48 |
| 1:B:304:GLU:C | 1:B:305:ILE:HD12 | 2.33 | 0.48 |
| 1:C:208:PRO:O | 1:C:212:ALA:HB3 | 2.13 | 0.48 |
| 1:D:194:GLN:O | 1:D:371:LYS:NZ | 2.44 | 0.48 |
| 1:D:302:SER:O | 1:D:305:ILE:N | 2.45 | 0.48 |
| 1:E:381:VAL:HG13 | 1:E:392:LYS:HG3 | 1.95 | 0.48 |
| 1:F:235:PRO:HG2 | 1:F:236:VAL:H | 1.79 | 0.48 |
| 1:F:432:GLN:NE2 | 1:F:436:GLN:HE22 | 2.12 | 0.48 |
| 1:F:496:PRO:O | 1:F:499:VAL:HG22 | 2.14 | 0.48 |
| 1:G:321:LYS:HD2 | 1:G:333:ILE:HG22 | 1.95 | 0.48 |
| 1:H:417:VAL:O | 1:H:418:ALA:C | 2.52 | 0.48 |
| 1:I:187:LEU:HD23 | 1:I:187:LEU:C | 2.33 | 0.48 |
| 1:J:413:ALA:HB1 | 1:J:417:VAL:HB | 1.95 | 0.48 |
| 1:K:218:PRO:HB3 | 1:K:246:PRO:HB2 | 1.95 | 0.48 |
| 1:K:411:VAL:HA | 1:K:497:THR:H | 1.79 | 0.48 |
| 1:K:66:PHE:HA | 1:K:520:MET:CE | 2.43 | 0.48 |
| 1:K:93:THR:O | 1:K:96:ALA:HB3 | 2.14 | 0.48 |
| 1:L:49:ILE:HD11 | 1:M:73:MET:HE3 | 1.95 | 0.48 |
| 1:M:364:LYS:HA | 1:M:367:GLU:OE1 | 2.13 | 0.48 |
| 1:M:7:LYS:HG3 | 1:M:66:PHE:CE2 | 2.49 | 0.48 |
| 1:N:248:LEU:HD22 | 1:N:249:ILE:H | 1.78 | 0.48 |
| 1:N:253:ASP:OD1 | 1:N:254:VAL:N | 2.30 | 0.48 |
| 2:T:37:ARG:NH1 | 2:T:37:ARG:HG2 | 2.28 | 0.48 |
| 2:U:17:VAL:CG1 | 2:U:34:LYS:HA | 2.43 | 0.48 |
| 2:U:78:ILE:HD12 | 2:U:78:ILE:N | 2.29 | 0.48 |
| 1:A:417:VAL:O | 1:A:420:ILE:CG2 | 2.59 | 0.48 |
| 1:A:41:ASP:O | 1:A:42:LYS:HG3 | 2.13 | 0.48 |
| 1:A:7:LYS:HD2 | 1:A:66:PHE:CE2 | 2.49 | 0.48 |
| 1:B:302:SER:O | 1:B:305:ILE:N | 2.44 | 0.48 |
| 1:B:119:GLY:O | 1:B:440:ILE:HG12 | 2.14 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:31:LEU:HD12 | 4:C:1:ADP:O1A | 2.13 | 0.48 |
| 1:C:203:TYR:HD1 | 1:C:203:TYR:H | 1.61 | 0.48 |
| 1:C:221:LEU:HD13 | 1:C:317:LEU:HD21 | 1.94 | 0.48 |
| 1:C:465:VAL:O | 1:C:466:ALA:C | 2.52 | 0.48 |
| 1:E:147:VAL:HA | 1:E:150:ILE:HG22 | 1.94 | 0.48 |
| 1:E:254:VAL:HG12 | 1:E:259:LEU:HG | 1.95 | 0.48 |
| 1:E:177:VAL:CG2 | 1:E:393:LYS:HG3 | 2.44 | 0.48 |
| 1:F:246:PRO:HA | 1:F:272:LYS:O | 2.14 | 0.48 |
| 1:F:69:MET:SD | 1:F:522:THR:HB | 2.54 | 0.48 |
| 1:H:258:ALA:O | 1:H:261:THR:OG1 | 2.30 | 0.48 |
| 1:H:383:ALA:CB | 1:H:389:MET:HA | 2.43 | 0.48 |
| 1:I:221:LEU:O | 1:I:222:LEU:HD23 | 2.14 | 0.48 |
| 1:I:293:ALA:HB2 | 1:I:300:VAL:HG13 | 1.96 | 0.48 |
| 1:J:216:GLU:C | 1:J:218:PRO:HD3 | 2.34 | 0.48 |
| 1:K:302:SER:HB2 | 1:K:305:ILE:HG13 | 1.96 | 0.48 |
| 1:K:420:ILE:CD1 | 1:K:448:GLU:HA | 2.44 | 0.48 |
| 1:L:345:ARG:HA | 1:L:348:GLN:NE2 | 2.29 | 0.48 |
| 1:M:27:VAL:HG11 | 1:M:93:THR:HG21 | 1.94 | 0.48 |
| 1:L:47:PRO:HG3 | 1:M:73:MET:HG3 | 1.95 | 0.48 |
| 1:N:305:ILE:O | 1:N:305:ILE:HG22 | 2.13 | 0.48 |
| 1:N:352:GLN:O | 1:N:355:GLU:OE1 | 2.32 | 0.48 |
| 1:H:281:PHE:CZ | 1:N:384:ALA:O | 2.67 | 0.48 |
| 2:P:14:ARG:CG | 2:P:15:LYS:H | 2.26 | 0.48 |
| 1:A:207:LYS:HB2 | 1:A:207:LYS:NZ | 2.29 | 0.48 |
| 1:A:366:GLN:HA | 1:A:369:VAL:HB | 1.94 | 0.48 |
| 1:B:222:LEU:HD22 | 1:B:300:VAL:HG22 | 1.96 | 0.48 |
| 1:B:259:LEU:O | 1:B:262:LEU:HB3 | 2.13 | 0.48 |
| 1:B:123:ALA:CB | 1:B:440:ILE:HG23 | 2.44 | 0.48 |
| 1:B:465:VAL:O | 1:B:466:ALA:C | 2.51 | 0.48 |
| 1:B:504:LEU:O | 1:B:504:LEU:HD13 | 2.13 | 0.48 |
| 1:C:339:GLU:N | 1:C:339:GLU:CD | 2.67 | 0.48 |
| 1:D:357:THR:HB | 1:D:361:ASP:HB2 | 1.95 | 0.48 |
| 1:F:162:ILE:HG21 | 1:F:403:THR:HG21 | 1.96 | 0.48 |
| 1:H:204:PHE:CD2 | 1:H:274:ALA:HB1 | 2.49 | 0.48 |
| 1:H:233:MET:CE | 1:H:309:LEU:HD13 | 2.44 | 0.48 |
| 1:I:386:GLU:HG2 | 1:I:390:LYS:HE2 | 1.96 | 0.48 |
| 1:J:352:GLN:O | 1:J:355:GLU:OE1 | 2.31 | 0.48 |
| 1:J:419:LEU:HA | 1:J:422:VAL:HG22 | 1.96 | 0.48 |
| 1:I:36:ARG:HB3 | 1:J:516:THR:O | 2.13 | 0.48 |
| 1:K:166:MET:HE2 | 1:K:171:LYS:CA | 2.30 | 0.48 |
| 1:K:216:GLU:C | 1:K:218:PRO:HD3 | 2.34 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:277:LYS:HZ2 | 1:K:277:LYS:HB2 | 1.79 | 0.48 |
| 1:K:350:ARG:HE | 1:K:369:VAL:HG11 | 1.79 | 0.48 |
| 1:L:247:LEU:O | 1:L:273:VAL:HB | 2.14 | 0.48 |
| 1:L:247:LEU:HD22 | 1:L:248:LEU:H | 1.79 | 0.48 |
| 1:L:293:ALA:O | 1:L:297:GLY:N | 2.47 | 0.48 |
| 1:L:389:MET:HE1 | 1:L:393:LYS:HB2 | 1.96 | 0.48 |
| 1:M:248:LEU:C | 1:M:248:LEU:HD13 | 2.33 | 0.48 |
| 1:M:213:VAL:O | 1:M:324:VAL:HA | 2.13 | 0.48 |
| 1:M:513:LEU:HD12 | 1:M:513:LEU:HA | 1.72 | 0.48 |
| 1:M:19:GLY:HA3 | 1:M:67:GLU:O | 2.14 | 0.48 |
| 2:R:11:ILE:HG12 | 2:R:85:ILE:HG12 | 1.96 | 0.48 |
| 2:S:20:LYS:HA | 2:S:28:THR:CG2 | 2.44 | 0.48 |
| 2:U:49:LEU:O | 2:U:55:LYS:NZ | 2.45 | 0.48 |
| 1:A:194:GLN:HG3 | 1:A:330:THR:O | 2.14 | 0.48 |
| 1:A:19:GLY:HA3 | 1:A:67:GLU:O | 2.13 | 0.48 |
| 1:B:365:LEU:HD22 | 1:B:366:GLN:HE22 | 1.78 | 0.48 |
| 1:B:368:ARG:O | 1:B:372:LEU:N | 2.47 | 0.48 |
| 1:C:281:PHE:N | 1:C:284:ARG:HD2 | 2.29 | 0.48 |
| 1:C:94:VAL:HG12 | 1:C:449:ALA:HB1 | 1.96 | 0.48 |
| 1:D:161:LEU:O | 1:D:164:GLU:HB2 | 2.14 | 0.48 |
| 1:D:400:LEU:HD13 | 1:D:400:LEU:C | 2.34 | 0.48 |
| 1:D:23:LEU:HD23 | 1:D:60:ILE:HB | 1.96 | 0.48 |
| 1:E:220:ILE:N | 1:E:220:ILE:CD1 | 2.76 | 0.48 |
| 1:F:479:ASN:O | 1:F:483:GLU:N | 2.46 | 0.48 |
| 1:G:147:VAL:HA | 1:G:150:ILE:HG22 | 1.96 | 0.48 |
| 1:G:216:GLU:O | 1:G:246:PRO:HG3 | 2.14 | 0.48 |
| 1:G:295:LEU:C | 1:G:295:LEU:HD23 | 2.34 | 0.48 |
| 1:H:215:LEU:HB3 | 1:H:218:PRO:CG | 2.41 | 0.48 |
| 1:H:215:LEU:HB2 | 1:H:323:VAL:HG13 | 1.96 | 0.48 |
| 1:H:420:ILE:HG13 | 1:H:451:LEU:HD22 | 1.95 | 0.48 |
| 1:H:55:SER:HA | 1:H:58:ARG:NH1 | 2.29 | 0.48 |
| 1:I:362:ARG:HB3 | 1:I:362:ARG:HH11 | 1.79 | 0.48 |
| 1:J:145:ALA:HA | 1:J:159:GLY:O | 2.13 | 0.48 |
| 1:J:187:LEU:HD23 | 1:J:187:LEU:C | 2.34 | 0.48 |
| 1:L:40:LEU:HD23 | 1:L:50:THR:HG22 | 1.95 | 0.48 |
| 1:M:194:GLN:HG2 | 1:M:195:PHE:N | 2.29 | 0.48 |
| 1:M:370:ALA:O | 1:M:371:LYS:C | 2.51 | 0.48 |
| 1:N:107:VAL:CG2 | 1:N:108:ALA:N | 2.77 | 0.48 |
| 1:N:284:ARG:NH1 | 1:N:284:ARG:H | 2.05 | 0.48 |
| 1:A:220:ILE:HD12 | 1:A:220:ILE:H | 1.78 | 0.47 |
| 1:A:496:PRO:O | 1:A:497:THR:C | 2.53 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:147:VAL:HA | 1:C:150:ILE:HG22 | 1.95 | 0.47 |
| 1:C:207:LYS:HB3 | 1:C:208:PRO:CD | 2.32 | 0.47 |
| 1:C:353:ILE:HG12 | 1:C:366:GLN:HE22 | 1.77 | 0.47 |
| 1:C:77:VAL:HG22 | 1:C:78:ALA:N | 2.29 | 0.47 |
| 1:D:149:THR:OG1 | 1:D:156:GLU:HA | 2.14 | 0.47 |
| 1:D:309:LEU:H | 1:D:309:LEU:CD1 | 2.26 | 0.47 |
| 1:D:37:ASN:OD1 | 1:D:51:LYS:HB2 | 2.14 | 0.47 |
| 1:D:496:PRO:HG2 | 1:D:499:VAL:CG1 | 2.44 | 0.47 |
| 1:G:116:LEU:O | 1:G:120:ILE:HG13 | 2.15 | 0.47 |
| 1:G:124:VAL:HG13 | 1:G:504:LEU:HD12 | 1.95 | 0.47 |
| 1:G:33:PRO:HD3 | 4:G:1:ADP:N7 | 2.29 | 0.47 |
| 1:H:194:GLN:HG2 | 1:H:195:PHE:N | 2.28 | 0.47 |
| 1:H:23:LEU:O | 1:H:27:VAL:HG12 | 2.13 | 0.47 |
| 1:H:476:TYR:HA | 1:H:486:GLY:O | 2.14 | 0.47 |
| 1:H:90:THR:O | 1:H:94:VAL:HG23 | 2.14 | 0.47 |
| 1:I:305:ILE:HG22 | 1:I:305:ILE:O | 2.13 | 0.47 |
| 1:J:391:GLU:O | 1:J:394:ALA:HB3 | 2.13 | 0.47 |
| 1:K:218:PRO:CG | 1:K:246:PRO:HB2 | 2.44 | 0.47 |
| 1:K:40:LEU:HD23 | 1:K:50:THR:HG22 | 1.96 | 0.47 |
| 1:L:496:PRO:O | 1:L:497:THR:C | 2.51 | 0.47 |
| 1:M:169:VAL:HG22 | 1:M:169:VAL:O | 2.14 | 0.47 |
| 1:M:262:LEU:HA | 1:M:265:ASN:HB3 | 1.96 | 0.47 |
| 1:N:479:ASN:OD1 | 1:N:481:ALA:HB3 | 2.14 | 0.47 |
| 2:O:47:ARG:HG2 | 2:O:49:LEU:H | 1.79 | 0.47 |
| 2:P:46:GLY:HA3 | 2:P:55:LYS:O | 2.14 | 0.47 |
| 2:Q:7:HIS:HA | 2:Q:45:ASN:N | 2.29 | 0.47 |
| 2:R:87:SER:OG | 2:R:89:SER:HB2 | 2.13 | 0.47 |
| 1:A:18:ARG:O | 1:A:22:VAL:HG23 | 2.14 | 0.47 |
| 1:B:235:PRO:HG2 | 1:B:236:VAL:HG23 | 1.94 | 0.47 |
| 1:B:247:LEU:HD13 | 1:B:248:LEU:O | 2.13 | 0.47 |
| 1:B:215:LEU:O | 1:B:322:ARG:HG3 | 2.14 | 0.47 |
| 1:B:357:THR:O | 1:B:359:ASP:N | 2.47 | 0.47 |
| 1:C:219:PHE:O | 1:C:247:LEU:HD22 | 2.15 | 0.47 |
| 1:C:23:LEU:CD1 | 1:C:23:LEU:C | 2.82 | 0.47 |
| 1:E:256:GLY:O | 1:E:257:GLU:C | 2.52 | 0.47 |
| 1:E:122:LYS:HE2 | 1:E:429:LEU:HD11 | 1.96 | 0.47 |
| 1:E:487:ASN:HB3 | 1:E:490:ASP:OD2 | 2.15 | 0.47 |
| 1:F:160:LYS:O | 1:F:164:GLU:HG3 | 2.14 | 0.47 |
| 1:F:221:LEU:C | 1:F:222:LEU:HD12 | 2.34 | 0.47 |
| 1:F:302:SER:CB | 1:F:305:ILE:HB | 2.42 | 0.47 |
| 1:F:215:LEU:O | 1:F:322:ARG:HG3 | 2.14 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:39:VAL:HA | 1:F:48:THR:O | 2.15 | 0.47 |
| 1:G:161:LEU:O | 1:G:164:GLU:HB2 | 2.14 | 0.47 |
| 1:G:23:LEU:CD1 | 1:G:23:LEU:C | 2.82 | 0.47 |
| 1:G:248:LEU:C | 1:G:248:LEU:HD13 | 2.34 | 0.47 |
| 1:G:72:GLN:NE2 | 1:G:72:GLN:CA | 2.75 | 0.47 |
| 1:H:353:ILE:HD11 | 1:H:369:VAL:HG21 | 1.95 | 0.47 |
| 1:H:358:SER:HB3 | 1:H:361:ASP:OD1 | 2.14 | 0.47 |
| 1:H:440:ILE:O | 1:H:443:ALA:HB3 | 2.14 | 0.47 |
| 1:H:494:LEU:CD2 | 1:H:494:LEU:N | 2.74 | 0.47 |
| 1:I:353:ILE:HA | 1:I:365:LEU:CD1 | 2.44 | 0.47 |
| 1:I:80:LYS:O | 1:I:83:ASP:HB2 | 2.14 | 0.47 |
| 1:J:219:PHE:O | 1:J:247:LEU:HD22 | 2.14 | 0.47 |
| 1:L:299:THR:HB | 1:L:316:ASP:HB3 | 1.97 | 0.47 |
| 1:M:285:ARG:HH11 | 1:M:285:ARG:HG2 | 1.78 | 0.47 |
| 1:N:249:ILE:HB | 1:N:275:ALA:HB1 | 1.93 | 0.47 |
| 1:N:411:VAL:HG21 | 1:N:494:LEU:HD12 | 1.96 | 0.47 |
| 2:S:17:VAL:HG11 | 2:S:33:ALA:O | 2.14 | 0.47 |
| 1:A:209:GLU:N | 1:A:209:GLU:CD | 2.68 | 0.47 |
| 1:A:237:LEU:C | 1:A:237:LEU:CD2 | 2.83 | 0.47 |
| 1:A:475:ASN:ND2 | 1:A:475:ASN:N | 2.62 | 0.47 |
| 1:B:115:ASP:HB3 | 1:B:436:GLN:HG3 | 1.95 | 0.47 |
| 1:B:88:GLY:HA2 | 4:B:1:ADP:O2B | 2.14 | 0.47 |
| 1:C:253:ASP:HB2 | 1:C:277:LYS:HE2 | 1.95 | 0.47 |
| 1:C:280:GLY:HA3 | 1:C:284:ARG:NH1 | 2.30 | 0.47 |
| 1:C:295:LEU:O | 1:C:295:LEU:HD23 | 2.14 | 0.47 |
| 1:C:177:VAL:CG1 | 1:C:397:GLU:HG2 | 2.43 | 0.47 |
| 1:D:233:MET:HE3 | 1:D:233:MET:O | 2.14 | 0.47 |
| 1:D:438:VAL:O | 1:D:442:VAL:HG23 | 2.14 | 0.47 |
| 1:E:349:ILE:O | 1:E:349:ILE:HG22 | 2.14 | 0.47 |
| 1:F:240:VAL:O | 1:F:244:GLY:N | 2.45 | 0.47 |
| 1:G:252:GLU:O | 1:G:253:ASP:CB | 2.61 | 0.47 |
| 1:H:348:GLN:O | 1:H:352:GLN:HG3 | 2.15 | 0.47 |
| 1:H:38:VAL:HG12 | 1:H:39:VAL:N | 2.29 | 0.47 |
| 1:J:190:VAL:HG22 | 1:J:191:GLU:N | 2.29 | 0.47 |
| 1:J:288:MET:HA | 1:J:288:MET:CE | 2.44 | 0.47 |
| 1:J:314:LEU:O | 1:J:316:ASP:N | 2.47 | 0.47 |
| 1:J:314:LEU:C | 1:J:316:ASP:H | 2.17 | 0.47 |
| 1:J:38:VAL:HG12 | 1:J:39:VAL:N | 2.29 | 0.47 |
| 1:K:131:LEU:CD1 | 1:K:422:VAL:HG11 | 2.43 | 0.47 |
| 1:L:240:VAL:HA | 1:L:243:ALA:CB | 2.43 | 0.47 |
| 1:L:515:ILE:O | 1:L:515:ILE:HG22 | 2.13 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:88:GLY:O | 1:M:89:THR:C | 2.53 | 0.47 |
| 1:N:381:VAL:HB | 1:N:389:MET:HE3 | 1.95 | 0.47 |
| 1:N:74:VAL:O | 1:N:75:LYS:C | 2.52 | 0.47 |
| 2:R:43:VAL:HG23 | 2:R:61:VAL:HG22 | 1.96 | 0.47 |
| 1:B:207:LYS:CB | 1:B:207:LYS:NZ | 2.77 | 0.47 |
| 1:C:30:THR:HB | 1:C:51:LYS:HG3 | 1.95 | 0.47 |
| 1:D:270:ILE:HD11 | 2:R:27:LEU:CD1 | 2.45 | 0.47 |
| 1:E:161:LEU:HD12 | 1:E:161:LEU:HA | 1.73 | 0.47 |
| 1:E:220:ILE:N | 1:E:318:GLY:O | 2.37 | 0.47 |
| 1:E:322:ARG:CG | 1:E:323:VAL:H | 2.14 | 0.47 |
| 1:D:519:CYS:HB3 | 1:E:38:VAL:HG13 | 1.97 | 0.47 |
| 1:F:212:ALA:HA | 1:F:325:ILE:O | 2.14 | 0.47 |
| 1:F:56:VAL:O | 1:F:57:ALA:C | 2.53 | 0.47 |
| 1:G:436:GLN:O | 1:G:440:ILE:HG13 | 2.14 | 0.47 |
| 1:I:222:LEU:CD1 | 1:I:293:ALA:HA | 2.44 | 0.47 |
| 1:I:299:THR:HB | 1:I:316:ASP:HB3 | 1.97 | 0.47 |
| 1:J:496:PRO:O | 1:J:499:VAL:HG22 | 2.13 | 0.47 |
| 1:K:109:ALA:HB3 | 1:K:111:MET:HE3 | 1.95 | 0.47 |
| 1:L:124:VAL:HG13 | 1:L:504:LEU:HD11 | 1.96 | 0.47 |
| 1:L:487:ASN:O | 1:L:491:MET:HG3 | 2.14 | 0.47 |
| 1:M:355:GLU:C | 1:M:357:THR:N | 2.67 | 0.47 |
| 1:N:284:ARG:N | 1:N:284:ARG:HH11 | 2.06 | 0.47 |
| 2:P:48:ILE:HG12 | 2:P:54:VAL:CG1 | 2.42 | 0.47 |
| 2:Q:47:ARG:HD2 | 2:Q:55:LYS:HD2 | 1.95 | 0.47 |
| 2:T:20:LYS:CD | 2:T:20:LYS:H | 2.26 | 0.47 |
| 1:A:468:THR:OG1 | 1:A:485:TYR:CE2 | 2.68 | 0.47 |
| 1:B:288:MET:O | 1:B:289:LEU:HG | 2.14 | 0.47 |
| 1:B:429:LEU:O | 1:B:430:ARG:NH1 | 2.40 | 0.47 |
| 1:D:417:VAL:HG13 | 1:D:418:ALA:N | 2.29 | 0.47 |
| 1:D:409:GLU:CD | 1:D:501:ARG:HH21 | 2.18 | 0.47 |
| 1:E:478:TYR:CE2 | 1:E:480:ALA:HA | 2.49 | 0.47 |
| 1:F:237:LEU:CD2 | 1:F:237:LEU:C | 2.83 | 0.47 |
| 1:F:313:THR:HG22 | 1:F:314:LEU:N | 2.30 | 0.47 |
| 1:F:355:GLU:HG3 | 1:F:357:THR:H | 1.78 | 0.47 |
| 1:F:413:ALA:HB1 | 1:F:417:VAL:HG11 | 1.96 | 0.47 |
| 1:F:510:VAL:CG2 | 1:F:511:ALA:N | 2.75 | 0.47 |
| 1:G:259:LEU:O | 1:G:262:LEU:HB3 | 2.15 | 0.47 |
| 1:G:353:ILE:HG12 | 1:G:366:GLN:HE22 | 1.79 | 0.47 |
| 1:H:161:LEU:N | 1:H:161:LEU:HD12 | 2.28 | 0.47 |
| 1:H:175:ILE:N | 1:H:175:ILE:CD1 | 2.77 | 0.47 |
| 1:I:102:GLU:HB2 | 1:I:442:VAL:HG13 | 1.96 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:222:LEU:HD22 | 1:I:289:LEU:CD1 | 2.44 | 0.47 |
| 1:I:385:THR:HG23 | 1:I:388:GLU:HB3 | 1.96 | 0.47 |
| 1:J:186:GLU:O | 1:J:379:ILE:HA | 2.14 | 0.47 |
| 1:J:214:GLU:HG2 | 1:J:324:VAL:HG12 | 1.97 | 0.47 |
| 1:J:364:LYS:HA | 1:J:367:GLU:OE1 | 2.15 | 0.47 |
| 1:J:16:MET:HG3 | 1:J:520:MET:SD | 2.54 | 0.47 |
| 1:K:228:SER:O | 1:K:257:GLU:HB3 | 2.14 | 0.47 |
| 1:K:313:THR:HG22 | 1:K:314:LEU:H | 1.79 | 0.47 |
| 1:L:350:ARG:HG3 | 1:L:350:ARG:NH1 | 2.29 | 0.47 |
| 1:L:32:GLY:CA | 1:L:454:ILE:HD12 | 2.42 | 0.47 |
| 1:N:353:ILE:HD11 | 1:N:369:VAL:HG21 | 1.97 | 0.47 |
| 2:R:48:ILE:HG12 | 2:R:54:VAL:CG1 | 2.43 | 0.47 |
| 2:T:17:VAL:HG13 | 2:T:34:LYS:HA | 1.95 | 0.47 |
| 1:A:265:ASN:HB3 | 1:A:271:VAL:CG2 | 2.45 | 0.47 |
| 1:A:263:VAL:HG12 | 1:A:267:MET:SD | 2.54 | 0.47 |
| 1:A:18:ARG:HB2 | 1:A:67:GLU:HG2 | 1.95 | 0.47 |
| 1:B:262:LEU:O | 1:B:266:THR:HG23 | 2.15 | 0.47 |
| 1:C:256:GLY:HA2 | 1:C:259:LEU:HD12 | 1.97 | 0.47 |
| 1:C:348:GLN:NE2 | 1:C:352:GLN:NE2 | 2.62 | 0.47 |
| 1:C:355:GLU:O | 1:C:362:ARG:NH2 | 2.46 | 0.47 |
| 1:D:234:LEU:N | 1:D:235:PRO:CD | 2.78 | 0.47 |
| 1:F:124:VAL:O | 1:F:128:VAL:HG23 | 2.15 | 0.47 |
| 1:F:280:GLY:CA | 1:F:284:ARG:HD2 | 2.45 | 0.47 |
| 1:F:44:PHE:HB2 | 1:F:45:GLY:H | 1.57 | 0.47 |
| 1:G:519:CYS:SG | 1:G:520:MET:N | 2.88 | 0.47 |
| 1:I:233:MET:HE2 | 1:I:309:LEU:HD13 | 1.96 | 0.47 |
| 1:I:38:VAL:HG12 | 1:I:39:VAL:N | 2.30 | 0.47 |
| 1:I:419:LEU:O | 1:I:422:VAL:HG22 | 2.14 | 0.47 |
| 1:I:66:PHE:HA | 1:I:520:MET:CE | 2.44 | 0.47 |
| 1:J:31:LEU:HG | 1:J:454:ILE:CD1 | 2.44 | 0.47 |
| 1:K:124:VAL:HG13 | 1:K:504:LEU:HD13 | 1.95 | 0.47 |
| 1:K:138:CYS:SG | 1:K:144:ILE:HD13 | 2.55 | 0.47 |
| 1:K:353:ILE:HA | 1:K:365:LEU:CD1 | 2.45 | 0.47 |
| 1:K:443:ALA:O | 1:K:447:MET:HG3 | 2.14 | 0.47 |
| 1:K:55:SER:O | 1:K:58:ARG:HB3 | 2.14 | 0.47 |
| 1:L:277:LYS:HZ3 | 1:L:277:LYS:HB2 | 1.78 | 0.47 |
| 1:L:291:ASP:O | 1:L:294:THR:HB | 2.15 | 0.47 |
| 1:L:432:GLN:OE1 | 1:L:432:GLN:N | 2.47 | 0.47 |
| 1:L:420:ILE:HD13 | 1:L:448:GLU:HA | 1.97 | 0.47 |
| 1:M:131:LEU:CD1 | 1:M:422:VAL:HG11 | 2.45 | 0.47 |
| 1:N:287:ALA:HB1 | 1:N:368:ARG:NH1 | 2.30 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:73:MET:HE1 | 1:N:514:MET:HG2 | 1.97 | 0.47 |
| 2:O:14:ARG:CD | 2:O:35:SER:HB3 | 2.42 | 0.47 |
| 2:O:5:PRO:HD3 | 2:O:42:ALA:CB | 2.42 | 0.47 |
| 2:U:59:VAL:HG23 | 2:U:59:VAL:O | 2.14 | 0.47 |
| 1:A:266:THR:HG22 | 1:A:273:VAL:N | 2.28 | 0.47 |
| 1:B:260:ALA:O | 1:B:263:VAL:HB | 2.14 | 0.47 |
| 1:B:252:GLU:O | 1:B:277:LYS:HE2 | 2.15 | 0.47 |
| 1:B:411:VAL:HG12 | 1:B:496:PRO:CA | 2.37 | 0.47 |
| 1:B:455:VAL:O | 1:B:458:CYS:HB2 | 2.15 | 0.47 |
| 1:B:510:VAL:CG2 | 1:B:511:ALA:N | 2.78 | 0.47 |
| 1:C:195:PHE:HD1 | 1:C:195:PHE:C | 2.17 | 0.47 |
| 1:C:221:LEU:C | 1:C:222:LEU:HD12 | 2.35 | 0.47 |
| 1:C:368:ARG:O | 1:C:372:LEU:N | 2.46 | 0.47 |
| 1:D:7:LYS:HD2 | 1:D:66:PHE:CE2 | 2.50 | 0.47 |
| 1:E:339:GLU:CD | 1:E:339:GLU:H | 2.18 | 0.47 |
| 1:E:418:ALA:O | 1:E:422:VAL:HG13 | 2.15 | 0.47 |
| 1:E:112:ASN:N | 1:E:435:ASP:OD2 | 2.43 | 0.47 |
| 1:E:510:VAL:CG2 | 1:E:511:ALA:N | 2.76 | 0.47 |
| 1:F:233:MET:C | 1:F:235:PRO:CD | 2.81 | 0.47 |
| 1:F:281:PHE:H | 1:F:284:ARG:CZ | 2.28 | 0.47 |
| 1:F:368:ARG:O | 1:F:372:LEU:N | 2.46 | 0.47 |
| 1:F:146:GLN:HE21 | 1:F:494:LEU:HD11 | 1.80 | 0.47 |
| 1:F:510:VAL:CG2 | 1:F:511:ALA:H | 2.28 | 0.47 |
| 1:F:76:GLU:OE1 | 1:G:387:VAL:HG13 | 2.14 | 0.47 |
| 1:G:346:VAL:CG1 | 1:G:350:ARG:HH22 | 2.27 | 0.47 |
| 1:H:293:ALA:O | 1:H:297:GLY:N | 2.47 | 0.47 |
| 1:H:513:LEU:HD12 | 1:H:513:LEU:HA | 1.66 | 0.47 |
| 1:J:461:GLU:HB3 | 1:J:464:VAL:HB | 1.95 | 0.47 |
| 1:J:65:LYS:O | 1:J:66:PHE:CB | 2.44 | 0.47 |
| 1:K:107:VAL:HG23 | 1:K:108:ALA:H | 1.78 | 0.47 |
| 1:K:187:LEU:HD23 | 1:K:187:LEU:C | 2.35 | 0.47 |
| 1:M:149:THR:HG22 | 1:M:156:GLU:HA | 1.95 | 0.47 |
| 1:M:145:ALA:HA | 1:M:159:GLY:O | 2.15 | 0.47 |
| 1:M:214:GLU:HG2 | 1:M:324:VAL:CG1 | 2.45 | 0.47 |
| 2:R:47:ARG:O | 2:R:54:VAL:HG13 | 2.14 | 0.47 |
| 2:U:43:VAL:HG12 | 2:U:57:LEU:HD12 | 1.95 | 0.47 |
| 2:U:60:LYS:N | 2:U:63:ASP:OD2 | 2.48 | 0.47 |
| 1:A:119:GLY:O | 1:A:440:ILE:HG12 | 2.14 | 0.47 |
| 1:A:482:THR:OG1 | 1:A:484:GLU:HG2 | 2.15 | 0.47 |
| 1:B:195:PHE:CD1 | 1:B:195:PHE:C | 2.88 | 0.47 |
| 1:B:204:PHE:CB | 1:B:274:ALA:HB2 | 2.45 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:391:GLU:O | 1:B:394:ALA:HB3 | 2.15 | 0.47 |
| 1:C:5:ASP:HB2 | 1:C:524:LEU:HD23 | 1.96 | 0.47 |
| 1:C:72:GLN:HB3 | 1:D:47:PRO:HD3 | 1.96 | 0.47 |
| 1:D:256:GLY:HA2 | 1:D:259:LEU:HD12 | 1.96 | 0.47 |
| 1:D:472:GLY:HA3 | 1:D:476:TYR:HD2 | 1.80 | 0.47 |
| 1:E:206:ASN:HB2 | 1:E:214:GLU:H | 1.78 | 0.47 |
| 1:E:257:GLU:O | 1:E:261:THR:HG22 | 2.15 | 0.47 |
| 1:E:428:ASP:HA | 1:E:430:ARG:HH12 | 1.80 | 0.47 |
| 1:F:100:ILE:O | 1:F:101:THR:C | 2.53 | 0.47 |
| 1:F:174:VAL:C | 1:F:175:ILE:HG13 | 2.34 | 0.47 |
| 1:F:202:PRO:HG2 | 1:F:203:TYR:CD1 | 2.50 | 0.47 |
| 1:F:225:LYS:C | 1:F:252:GLU:HB2 | 2.35 | 0.47 |
| 1:F:304:GLU:HB2 | 1:F:305:ILE:HD12 | 1.96 | 0.47 |
| 1:F:475:ASN:ND2 | 1:F:475:ASN:N | 2.63 | 0.47 |
| 1:G:428:ASP:C | 1:G:430:ARG:NH1 | 2.68 | 0.47 |
| 1:H:15:LYS:HD2 | 1:H:67:GLU:HG3 | 1.97 | 0.47 |
| 1:H:84:ALA:O | 1:H:498:LYS:HE2 | 2.14 | 0.47 |
| 1:I:231:ARG:O | 1:I:234:LEU:HG | 2.15 | 0.47 |
| 1:I:41:ASP:HB2 | 1:J:69:MET:CE | 2.45 | 0.47 |
| 1:J:270:ILE:HG22 | 1:J:271:VAL:H | 1.77 | 0.47 |
| 1:K:107:VAL:HG11 | 1:K:515:ILE:HG23 | 1.96 | 0.47 |
| 1:K:221:LEU:HB3 | 1:K:249:ILE:HA | 1.96 | 0.47 |
| 1:L:391:GLU:O | 1:L:394:ALA:HB3 | 2.14 | 0.47 |
| 1:L:476:TYR:HA | 1:L:486:GLY:O | 2.14 | 0.47 |
| 1:M:109:ALA:HB3 | 1:M:111:MET:CE | 2.44 | 0.47 |
| 1:M:449:ALA:CB | 1:M:450:PRO:HD3 | 2.29 | 0.47 |
| 1:N:501:ARG:O | 1:N:502:SER:C | 2.52 | 0.47 |
| 2:O:48:ILE:HG12 | 2:O:54:VAL:HG13 | 1.96 | 0.47 |
| 2:O:83:VAL:C | 2:O:84:LEU:HD12 | 2.35 | 0.47 |
| 2:Q:84:LEU:N | 2:Q:84:LEU:CD1 | 2.76 | 0.47 |
| 2:R:40:VAL:CG2 | 2:R:63:ASP:HB2 | 2.44 | 0.47 |
| 2:S:37:ARG:NH1 | 2:S:37:ARG:HG2 | 2.30 | 0.47 |
| 2:U:3:ILE:H | 2:U:3:ILE:HD12 | 1.79 | 0.47 |
| 2:U:52:GLY:O | 2:U:53:GLU:HB2 | 2.13 | 0.47 |
| 1:A:293:ALA:O | 1:A:297:GLY:N | 2.47 | 0.47 |
| 1:A:383:ALA:N | 1:A:389:MET:HE1 | 2.29 | 0.47 |
| 1:B:239:ALA:O | 1:B:242:LYS:HB3 | 2.15 | 0.47 |
| 1:B:409:GLU:CD | 1:B:501:ARG:HH21 | 2.18 | 0.47 |
| 1:E:289:LEU:N | 1:E:290:GLN:OE1 | 2.43 | 0.47 |
| 1:E:308:GLU:O | 1:E:309:LEU:O | 2.33 | 0.47 |
| 1:E:411:VAL:HG12 | 1:E:496:PRO:CA | 2.40 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:417:VAL:C | 1:E:420:ILE:HG22 | 2.34 | 0.47 |
| 1:F:222:LEU:CD2 | 1:F:300:VAL:HG22 | 2.40 | 0.47 |
| 1:G:117:LYS:HG2 | 1:G:121:ASP:OD2 | 2.14 | 0.47 |
| 1:G:130:GLU:O | 1:G:134:LEU:HD13 | 2.15 | 0.47 |
| 1:G:234:LEU:HA | 1:G:237:LEU:HB3 | 1.96 | 0.47 |
| 1:H:17:LEU:HA | 1:H:20:VAL:CG1 | 2.45 | 0.47 |
| 1:H:218:PRO:HB3 | 1:H:246:PRO:C | 2.35 | 0.47 |
| 1:I:402:ALA:HA | 1:I:496:PRO:HG2 | 1.96 | 0.47 |
| 1:I:441:LYS:O | 1:I:442:VAL:C | 2.51 | 0.47 |
| 1:I:450:PRO:O | 1:I:454:ILE:HG12 | 2.15 | 0.47 |
| 1:I:69:MET:O | 1:I:73:MET:HG3 | 2.14 | 0.47 |
| 1:J:161:LEU:HD12 | 1:J:161:LEU:N | 2.30 | 0.47 |
| 1:J:228:SER:HA | 1:J:255:GLU:HB2 | 1.96 | 0.47 |
| 1:J:266:THR:HB | 1:J:272:LYS:HG3 | 1.96 | 0.47 |
| 1:K:193:MET:HB3 | 1:K:332:ILE:HD11 | 1.96 | 0.47 |
| 1:K:290:GLN:HA | 1:K:290:GLN:OE1 | 2.15 | 0.47 |
| 1:K:385:THR:CG2 | 1:K:388:GLU:HB3 | 2.44 | 0.47 |
| 1:K:38:VAL:HG12 | 1:K:39:VAL:N | 2.30 | 0.47 |
| 1:L:305:ILE:O | 1:L:305:ILE:HG22 | 2.15 | 0.47 |
| 1:L:270:ILE:HG23 | 1:M:229:ASN:ND2 | 2.29 | 0.47 |
| 1:M:308:GLU:OE2 | 1:M:310:GLU:HG3 | 2.15 | 0.47 |
| 1:M:336:VAL:O | 1:M:336:VAL:HG12 | 2.15 | 0.47 |
| 1:M:501:ARG:NH1 | 1:M:505:GLN:OE1 | 2.48 | 0.47 |
| 1:N:64:ASP:C | 1:N:65:LYS:O | 2.51 | 0.47 |
| 2:Q:78:ILE:N | 2:Q:78:ILE:HD12 | 2.30 | 0.47 |
| 1:A:417:VAL:HG13 | 1:A:418:ALA:N | 2.28 | 0.47 |
| 1:A:479:ASN:O | 1:A:483:GLU:N | 2.47 | 0.47 |
| 1:B:234:LEU:HA | 1:B:237:LEU:HB3 | 1.96 | 0.47 |
| 1:B:366:GLN:HA | 1:B:369:VAL:HG21 | 1.97 | 0.47 |
| 1:C:256:GLY:O | 1:C:257:GLU:C | 2.53 | 0.47 |
| 1:C:194:GLN:NE2 | 1:C:329:THR:HG21 | 2.30 | 0.47 |
| 1:C:358:SER:HA | 1:C:362:ARG:CD | 2.45 | 0.47 |
| 1:C:434:GLU:O | 1:C:435:ASP:C | 2.53 | 0.47 |
| 1:C:456:LEU:HD13 | 1:C:462:PRO:CG | 2.45 | 0.47 |
| 1:E:326:ASN:OD1 | 1:E:329:THR:N | 2.48 | 0.47 |
| 1:F:421:ARG:HA | 1:F:421:ARG:HD3 | 1.74 | 0.47 |
| 1:F:428:ASP:HA | 1:F:430:ARG:HH12 | 1.80 | 0.47 |
| 1:F:73:MET:O | 1:F:74:VAL:C | 2.53 | 0.47 |
| 1:G:266:THR:HG22 | 1:G:273:VAL:N | 2.30 | 0.47 |
| 1:G:272:LYS:HZ2 | 1:G:272:LYS:HB2 | 1.80 | 0.47 |
| 1:G:417:VAL:O | 1:G:420:ILE:CG2 | 2.56 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:160:LYS:HG2 | 1:H:164:GLU:OE2 | 2.14 | 0.47 |
| 1:H:266:THR:O | 1:H:268:ARG:N | 2.48 | 0.47 |
| 1:H:301:ILE:HG21 | 1:H:309:LEU:HD23 | 1.96 | 0.47 |
| 1:H:317:LEU:CD1 | 1:H:317:LEU:N | 2.78 | 0.47 |
| 1:I:247:LEU:HB3 | 1:I:273:VAL:HG11 | 1.96 | 0.47 |
| 1:I:336:VAL:HG12 | 1:I:336:VAL:O | 2.14 | 0.47 |
| 1:I:357:THR:O | 1:I:357:THR:HG22 | 2.15 | 0.47 |
| 1:I:478:TYR:HB2 | 1:I:485:TYR:CE2 | 2.50 | 0.47 |
| 1:I:5:ASP:HB2 | 1:I:524:LEU:CD2 | 2.41 | 0.47 |
| 1:I:74:VAL:O | 1:I:75:LYS:C | 2.54 | 0.47 |
| 1:J:230:ILE:HG12 | 1:J:261:THR:HG21 | 1.97 | 0.47 |
| 1:J:419:LEU:HD21 | 1:J:500:THR:CG2 | 2.45 | 0.47 |
| 1:K:288:MET:HA | 1:K:288:MET:HE3 | 1.97 | 0.47 |
| 1:L:106:ALA:HA | 1:L:111:MET:CE | 2.45 | 0.47 |
| 1:L:131:LEU:HD12 | 1:L:422:VAL:HG11 | 1.97 | 0.47 |
| 1:L:202:PRO:C | 1:L:204:PHE:N | 2.68 | 0.47 |
| 1:K:36:ARG:HB3 | 1:L:516:THR:O | 2.13 | 0.47 |
| 1:M:189:VAL:O | 1:M:189:VAL:HG23 | 2.15 | 0.47 |
| 1:N:163:ALA:O | 1:N:167:ASP:HB2 | 2.15 | 0.47 |
| 1:N:230:ILE:CD1 | 1:N:257:GLU:HG2 | 2.44 | 0.47 |
| 2:P:20:LYS:H | 2:P:20:LYS:CD | 2.28 | 0.47 |
| 2:P:50:GLU:OE1 | 2:Q:50:GLU:HA | 2.15 | 0.47 |
| 2:T:71:TYR:O | 2:T:73:VAL:N | 2.48 | 0.47 |
| 1:A:218:PRO:HA | 1:A:246:PRO:O | 2.15 | 0.47 |
| 1:A:247:LEU:HD13 | 1:A:248:LEU:N | 2.29 | 0.47 |
| 1:A:329:THR:HG22 | 1:A:330:THR:N | 2.30 | 0.47 |
| 1:A:414:GLY:HA2 | 1:A:495:ASP:OD2 | 2.14 | 0.47 |
| 1:B:199:TYR:O | 1:B:199:TYR:CD1 | 2.68 | 0.47 |
| 1:B:271:VAL:HG23 | 1:B:271:VAL:O | 2.14 | 0.47 |
| 1:C:187:LEU:HD12 | 1:C:188:ASP:N | 2.30 | 0.47 |
| 1:C:352:GLN:HB3 | 1:C:365:LEU:HD11 | 1.97 | 0.47 |
| 1:C:486:GLY:CA | 1:C:491:MET:CE | 2.93 | 0.47 |
| 1:D:237:LEU:C | 1:D:237:LEU:CD2 | 2.83 | 0.47 |
| 1:E:272:LYS:HB2 | 1:E:272:LYS:NZ | 2.30 | 0.47 |
| 1:E:277:LYS:HG2 | 1:E:278:ALA:N | 2.30 | 0.47 |
| 1:E:353:ILE:HG22 | 1:E:354:GLU:N | 2.30 | 0.47 |
| 1:F:260:ALA:O | 1:F:263:VAL:HB | 2.15 | 0.47 |
| 1:F:278:ALA:HB1 | 1:F:279:PRO:HD2 | 1.96 | 0.47 |
| 1:F:308:GLU:O | 1:F:309:LEU:O | 2.33 | 0.47 |
| 1:F:400:LEU:HD13 | 1:F:400:LEU:O | 2.15 | 0.47 |
| 1:H:37:ASN:ND2 | 1:H:37:ASN:H | 2.13 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:254:VAL:O | 1:J:259:LEU:HD12 | 2.15 | 0.47 |
| 1:K:153:ASN:O | 1:K:154:SER:HB2 | 2.15 | 0.47 |
| 1:K:199:TYR:C | 1:K:200:LEU:HD12 | 2.35 | 0.47 |
| 1:K:228:SER:O | 1:K:258:ALA:N | 2.47 | 0.47 |
| 1:K:322:ARG:HB2 | 1:K:333:ILE:HB | 1.97 | 0.47 |
| 1:L:290:GLN:HG3 | 1:L:345:ARG:HE | 1.79 | 0.47 |
| 1:M:414:GLY:N | 1:M:494:LEU:HA | 2.31 | 0.47 |
| 1:M:66:PHE:N | 1:M:69:MET:HG3 | 2.28 | 0.47 |
| 1:N:191:GLU:O | 1:N:334:ASP:HA | 2.15 | 0.47 |
| 1:N:345:ARG:O | 1:N:348:GLN:HB2 | 2.15 | 0.47 |
| 1:N:420:ILE:CD1 | 1:N:448:GLU:HG2 | 2.45 | 0.47 |
| 2:Q:47:ARG:HD3 | 2:Q:49:LEU:CG | 2.45 | 0.47 |
| 2:Q:71:TYR:O | 2:Q:73:VAL:N | 2.48 | 0.47 |
| 2:S:47:ARG:HG2 | 2:S:48:ILE:N | 2.30 | 0.47 |
| 2:U:4:ARG:HD2 | 2:U:5:PRO:HD2 | 1.96 | 0.47 |
| 1:A:210:THR:HG22 | 1:A:210:THR:O | 2.15 | 0.46 |
| 1:A:249:ILE:C | 1:A:250:ILE:HG13 | 2.35 | 0.46 |
| 1:A:30:THR:HB | 1:A:51:LYS:HG3 | 1.96 | 0.46 |
| 1:A:346:VAL:O | 1:A:350:ARG:NH1 | 2.47 | 0.46 |
| 1:A:404:ARG:NH1 | 1:A:404:ARG:HG3 | 2.28 | 0.46 |
| 1:B:127:ALA:O | 1:B:131:LEU:HG | 2.15 | 0.46 |
| 1:B:195:PHE:HD1 | 1:B:195:PHE:C | 2.18 | 0.46 |
| 1:B:221:LEU:C | 1:B:222:LEU:HD12 | 2.36 | 0.46 |
| 1:E:206:ASN:HB3 | 1:E:214:GLU:N | 2.30 | 0.46 |
| 1:E:353:ILE:O | 1:E:355:GLU:N | 2.47 | 0.46 |
| 1:E:111:MET:CE | 1:E:438:VAL:HG21 | 2.44 | 0.46 |
| 1:F:127:ALA:O | 1:F:131:LEU:HG | 2.14 | 0.46 |
| 1:F:314:LEU:C | 1:F:314:LEU:HD12 | 2.33 | 0.46 |
| 1:F:444:LEU:HD23 | 1:F:447:MET:HE3 | 1.97 | 0.46 |
| 1:F:54:VAL:HG13 | 1:F:55:SER:N | 2.29 | 0.46 |
| 1:G:94:VAL:HG12 | 1:G:449:ALA:HB1 | 1.97 | 0.46 |
| 1:H:353:ILE:HA | 1:H:365:LEU:CD1 | 2.45 | 0.46 |
| 1:K:222:LEU:HD22 | 1:K:289:LEU:CD1 | 2.46 | 0.46 |
| 1:K:285:ARG:HH11 | 1:K:285:ARG:HG2 | 1.80 | 0.46 |
| 1:K:352:GLN:O | 1:K:355:GLU:OE1 | 2.33 | 0.46 |
| 1:L:144:ILE:HG21 | 1:L:163:ALA:HA | 1.96 | 0.46 |
| 1:L:233:MET:HB3 | 1:L:237:LEU:HB2 | 1.98 | 0.46 |
| 1:M:157:THR:O | 1:M:161:LEU:HD13 | 2.15 | 0.46 |
| 1:N:206:ASN:ND2 | 1:N:207:LYS:HE2 | 2.30 | 0.46 |
| 1:N:267:MET:O | 1:N:267:MET:HG3 | 2.15 | 0.46 |
| 1:N:298:GLY:HA2 | 1:N:317:LEU:O | 2.15 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:325:ILE:HG22 | 1:N:326:ASN:N | 2.29 | 0.46 |
| 2:O:73:VAL:O | 2:O:74:LYS:HD3 | 2.15 | 0.46 |
| 2:Q:47:ARG:O | 2:Q:55:LYS:HE3 | 2.15 | 0.46 |
| 2:Q:47:ARG:HB3 | 2:Q:55:LYS:HG2 | 1.97 | 0.46 |
| 2:Q:87:SER:C | 2:Q:89:SER:N | 2.67 | 0.46 |
| 2:R:11:ILE:HB | 2:R:42:ALA:HB3 | 1.98 | 0.46 |
| 2:R:59:VAL:HG23 | 2:R:59:VAL:O | 2.15 | 0.46 |
| 2:T:17:VAL:CG1 | 2:T:34:LYS:HA | 2.45 | 0.46 |
| 2:U:5:PRO:HD3 | 2:U:42:ALA:HB1 | 1.96 | 0.46 |
| 1:A:299:THR:N | 1:A:316:ASP:O | 2.48 | 0.46 |
| 1:A:315:GLU:OE1 | 1:A:316:ASP:N | 2.49 | 0.46 |
| 1:B:112:ASN:HD21 | 1:B:114:MET:HB3 | 1.79 | 0.46 |
| 1:B:4:LYS:HG3 | 1:C:59:GLU:O | 2.14 | 0.46 |
| 1:C:10:ASN:O | 1:C:14:VAL:HG23 | 2.15 | 0.46 |
| 1:C:195:PHE:CD1 | 1:C:195:PHE:C | 2.88 | 0.46 |
| 1:D:205:ILE:HD13 | 1:D:211:GLY:HA2 | 1.96 | 0.46 |
| 1:D:245:LYS:HE2 | 1:D:245:LYS:CA | 2.36 | 0.46 |
| 1:D:84:ALA:HB2 | 1:D:506:TYR:CE2 | 2.49 | 0.46 |
| 1:E:96:ALA:O | 1:E:97:GLN:C | 2.54 | 0.46 |
| 1:F:131:LEU:HD23 | 1:F:422:VAL:HG11 | 1.94 | 0.46 |
| 1:G:302:SER:C | 1:G:304:GLU:N | 2.68 | 0.46 |
| 1:G:327:LYS:N | 1:G:327:LYS:HD3 | 2.30 | 0.46 |
| 1:G:403:THR:O | 1:G:404:ARG:C | 2.54 | 0.46 |
| 1:G:433:ASN:OD1 | 1:G:436:GLN:HB2 | 2.15 | 0.46 |
| 1:G:52:ASP:OD1 | 1:G:54:VAL:HG12 | 2.16 | 0.46 |
| 1:H:402:ALA:O | 1:H:406:ALA:N | 2.32 | 0.46 |
| 1:I:417:VAL:O | 1:I:418:ALA:C | 2.53 | 0.46 |
| 1:J:222:LEU:HD11 | 1:J:293:ALA:HA | 1.97 | 0.46 |
| 1:J:336:VAL:O | 1:J:336:VAL:HG12 | 2.14 | 0.46 |
| 1:L:175:ILE:HD13 | 1:L:404:ARG:NH2 | 2.30 | 0.46 |
| 1:L:188:ASP:O | 1:L:378:VAL:HG22 | 2.15 | 0.46 |
| 1:L:7:LYS:HG3 | 1:L:66:PHE:CE2 | 2.50 | 0.46 |
| 1:M:112:ASN:HA | 1:M:113:PRO:HD3 | 1.67 | 0.46 |
| 1:N:180:GLY:HA2 | 1:N:380:LYS:HB3 | 1.97 | 0.46 |
| 1:N:433:ASN:HD22 | 1:N:434:GLU:H | 1.63 | 0.46 |
| 2:P:5:PRO:HD3 | 2:P:42:ALA:HB1 | 1.97 | 0.46 |
| 2:P:69:ASP:HA | 2:P:73:VAL:HG21 | 1.98 | 0.46 |
| 1:A:134:LEU:N | 1:A:134:LEU:CD1 | 2.78 | 0.46 |
| 1:A:253:ASP:CG | 1:A:254:VAL:N | 2.69 | 0.46 |
| 1:A:510:VAL:O | 1:A:511:ALA:C | 2.53 | 0.46 |
| 1:B:223:ALA:HB3 | 1:B:251:ALA:CB | 2.42 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:227:ILE:HG22 | 1:B:227:ILE:O | 2.14 | 0.46 |
| 1:B:95:LEU:O | 1:B:99:ILE:HG13 | 2.16 | 0.46 |
| 1:C:329:THR:HG22 | 1:C:330:THR:N | 2.30 | 0.46 |
| 1:D:280:GLY:CA | 1:D:284:ARG:HD2 | 2.46 | 0.46 |
| 1:D:309:LEU:O | 1:D:310:GLU:C | 2.53 | 0.46 |
| 1:D:313:THR:HG22 | 1:D:314:LEU:N | 2.30 | 0.46 |
| 1:D:358:SER:HA | 1:D:362:ARG:HD2 | 1.96 | 0.46 |
| 1:D:468:THR:OG1 | 1:D:485:TYR:CE2 | 2.68 | 0.46 |
| 1:D:74:VAL:O | 1:D:77:VAL:CG1 | 2.54 | 0.46 |
| 1:E:208:PRO:HD2 | 1:E:212:ALA:HB1 | 1.96 | 0.46 |
| 1:E:62:LEU:N | 1:E:62:LEU:CD1 | 2.79 | 0.46 |
| 1:F:325:ILE:N | 1:F:325:ILE:CD1 | 2.78 | 0.46 |
| 1:F:366:GLN:HA | 1:F:369:VAL:HB | 1.98 | 0.46 |
| 1:G:200:LEU:HD21 | 1:G:253:ASP:OD1 | 2.16 | 0.46 |
| 1:G:501:ARG:O | 1:G:505:GLN:HG3 | 2.15 | 0.46 |
| 1:I:353:ILE:HA | 1:I:365:LEU:HD12 | 1.97 | 0.46 |
| 1:I:66:PHE:N | 1:I:69:MET:HG3 | 2.27 | 0.46 |
| 1:J:302:SER:HB2 | 1:J:305:ILE:CG1 | 2.45 | 0.46 |
| 1:J:314:LEU:C | 1:J:316:ASP:N | 2.69 | 0.46 |
| 1:J:317:LEU:N | 1:J:317:LEU:HD12 | 2.30 | 0.46 |
| 1:J:186:GLU:OE1 | 1:J:380:LYS:HD2 | 2.14 | 0.46 |
| 1:J:433:ASN:HD22 | 1:J:434:GLU:H | 1.63 | 0.46 |
| 1:J:15:LYS:HD2 | 1:J:67:GLU:HG3 | 1.98 | 0.46 |
| 1:K:72:GLN:HE21 | 1:K:72:GLN:HA | 1.78 | 0.46 |
| 1:L:112:ASN:HA | 1:L:113:PRO:HD3 | 1.73 | 0.46 |
| 1:L:360:TYR:O | 1:L:364:LYS:HB2 | 2.15 | 0.46 |
| 1:L:399:ALA:O | 1:L:400:LEU:C | 2.54 | 0.46 |
| 1:M:284:ARG:HE | 1:M:364:LYS:NZ | 2.14 | 0.46 |
| 1:M:350:ARG:HE | 1:M:369:VAL:HG11 | 1.80 | 0.46 |
| 1:M:84:ALA:O | 1:M:498:LYS:HE2 | 2.14 | 0.46 |
| 1:N:220:ILE:N | 1:N:318:GLY:O | 2.48 | 0.46 |
| 1:A:326:ASN:HD21 | 1:A:328:ASP:HB2 | 1.79 | 0.46 |
| 1:A:421:ARG:HA | 1:A:421:ARG:HD3 | 1.76 | 0.46 |
| 1:B:199:TYR:CE2 | 1:B:205:ILE:HG12 | 2.50 | 0.46 |
| 1:C:290:GLN:O | 1:C:294:THR:HG23 | 2.15 | 0.46 |
| 1:C:357:THR:O | 1:C:359:ASP:N | 2.48 | 0.46 |
| 1:C:357:THR:HB | 1:C:361:ASP:CB | 2.45 | 0.46 |
| 1:C:438:VAL:O | 1:C:442:VAL:HG23 | 2.16 | 0.46 |
| 1:D:140:ASP:OD1 | 1:D:142:LYS:HB3 | 2.15 | 0.46 |
| 1:D:475:ASN:ND2 | 1:D:475:ASN:N | 2.63 | 0.46 |
| 1:D:87:ASP:OD1 | 1:D:88:GLY:N | 2.46 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:134:LEU:N | 1:E:134:LEU:CD1 | 2.79 | 0.46 |
| 1:E:240:VAL:O | 1:E:244:GLY:N | 2.45 | 0.46 |
| 1:F:295:LEU:C | 1:F:295:LEU:HD23 | 2.36 | 0.46 |
| 1:F:381:VAL:HG21 | 1:F:393:LYS:CA | 2.45 | 0.46 |
| 1:G:284:ARG:HG2 | 1:G:288:MET:HE1 | 1.97 | 0.46 |
| 1:G:28:LYS:O | 1:G:30:THR:N | 2.49 | 0.46 |
| 1:G:219:PHE:HB3 | 1:G:317:LEU:HD13 | 1.96 | 0.46 |
| 1:I:236:VAL:HG23 | 1:I:237:LEU:H | 1.79 | 0.46 |
| 1:K:421:ARG:HD2 | 1:K:474:GLY:O | 2.16 | 0.46 |
| 1:L:203:TYR:CB | 1:L:263:VAL:HG13 | 2.43 | 0.46 |
| 1:L:325:ILE:HG13 | 1:L:330:THR:HG23 | 1.97 | 0.46 |
| 1:L:478:TYR:HA | 1:L:485:TYR:HA | 1.98 | 0.46 |
| 1:M:247:LEU:HD22 | 1:M:248:LEU:N | 2.30 | 0.46 |
| 1:M:301:ILE:CD1 | 1:M:301:ILE:N | 2.71 | 0.46 |
| 1:M:433:ASN:HD22 | 1:M:434:GLU:H | 1.63 | 0.46 |
| 1:N:363:GLU:O | 1:N:366:GLN:HB3 | 2.15 | 0.46 |
| 1:N:494:LEU:O | 1:N:495:ASP:OD1 | 2.34 | 0.46 |
| 2:O:40:VAL:CG2 | 2:O:63:ASP:HB2 | 2.44 | 0.46 |
| 2:Q:53:GLU:N | 2:Q:53:GLU:OE1 | 2.49 | 0.46 |
| 1:A:208:PRO:HB2 | 1:A:212:ALA:CB | 2.45 | 0.46 |
| 1:A:215:LEU:HB3 | 1:A:246:PRO:CB | 2.40 | 0.46 |
| 1:A:233:MET:HE2 | 1:A:237:LEU:HB2 | 1.98 | 0.46 |
| 1:B:209:GLU:N | 1:B:209:GLU:CD | 2.69 | 0.46 |
| 1:C:430:ARG:HH11 | 1:C:430:ARG:HG2 | 1.80 | 0.46 |
| 1:D:183:LEU:O | 1:D:382:GLY:HA3 | 2.16 | 0.46 |
| 1:D:199:TYR:OH | 1:D:211:GLY:CA | 2.64 | 0.46 |
| 1:D:413:ALA:HB1 | 1:D:417:VAL:HG11 | 1.98 | 0.46 |
| 1:D:456:LEU:HD13 | 1:D:462:PRO:HG2 | 1.97 | 0.46 |
| 1:E:72:GLN:CA | 1:E:72:GLN:HE21 | 2.28 | 0.46 |
| 1:F:219:PHE:CE2 | 1:F:245:LYS:HB2 | 2.51 | 0.46 |
| 1:F:271:VAL:HG23 | 1:F:271:VAL:O | 2.16 | 0.46 |
| 1:F:353:ILE:HG22 | 1:F:354:GLU:N | 2.31 | 0.46 |
| 1:G:256:GLY:HA2 | 1:G:259:LEU:HD12 | 1.96 | 0.46 |
| 1:H:305:ILE:HG22 | 1:H:305:ILE:O | 2.16 | 0.46 |
| 1:H:314:LEU:C | 1:H:316:ASP:N | 2.69 | 0.46 |
| 1:H:433:ASN:HD22 | 1:H:434:GLU:H | 1.62 | 0.46 |
| 1:H:487:ASN:O | 1:H:491:MET:HG3 | 2.15 | 0.46 |
| 1:H:496:PRO:O | 1:H:497:THR:C | 2.53 | 0.46 |
| 1:I:494:LEU:CD2 | 1:I:494:LEU:N | 2.78 | 0.46 |
| 1:I:496:PRO:O | 1:I:497:THR:C | 2.54 | 0.46 |
| 1:J:202:PRO:C | 1:J:204:PHE:H | 2.19 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:214:GLU:HG2 | 1:J:324:VAL:CG1 | 2.45 | 0.46 |
| 1:K:420:ILE:HD13 | 1:K:448:GLU:HA | 1.98 | 0.46 |
| 1:L:270:ILE:HA | 1:M:257:GLU:OE2 | 2.16 | 0.46 |
| 1:L:287:ALA:O | 1:L:290:GLN:N | 2.49 | 0.46 |
| 1:L:433:ASN:HD22 | 1:L:434:GLU:H | 1.64 | 0.46 |
| 1:M:287:ALA:HB1 | 1:M:368:ARG:HH22 | 1.77 | 0.46 |
| 1:M:353:ILE:O | 1:M:353:ILE:HG22 | 2.16 | 0.46 |
| 1:N:102:GLU:HB2 | 1:N:442:VAL:HG13 | 1.96 | 0.46 |
| 1:N:478:TYR:HB2 | 1:N:485:TYR:CE2 | 2.50 | 0.46 |
| 1:N:69:MET:HE2 | 1:N:522:THR:HB | 1.95 | 0.46 |
| 2:Q:14:ARG:NH2 | 2:Q:69:ASP:OD2 | 2.44 | 0.46 |
| 2:Q:86:MET:HG3 | 2:Q:90:ASP:HB2 | 1.97 | 0.46 |
| 2:S:75:SER:OG | 2:S:82:GLU:OE1 | 2.34 | 0.46 |
| 2:T:84:LEU:CD1 | 2:T:84:LEU:N | 2.79 | 0.46 |
| 2:U:68:ASN:O | 2:U:70:GLY:N | 2.47 | 0.46 |
| 1:C:200:LEU:O | 1:C:202:PRO:CD | 2.63 | 0.46 |
| 1:C:421:ARG:HA | 1:C:421:ARG:HD3 | 1.76 | 0.46 |
| 1:C:510:VAL:CG2 | 1:C:511:ALA:H | 2.28 | 0.46 |
| 1:C:3:ALA:HB3 | 1:C:524:LEU:HD12 | 1.98 | 0.46 |
| 1:D:241:ALA:HA | 1:D:271:VAL:HG12 | 1.97 | 0.46 |
| 1:D:417:VAL:C | 1:D:420:ILE:HG22 | 2.36 | 0.46 |
| 1:E:128:VAL:HG12 | 1:E:132:LYS:HE2 | 1.97 | 0.46 |
| 1:E:365:LEU:HD22 | 1:E:366:GLN:NE2 | 2.30 | 0.46 |
| 1:E:417:VAL:O | 1:E:418:ALA:C | 2.54 | 0.46 |
| 1:E:452:ARG:HB2 | 1:E:462:PRO:CB | 2.40 | 0.46 |
| 1:F:346:VAL:HA | 1:F:349:ILE:HD12 | 1.97 | 0.46 |
| 1:G:428:ASP:HA | 1:G:430:ARG:HH12 | 1.81 | 0.46 |
| 1:H:197:ARG:HG2 | 1:H:277:LYS:O | 2.14 | 0.46 |
| 1:H:487:ASN:OD1 | 1:H:489:ILE:HB | 2.16 | 0.46 |
| 1:I:287:ALA:O | 1:I:290:GLN:N | 2.48 | 0.46 |
| 1:J:226:LYS:CA | 1:J:252:GLU:HB2 | 2.46 | 0.46 |
| 1:J:441:LYS:O | 1:J:442:VAL:C | 2.53 | 0.46 |
| 1:K:248:LEU:HD11 | 1:K:250:ILE:HG13 | 1.98 | 0.46 |
| 1:K:314:LEU:C | 1:K:316:ASP:N | 2.69 | 0.46 |
| 1:L:149:THR:CG2 | 1:L:159:GLY:HA3 | 2.30 | 0.46 |
| 1:L:66:PHE:HA | 1:L:520:MET:HE1 | 1.97 | 0.46 |
| 1:K:41:ASP:HB2 | 1:L:69:MET:HE2 | 1.98 | 0.46 |
| 1:M:205:ILE:HG23 | 1:M:212:ALA:O | 2.16 | 0.46 |
| 1:M:197:ARG:NE | 1:M:277:LYS:HZ3 | 2.14 | 0.46 |
| 1:N:128:VAL:O | 1:N:132:LYS:HG3 | 2.16 | 0.46 |
| 1:N:419:LEU:HD21 | 1:N:500:THR:HG23 | 1.96 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:11:ILE:HB | 2:P:42:ALA:HB3 | 1.97 | 0.46 |
| 2:R:13:LYS:HB3 | 2:R:41:LEU:HD11 | 1.97 | 0.46 |
| 2:R:73:VAL:O | 2:R:74:LYS:HD3 | 2.16 | 0.46 |
| 1:A:116:LEU:O | 1:A:120:ILE:HG13 | 2.16 | 0.46 |
| 1:A:179:ASP:OD1 | 1:A:389:MET:HG3 | 2.15 | 0.46 |
| 1:A:56:VAL:O | 1:A:57:ALA:C | 2.54 | 0.46 |
| 1:B:272:LYS:HB2 | 1:B:272:LYS:HZ2 | 1.81 | 0.46 |
| 1:B:284:ARG:HG2 | 1:B:288:MET:CE | 2.46 | 0.46 |
| 1:B:433:ASN:HD21 | 1:B:435:ASP:HB2 | 1.81 | 0.46 |
| 1:C:495:ASP:CG | 4:C:1:ADP:HO2' | 2.18 | 0.46 |
| 1:C:326:ASN:OD1 | 1:C:329:THR:N | 2.49 | 0.46 |
| 1:C:177:VAL:CG2 | 1:C:393:LYS:HG3 | 2.45 | 0.46 |
| 1:C:54:VAL:HG13 | 1:C:55:SER:N | 2.31 | 0.46 |
| 1:D:219:PHE:O | 1:D:247:LEU:HD22 | 2.15 | 0.46 |
| 1:E:321:LYS:HB2 | 1:E:333:ILE:HB | 1.96 | 0.46 |
| 1:F:258:ALA:O | 1:F:261:THR:HG23 | 2.16 | 0.46 |
| 1:F:449:ALA:O | 1:F:450:PRO:C | 2.51 | 0.46 |
| 1:F:87:ASP:OD1 | 1:F:88:GLY:N | 2.47 | 0.46 |
| 1:G:249:ILE:HG22 | 1:G:250:ILE:N | 2.31 | 0.46 |
| 1:G:255:GLU:O | 1:G:259:LEU:HG | 2.15 | 0.46 |
| 1:G:345:ARG:O | 1:G:349:ILE:HG13 | 2.16 | 0.46 |
| 1:G:355:GLU:C | 1:G:357:THR:H | 2.18 | 0.46 |
| 1:H:39:VAL:HG22 | 1:H:49:ILE:HG12 | 1.97 | 0.46 |
| 1:H:72:GLN:NE2 | 1:H:75:LYS:HD3 | 2.31 | 0.46 |
| 1:I:255:GLU:O | 1:I:256:GLY:C | 2.53 | 0.46 |
| 1:H:270:ILE:HA | 1:I:257:GLU:OE2 | 2.16 | 0.46 |
| 1:I:434:GLU:O | 1:I:438:VAL:HG23 | 2.15 | 0.46 |
| 1:I:466:ALA:O | 1:I:470:LYS:HG2 | 2.15 | 0.46 |
| 1:J:239:ALA:CB | 1:J:314:LEU:HD11 | 2.30 | 0.46 |
| 1:K:317:LEU:N | 1:K:317:LEU:HD12 | 2.31 | 0.46 |
| 1:L:421:ARG:HD2 | 1:L:474:GLY:O | 2.15 | 0.46 |
| 1:M:225:LYS:HE2 | 1:M:309:LEU:CD1 | 2.43 | 0.46 |
| 1:M:232:GLU:HA | 1:M:310:GLU:CG | 2.46 | 0.46 |
| 1:M:197:ARG:H | 1:M:329:THR:HA | 1.81 | 0.46 |
| 1:M:422:VAL:O | 1:M:426:LEU:CD2 | 2.63 | 0.46 |
| 1:M:15:LYS:HD2 | 1:M:67:GLU:HG3 | 1.97 | 0.46 |
| 1:N:203:TYR:HB2 | 1:N:263:VAL:HG13 | 1.98 | 0.46 |
| 1:N:362:ARG:HB3 | 1:N:362:ARG:HH11 | 1.80 | 0.46 |
| 1:N:434:GLU:O | 1:N:438:VAL:HG23 | 2.16 | 0.46 |
| 2:P:78:ILE:N | 2:P:78:ILE:CD1 | 2.79 | 0.46 |
| 2:R:17:VAL:HG11 | 2:R:33:ALA:O | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:206:ASN:CB | 1:A:213:VAL:HA | 2.46 | 0.46 |
| 1:A:219:PHE:CB | 1:A:317:LEU:HD13 | 2.42 | 0.46 |
| 1:A:385:THR:OG1 | 1:A:388:GLU:CB | 2.64 | 0.46 |
| 1:B:433:ASN:OD1 | 1:B:436:GLN:HB2 | 2.15 | 0.46 |
| 1:C:284:ARG:O | 1:C:287:ALA:HB3 | 2.16 | 0.46 |
| 1:D:52:ASP:OD1 | 1:D:54:VAL:HG12 | 2.16 | 0.46 |
| 1:D:69:MET:O | 1:D:73:MET:HG3 | 2.16 | 0.46 |
| 1:D:95:LEU:O | 1:D:98:ALA:HB3 | 2.15 | 0.46 |
| 1:E:206:ASN:H | 1:E:213:VAL:HA | 1.80 | 0.46 |
| 1:E:229:ASN:C | 1:E:231:ARG:H | 2.19 | 0.46 |
| 1:E:304:GLU:HB2 | 1:E:305:ILE:HD12 | 1.97 | 0.46 |
| 1:F:256:GLY:O | 1:F:257:GLU:C | 2.53 | 0.46 |
| 1:F:277:LYS:HG2 | 1:F:278:ALA:N | 2.30 | 0.46 |
| 1:F:281:PHE:H | 1:F:284:ARG:HD2 | 1.81 | 0.46 |
| 1:F:411:VAL:HG12 | 1:F:496:PRO:CA | 2.39 | 0.46 |
| 1:G:194:GLN:HG3 | 1:G:331:THR:OG1 | 2.16 | 0.46 |
| 1:G:16:MET:O | 1:G:20:VAL:HG23 | 2.16 | 0.46 |
| 1:G:210:THR:HG22 | 1:G:210:THR:O | 2.15 | 0.46 |
| 1:G:287:ALA:O | 1:G:290:GLN:NE2 | 2.44 | 0.46 |
| 1:G:409:GLU:CD | 1:G:501:ARG:HH21 | 2.18 | 0.46 |
| 1:H:277:LYS:HZ2 | 1:H:277:LYS:HB2 | 1.79 | 0.46 |
| 1:I:112:ASN:HA | 1:I:113:PRO:HD3 | 1.73 | 0.46 |
| 1:I:317:LEU:CD1 | 1:I:317:LEU:N | 2.79 | 0.46 |
| 1:I:69:MET:HE2 | 1:I:522:THR:CB | 2.38 | 0.46 |
| 1:K:303:GLU:C | 1:K:305:ILE:N | 2.68 | 0.46 |
| 1:K:69:MET:HE2 | 1:K:522:THR:HB | 1.94 | 0.46 |
| 1:L:317:LEU:N | 1:L:317:LEU:HD12 | 2.31 | 0.46 |
| 1:L:130:GLU:OE2 | 1:L:425:LYS:HB3 | 2.15 | 0.46 |
| 1:L:479:ASN:O | 1:L:483:GLU:N | 2.48 | 0.46 |
| 1:L:88:GLY:O | 1:L:89:THR:C | 2.55 | 0.46 |
| 1:N:221:LEU:HD13 | 1:N:223:ALA:N | 2.30 | 0.46 |
| 1:M:270:ILE:HG23 | 1:N:229:ASN:ND2 | 2.31 | 0.46 |
| 1:N:247:LEU:HD13 | 1:N:248:LEU:N | 2.30 | 0.46 |
| 1:N:277:LYS:HZ3 | 1:N:277:LYS:HB2 | 1.81 | 0.46 |
| 1:N:478:TYR:HA | 1:N:485:TYR:HA | 1.98 | 0.46 |
| 2:P:58:ASP:N | 2:P:88:GLU:OE2 | 2.45 | 0.46 |
| 1:A:211:GLY:O | 1:A:325:ILE:O | 2.34 | 0.46 |
| 1:A:449:ALA:HB3 | 1:A:450:PRO:CD | 2.43 | 0.46 |
| 1:A:449:ALA:O | 1:A:450:PRO:C | 2.54 | 0.46 |
| 1:A:496:PRO:HG2 | 1:A:499:VAL:CG1 | 2.45 | 0.46 |
| 1:B:177:VAL:HG22 | 1:B:393:LYS:HG3 | 1.97 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:210:THR:O | 1:B:210:THR:HG22 | 2.16 | 0.46 |
| 1:B:234:LEU:O | 1:B:238:GLU:N | 2.47 | 0.46 |
| 1:C:262:LEU:O | 1:C:266:THR:HG23 | 2.16 | 0.46 |
| 1:C:281:PHE:HB2 | 1:C:284:ARG:NH2 | 2.31 | 0.46 |
| 1:C:183:LEU:O | 1:C:382:GLY:HA3 | 2.15 | 0.46 |
| 1:C:449:ALA:HB3 | 1:C:450:PRO:CD | 2.41 | 0.46 |
| 1:D:128:VAL:HG12 | 1:D:132:LYS:HE2 | 1.98 | 0.46 |
| 1:D:200:LEU:O | 1:D:202:PRO:HD2 | 2.16 | 0.46 |
| 1:D:320:ALA:HA | 1:D:334:ASP:O | 2.16 | 0.46 |
| 1:D:474:GLY:C | 1:D:475:ASN:HD22 | 2.19 | 0.46 |
| 1:E:116:LEU:O | 1:E:120:ILE:HG13 | 2.16 | 0.46 |
| 1:E:366:GLN:HA | 1:E:369:VAL:HG21 | 1.98 | 0.46 |
| 1:E:430:ARG:HH11 | 1:E:430:ARG:HG2 | 1.80 | 0.46 |
| 1:F:88:GLY:C | 4:F:1:ADP:O2B | 2.54 | 0.46 |
| 1:F:428:ASP:C | 1:F:430:ARG:NH1 | 2.70 | 0.46 |
| 1:F:434:GLU:OE2 | 1:F:438:VAL:HG23 | 2.15 | 0.46 |
| 1:F:5:ASP:O | 1:F:66:PHE:HZ | 1.99 | 0.46 |
| 1:F:77:VAL:HG22 | 1:F:78:ALA:N | 2.31 | 0.46 |
| 1:G:209:GLU:O | 1:G:210:THR:HB | 2.16 | 0.46 |
| 1:G:350:ARG:O | 1:G:354:GLU:HG2 | 2.16 | 0.46 |
| 1:G:115:ASP:HB3 | 1:G:436:GLN:HG3 | 1.96 | 0.46 |
| 1:H:414:GLY:N | 1:H:494:LEU:HA | 2.30 | 0.46 |
| 1:H:131:LEU:CD1 | 1:H:422:VAL:HG11 | 2.45 | 0.46 |
| 1:H:422:VAL:O | 1:H:426:LEU:CD2 | 2.64 | 0.46 |
| 1:H:64:ASP:C | 1:H:65:LYS:O | 2.50 | 0.46 |
| 1:J:193:MET:CG | 1:J:194:GLN:N | 2.78 | 0.46 |
| 1:J:200:LEU:N | 1:J:200:LEU:HD12 | 2.31 | 0.46 |
| 1:K:122:LYS:O | 1:K:125:THR:HB | 2.15 | 0.46 |
| 1:K:184:GLN:HA | 1:K:184:GLN:OE1 | 2.15 | 0.46 |
| 1:K:189:VAL:HG23 | 1:K:189:VAL:O | 2.15 | 0.46 |
| 1:K:296:THR:HB | 1:K:319:GLN:N | 2.31 | 0.46 |
| 1:K:353:ILE:HD11 | 1:K:369:VAL:CG2 | 2.46 | 0.46 |
| 1:L:102:GLU:HB2 | 1:L:442:VAL:HG13 | 1.97 | 0.46 |
| 1:L:352:GLN:O | 1:L:355:GLU:OE1 | 2.34 | 0.46 |
| 1:L:131:LEU:CD1 | 1:L:422:VAL:HG11 | 2.46 | 0.46 |
| 1:M:227:ILE:HD12 | 1:M:309:LEU:HD11 | 1.97 | 0.46 |
| 1:M:391:GLU:O | 1:M:394:ALA:HB3 | 2.16 | 0.46 |
| 2:O:14:ARG:CB | 2:O:14:ARG:HH11 | 2.29 | 0.46 |
| 2:O:48:ILE:HG12 | 2:O:54:VAL:CG1 | 2.45 | 0.46 |
| 2:S:7:HIS:HA | 2:S:45:ASN:N | 2.30 | 0.46 |
| 2:S:12:VAL:CG2 | 2:S:84:LEU:HB2 | 2.45 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:279:PRO:HD2 | 1:A:285:ARG:CB | 2.46 | 0.46 |
| 1:A:305:ILE:CD1 | 1:A:305:ILE:N | 2.75 | 0.46 |
| 1:A:355:GLU:HG2 | 1:A:361:ASP:OD2 | 2.15 | 0.46 |
| 1:D:134:LEU:N | 1:D:134:LEU:HD12 | 2.31 | 0.46 |
| 1:E:267:MET:N | 1:E:267:MET:HE3 | 2.31 | 0.46 |
| 1:E:368:ARG:HD3 | 1:E:372:LEU:HD11 | 1.98 | 0.46 |
| 1:E:381:VAL:CG1 | 1:E:392:LYS:HG2 | 2.45 | 0.46 |
| 1:E:417:VAL:CA | 1:E:420:ILE:HG22 | 2.46 | 0.46 |
| 1:F:144:ILE:O | 1:F:147:VAL:HG22 | 2.16 | 0.46 |
| 1:F:433:ASN:HD21 | 1:F:435:ASP:HB2 | 1.81 | 0.46 |
| 1:G:124:VAL:HG22 | 1:G:504:LEU:HD11 | 1.98 | 0.46 |
| 1:A:385:THR:HG23 | 1:G:509:SER:OG | 2.16 | 0.46 |
| 1:H:221:LEU:HD13 | 1:H:223:ALA:H | 1.80 | 0.46 |
| 1:H:301:ILE:HD12 | 1:H:301:ILE:H | 1.80 | 0.46 |
| 1:H:353:ILE:HA | 1:H:365:LEU:HD12 | 1.98 | 0.46 |
| 1:H:362:ARG:NH1 | 1:H:362:ARG:HB3 | 2.31 | 0.46 |
| 1:J:506:TYR:O | 1:J:509:SER:HB3 | 2.16 | 0.46 |
| 1:K:302:SER:O | 1:K:305:ILE:HB | 2.16 | 0.46 |
| 1:L:218:PRO:HB3 | 1:L:246:PRO:HB2 | 1.98 | 0.46 |
| 1:L:72:GLN:NE2 | 1:L:75:LYS:HD3 | 2.30 | 0.46 |
| 1:M:363:GLU:O | 1:M:366:GLN:HB3 | 2.15 | 0.46 |
| 1:M:385:THR:CG2 | 1:M:388:GLU:H | 2.22 | 0.46 |
| 1:M:419:LEU:HD21 | 1:M:500:THR:CG2 | 2.46 | 0.46 |
| 1:N:432:GLN:OE1 | 1:N:432:GLN:N | 2.49 | 0.46 |
| 2:P:49:LEU:O | 2:P:55:LYS:NZ | 2.48 | 0.46 |
| 2:P:78:ILE:HG22 | 2:P:79:ASP:OD2 | 2.17 | 0.46 |
| 2:S:96:GLU:OE1 | 2:T:4:ARG:HB2 | 2.16 | 0.46 |
| 1:A:289:LEU:O | 1:A:290:GLN:C | 2.55 | 0.45 |
| 1:A:450:PRO:O | 1:A:454:ILE:HG13 | 2.16 | 0.45 |
| 1:B:177:VAL:HG11 | 1:B:397:GLU:CG | 2.44 | 0.45 |
| 1:B:256:GLY:O | 1:B:257:GLU:C | 2.55 | 0.45 |
| 1:B:313:THR:CG2 | 1:B:315:GLU:HG3 | 2.46 | 0.45 |
| 1:B:421:ARG:HA | 1:B:421:ARG:HD3 | 1.78 | 0.45 |
| 1:D:358:SER:HA | 1:D:362:ARG:CD | 2.46 | 0.45 |
| 1:D:77:VAL:HG22 | 1:D:78:ALA:N | 2.30 | 0.45 |
| 1:F:235:PRO:O | 1:F:239:ALA:HB2 | 2.17 | 0.45 |
| 1:F:262:LEU:O | 1:F:266:THR:HG23 | 2.15 | 0.45 |
| 1:F:281:PHE:O | 1:F:284:ARG:HB3 | 2.16 | 0.45 |
| 1:F:183:LEU:O | 1:F:382:GLY:HA3 | 2.16 | 0.45 |
| 1:F:434:GLU:O | 1:F:437:ASN:N | 2.50 | 0.45 |
| 1:G:199:TYR:HE2 | 1:G:205:ILE:HG12 | 1.79 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:434:GLU:O | 1:G:435:ASP:C | 2.54 | 0.45 |
| 1:H:286:LYS:CE | 1:H:286:LYS:HA | 2.40 | 0.45 |
| 1:H:126:ALA:HB1 | 1:H:426:LEU:HD13 | 1.97 | 0.45 |
| 1:I:101:THR:HG22 | 1:I:105:LYS:HE3 | 1.98 | 0.45 |
| 1:I:130:GLU:OE2 | 1:I:425:LYS:HB3 | 2.16 | 0.45 |
| 1:I:292:ILE:O | 1:I:293:ALA:C | 2.54 | 0.45 |
| 1:I:411:VAL:HG21 | 1:I:494:LEU:CD1 | 2.44 | 0.45 |
| 1:J:17:LEU:HA | 1:J:20:VAL:CG1 | 2.46 | 0.45 |
| 1:J:257:GLU:O | 1:J:261:THR:HG23 | 2.16 | 0.45 |
| 1:J:28:LYS:HD2 | 1:J:453:GLN:OE1 | 2.15 | 0.45 |
| 1:K:32:GLY:CA | 1:K:454:ILE:HG23 | 2.46 | 0.45 |
| 1:K:364:LYS:O | 1:K:365:LEU:C | 2.52 | 0.45 |
| 1:K:65:LYS:O | 1:K:66:PHE:CB | 2.46 | 0.45 |
| 1:L:175:ILE:N | 1:L:175:ILE:CD1 | 2.75 | 0.45 |
| 1:L:81:ALA:HA | 1:L:506:TYR:CD2 | 2.51 | 0.45 |
| 1:M:107:VAL:CG2 | 1:M:108:ALA:H | 2.29 | 0.45 |
| 1:M:225:LYS:HG3 | 1:M:227:ILE:HD13 | 1.97 | 0.45 |
| 1:M:256:GLY:HA2 | 1:M:260:ALA:H | 1.80 | 0.45 |
| 1:N:16:MET:HG3 | 1:N:520:MET:SD | 2.56 | 0.45 |
| 1:N:95:LEU:O | 1:N:96:ALA:C | 2.54 | 0.45 |
| 2:Q:41:LEU:O | 2:Q:61:VAL:HG13 | 2.16 | 0.45 |
| 2:T:50:GLU:OE2 | 2:U:51:ASN:HB3 | 2.16 | 0.45 |
| 1:A:314:LEU:HD12 | 1:A:315:GLU:H | 1.75 | 0.45 |
| 1:A:368:ARG:O | 1:A:372:LEU:HG | 2.15 | 0.45 |
| 1:B:112:ASN:ND2 | 1:B:115:ASP:H | 2.14 | 0.45 |
| 1:B:413:ALA:CB | 1:B:417:VAL:CG1 | 2.94 | 0.45 |
| 1:B:417:VAL:C | 1:B:420:ILE:HG22 | 2.35 | 0.45 |
| 1:B:487:ASN:OD1 | 1:B:489:ILE:N | 2.48 | 0.45 |
| 1:C:183:LEU:HD22 | 1:C:384:ALA:HA | 1.98 | 0.45 |
| 1:C:397:GLU:O | 1:C:398:ASP:C | 2.54 | 0.45 |
| 1:C:443:ALA:O | 1:C:447:MET:HG3 | 2.16 | 0.45 |
| 1:D:209:GLU:O | 1:D:210:THR:HB | 2.16 | 0.45 |
| 1:D:321:LYS:HD2 | 1:D:333:ILE:CG2 | 2.43 | 0.45 |
| 1:E:130:GLU:HB3 | 1:E:422:VAL:HB | 1.98 | 0.45 |
| 1:E:248:LEU:C | 1:E:248:LEU:HD13 | 2.36 | 0.45 |
| 1:E:326:ASN:ND2 | 1:E:328:ASP:N | 2.63 | 0.45 |
| 1:E:482:THR:OG1 | 1:E:484:GLU:HG2 | 2.16 | 0.45 |
| 1:E:77:VAL:HG22 | 1:E:78:ALA:N | 2.30 | 0.45 |
| 1:F:281:PHE:H | 1:F:284:ARG:NE | 2.14 | 0.45 |
| 1:F:406:ALA:HB2 | 1:F:496:PRO:HB3 | 1.99 | 0.45 |
| 1:G:31:LEU:HD12 | 4:G:1:ADP:O1A | 2.16 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:421:ARG:HA | 1:G:421:ARG:HD3 | 1.78 | 0.45 |
| 1:H:221:LEU:HB3 | 1:H:249:ILE:HA | 1.96 | 0.45 |
| 1:H:55:SER:O | 1:H:58:ARG:HB3 | 2.16 | 0.45 |
| 1:J:512:GLY:HA2 | 1:J:515:ILE:HD12 | 1.98 | 0.45 |
| 1:K:253:ASP:OD1 | 1:K:254:VAL:N | 2.38 | 0.45 |
| 1:K:472:GLY:HA3 | 1:K:476:TYR:CD2 | 2.51 | 0.45 |
| 1:L:326:ASN:O | 1:L:327:LYS:C | 2.55 | 0.45 |
| 1:M:117:LYS:HG2 | 1:M:121:ASP:OD2 | 2.17 | 0.45 |
| 1:M:197:ARG:HE | 1:M:277:LYS:HB2 | 1.81 | 0.45 |
| 1:M:232:GLU:CB | 1:M:309:LEU:HD12 | 2.45 | 0.45 |
| 1:M:425:LYS:O | 1:M:427:ALA:N | 2.48 | 0.45 |
| 1:N:37:ASN:HB3 | 1:N:51:LYS:HG3 | 1.97 | 0.45 |
| 2:O:43:VAL:CG1 | 2:O:57:LEU:HD12 | 2.46 | 0.45 |
| 1:B:270:ILE:HD13 | 2:P:27:LEU:HB2 | 1.98 | 0.45 |
| 2:Q:83:VAL:C | 2:Q:84:LEU:HD12 | 2.36 | 0.45 |
| 2:R:13:LYS:HG3 | 2:R:13:LYS:O | 2.16 | 0.45 |
| 2:R:20:LYS:HA | 2:R:28:THR:CG2 | 2.46 | 0.45 |
| 2:S:27:LEU:HD23 | 2:S:27:LEU:O | 2.16 | 0.45 |
| 1:B:295:LEU:O | 1:B:337:GLY:CA | 2.62 | 0.45 |
| 1:B:381:VAL:CG1 | 1:B:392:LYS:HG3 | 2.46 | 0.45 |
| 1:B:56:VAL:O | 1:B:57:ALA:C | 2.53 | 0.45 |
| 1:C:218:PRO:CA | 1:C:246:PRO:HG2 | 2.45 | 0.45 |
| 1:C:512:GLY:O | 1:C:515:ILE:HG12 | 2.15 | 0.45 |
| 1:D:289:LEU:N | 1:D:290:GLN:OE1 | 2.44 | 0.45 |
| 1:E:207:LYS:HB2 | 1:E:207:LYS:NZ | 2.31 | 0.45 |
| 1:E:333:ILE:O | 1:E:334:ASP:HB2 | 2.17 | 0.45 |
| 1:E:413:ALA:CB | 1:E:417:VAL:CG1 | 2.94 | 0.45 |
| 1:E:9:GLY:HA2 | 1:E:13:ARG:NH1 | 2.32 | 0.45 |
| 1:F:434:GLU:HA | 1:F:437:ASN:HD22 | 1.80 | 0.45 |
| 1:G:194:GLN:HG2 | 1:G:195:PHE:N | 2.31 | 0.45 |
| 1:G:302:SER:HB2 | 1:G:305:ILE:HB | 1.98 | 0.45 |
| 1:G:420:ILE:HD11 | 1:G:470:LYS:CG | 2.47 | 0.45 |
| 1:H:149:THR:HG22 | 1:H:156:GLU:O | 2.16 | 0.45 |
| 1:I:385:THR:CG2 | 1:I:388:GLU:HB3 | 2.47 | 0.45 |
| 1:I:65:LYS:O | 1:I:66:PHE:CB | 2.42 | 0.45 |
| 1:J:449:ALA:HB3 | 1:J:450:PRO:CD | 2.38 | 0.45 |
| 1:K:494:LEU:CD2 | 1:K:494:LEU:N | 2.78 | 0.45 |
| 1:L:191:GLU:OE1 | 1:L:342:ILE:HG21 | 2.17 | 0.45 |
| 1:M:227:ILE:O | 1:M:254:VAL:HA | 2.17 | 0.45 |
| 1:M:228:SER:HA | 1:M:255:GLU:HB2 | 1.98 | 0.45 |
| 1:M:358:SER:HB3 | 1:M:361:ASP:HB2 | 1.98 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:22:ALA:O | 2:R:26:VAL:HB | 2.16 | 0.45 |
| 2:R:47:ARG:HB3 | 2:R:55:LYS:CG | 2.46 | 0.45 |
| 2:U:5:PRO:CD | 2:U:42:ALA:HB1 | 2.45 | 0.45 |
| 2:U:76:GLU:O | 2:U:83:VAL:HG22 | 2.16 | 0.45 |
| 2:U:8:ASP:O | 2:U:87:SER:HA | 2.16 | 0.45 |
| 1:A:209:GLU:O | 1:A:210:THR:HB | 2.16 | 0.45 |
| 1:B:352:GLN:C | 1:B:365:LEU:HD11 | 2.37 | 0.45 |
| 1:B:381:VAL:CG1 | 1:B:392:LYS:HG2 | 2.45 | 0.45 |
| 1:C:215:LEU:O | 1:C:322:ARG:HA | 2.17 | 0.45 |
| 1:C:193:MET:O | 1:C:331:THR:HG23 | 2.17 | 0.45 |
| 1:C:510:VAL:O | 1:C:511:ALA:C | 2.53 | 0.45 |
| 1:D:430:ARG:HG2 | 1:D:430:ARG:NH1 | 2.32 | 0.45 |
| 1:E:128:VAL:CG1 | 1:E:132:LYS:HE2 | 2.46 | 0.45 |
| 1:E:455:VAL:O | 1:E:458:CYS:HB2 | 2.16 | 0.45 |
| 1:G:366:GLN:O | 1:G:369:VAL:HB | 2.16 | 0.45 |
| 1:G:383:ALA:N | 1:G:389:MET:HE1 | 2.31 | 0.45 |
| 1:H:190:VAL:HG21 | 1:H:334:ASP:CG | 2.37 | 0.45 |
| 1:I:219:PHE:CB | 1:I:317:LEU:HD23 | 2.46 | 0.45 |
| 1:J:399:ALA:O | 1:J:400:LEU:C | 2.54 | 0.45 |
| 1:K:220:ILE:HG23 | 1:K:248:LEU:HD12 | 1.97 | 0.45 |
| 1:K:364:LYS:HD2 | 1:K:367:GLU:OE1 | 2.15 | 0.45 |
| 1:K:175:ILE:HD13 | 1:K:404:ARG:NH2 | 2.31 | 0.45 |
| 1:L:222:LEU:HD11 | 1:L:293:ALA:HA | 1.99 | 0.45 |
| 1:L:69:MET:O | 1:L:73:MET:HG3 | 2.16 | 0.45 |
| 1:M:286:LYS:CE | 1:M:286:LYS:HA | 2.39 | 0.45 |
| 1:A:162:ILE:HG21 | 1:A:403:THR:HG21 | 1.97 | 0.45 |
| 1:A:472:GLY:HA3 | 1:A:476:TYR:HD2 | 1.80 | 0.45 |
| 1:B:88:GLY:C | 4:B:1:ADP:O2B | 2.55 | 0.45 |
| 1:B:339:GLU:HA | 1:B:342:ILE:HB | 1.97 | 0.45 |
| 1:C:347:ALA:O | 1:C:350:ARG:HG2 | 2.15 | 0.45 |
| 1:C:474:GLY:C | 1:C:475:ASN:HD22 | 2.20 | 0.45 |
| 1:D:233:MET:HE1 | 1:D:237:LEU:HB2 | 1.98 | 0.45 |
| 1:D:239:ALA:HB1 | 1:D:314:LEU:HB3 | 1.99 | 0.45 |
| 1:D:451:LEU:O | 1:D:454:ILE:HB | 2.17 | 0.45 |
| 1:E:194:GLN:HG2 | 1:E:195:PHE:N | 2.30 | 0.45 |
| 1:E:221:LEU:HD13 | 1:E:317:LEU:CD2 | 2.46 | 0.45 |
| 1:E:417:VAL:HA | 1:E:420:ILE:CG2 | 2.46 | 0.45 |
| 1:F:147:VAL:HG12 | 1:F:494:LEU:HB2 | 1.98 | 0.45 |
| 1:F:216:GLU:O | 1:F:246:PRO:HG3 | 2.17 | 0.45 |
| 1:F:465:VAL:O | 1:F:466:ALA:C | 2.55 | 0.45 |
| 1:F:485:TYR:N | 1:F:485:TYR:CD1 | 2.85 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:37:ASN:OD1 | 1:G:51:LYS:HB2 | 2.17 | 0.45 |
| 1:H:24:ALA:HA | 1:H:27:VAL:HG12 | 1.97 | 0.45 |
| 1:I:123:ALA:HB2 | 1:I:440:ILE:HG23 | 1.99 | 0.45 |
| 1:I:16:MET:HG3 | 1:I:520:MET:SD | 2.57 | 0.45 |
| 1:I:288:MET:HA | 1:I:288:MET:HE3 | 1.97 | 0.45 |
| 1:J:165:ALA:O | 1:J:168:LYS:HB2 | 2.16 | 0.45 |
| 1:J:301:ILE:N | 1:J:301:ILE:CD1 | 2.80 | 0.45 |
| 1:K:226:LYS:CA | 1:K:252:GLU:HB2 | 2.45 | 0.45 |
| 1:L:302:SER:HB2 | 1:L:305:ILE:HG13 | 1.99 | 0.45 |
| 1:L:233:MET:HE1 | 1:L:309:LEU:HD13 | 1.99 | 0.45 |
| 1:L:362:ARG:NH1 | 1:L:362:ARG:CB | 2.79 | 0.45 |
| 1:M:106:ALA:HA | 1:M:111:MET:HE1 | 1.99 | 0.45 |
| 1:M:204:PHE:CD2 | 1:M:274:ALA:HB1 | 2.52 | 0.45 |
| 1:M:232:GLU:OE1 | 1:M:232:GLU:N | 2.35 | 0.45 |
| 1:M:360:TYR:O | 1:M:364:LYS:HB2 | 2.16 | 0.45 |
| 1:N:178:GLU:O | 1:N:380:LYS:HA | 2.17 | 0.45 |
| 1:N:80:LYS:O | 1:N:83:ASP:HB2 | 2.17 | 0.45 |
| 2:O:50:GLU:OE1 | 2:P:50:GLU:HA | 2.16 | 0.45 |
| 2:O:58:ASP:N | 2:O:88:GLU:OE2 | 2.39 | 0.45 |
| 2:P:11:ILE:HG12 | 2:P:85:ILE:HG12 | 1.99 | 0.45 |
| 2:R:60:LYS:N | 2:R:63:ASP:OD2 | 2.50 | 0.45 |
| 2:T:14:ARG:CB | 2:T:14:ARG:NH1 | 2.80 | 0.45 |
| 2:T:68:ASN:HD22 | 2:U:74:LYS:CE | 2.27 | 0.45 |
| 1:A:232:GLU:O | 1:A:310:GLU:OE2 | 2.35 | 0.45 |
| 1:B:23:LEU:C | 1:B:23:LEU:CD1 | 2.84 | 0.45 |
| 1:C:302:SER:O | 1:C:305:ILE:N | 2.47 | 0.45 |
| 1:D:308:GLU:O | 1:D:309:LEU:O | 2.35 | 0.45 |
| 1:E:295:LEU:CD2 | 1:E:295:LEU:C | 2.84 | 0.45 |
| 1:E:348:GLN:NE2 | 1:E:352:GLN:HE22 | 2.12 | 0.45 |
| 1:E:499:VAL:CG2 | 1:E:500:THR:H | 2.30 | 0.45 |
| 1:F:250:ILE:O | 1:F:251:ALA:HB2 | 2.17 | 0.45 |
| 1:F:321:LYS:HG3 | 1:F:334:ASP:HB3 | 1.98 | 0.45 |
| 1:H:354:GLU:CG | 1:H:355:GLU:N | 2.79 | 0.45 |
| 1:I:219:PHE:HA | 1:I:319:GLN:HG2 | 1.99 | 0.45 |
| 1:I:228:SER:HA | 1:I:255:GLU:HB2 | 1.97 | 0.45 |
| 1:J:227:ILE:HD12 | 1:J:309:LEU:HD11 | 1.98 | 0.45 |
| 1:J:323:VAL:HG23 | 1:J:331:THR:O | 2.16 | 0.45 |
| 1:K:363:GLU:O | 1:K:366:GLN:HB3 | 2.17 | 0.45 |
| 1:K:475:ASN:ND2 | 1:K:489:ILE:HD12 | 2.31 | 0.45 |
| 1:L:84:ALA:O | 1:L:498:LYS:HE2 | 2.16 | 0.45 |
| 1:M:30:THR:HB | 1:M:51:LYS:O | 2.16 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:192:GLY:C | 1:N:376:VAL:HG23 | 2.37 | 0.45 |
| 1:N:77:VAL:HG11 | 1:N:510:VAL:HB | 1.99 | 0.45 |
| 2:O:14:ARG:CB | 2:O:14:ARG:NH1 | 2.80 | 0.45 |
| 2:O:37:ARG:NH1 | 2:O:37:ARG:HG2 | 2.29 | 0.45 |
| 2:R:37:ARG:NH1 | 2:R:37:ARG:HG2 | 2.32 | 0.45 |
| 2:S:57:LEU:HD22 | 2:S:88:GLU:HB2 | 1.98 | 0.45 |
| 1:A:150:ILE:HG23 | 1:A:151:SER:N | 2.32 | 0.45 |
| 1:A:285:ARG:HG3 | 1:A:286:LYS:HG3 | 1.99 | 0.45 |
| 1:B:285:ARG:O | 1:B:289:LEU:HG | 2.17 | 0.45 |
| 1:B:309:LEU:N | 1:B:309:LEU:HD12 | 2.31 | 0.45 |
| 1:B:417:VAL:CA | 1:B:420:ILE:HG22 | 2.47 | 0.45 |
| 1:C:304:GLU:C | 1:C:305:ILE:HD12 | 2.36 | 0.45 |
| 1:D:219:PHE:CE2 | 1:D:245:LYS:HB2 | 2.52 | 0.45 |
| 1:D:434:GLU:O | 1:D:437:ASN:N | 2.49 | 0.45 |
| 1:E:267:MET:HA | 1:E:267:MET:CE | 2.46 | 0.45 |
| 1:E:329:THR:CG2 | 1:E:330:THR:N | 2.80 | 0.45 |
| 1:E:400:LEU:O | 1:E:400:LEU:HD13 | 2.16 | 0.45 |
| 1:F:215:LEU:C | 1:F:322:ARG:HG3 | 2.37 | 0.45 |
| 1:F:219:PHE:O | 1:F:247:LEU:HD22 | 2.17 | 0.45 |
| 1:G:178:GLU:CD | 1:G:378:VAL:HG11 | 2.36 | 0.45 |
| 1:G:315:GLU:OE1 | 1:G:316:ASP:N | 2.49 | 0.45 |
| 1:G:362:ARG:O | 1:G:366:GLN:OE1 | 2.34 | 0.45 |
| 1:G:183:LEU:HD22 | 1:G:384:ALA:HA | 1.99 | 0.45 |
| 1:H:104:LEU:HD12 | 1:H:104:LEU:HA | 1.72 | 0.45 |
| 1:H:230:ILE:CG1 | 1:H:258:ALA:HA | 2.23 | 0.45 |
| 1:I:259:LEU:C | 1:I:259:LEU:HD23 | 2.37 | 0.45 |
| 1:I:422:VAL:HG23 | 1:I:423:ALA:N | 2.32 | 0.45 |
| 1:J:303:GLU:C | 1:J:305:ILE:H | 2.20 | 0.45 |
| 1:J:324:VAL:HG22 | 1:J:331:THR:HG23 | 1.98 | 0.45 |
| 1:K:214:GLU:HG2 | 1:K:324:VAL:HG12 | 1.99 | 0.45 |
| 1:K:191:GLU:HG3 | 1:K:339:GLU:OE2 | 2.17 | 0.45 |
| 1:L:65:LYS:O | 1:L:66:PHE:CB | 2.51 | 0.45 |
| 1:M:205:ILE:CA | 1:M:213:VAL:HG22 | 2.39 | 0.45 |
| 1:M:233:MET:HE1 | 1:M:309:LEU:HD13 | 1.98 | 0.45 |
| 1:M:385:THR:CG2 | 1:M:388:GLU:HB3 | 2.47 | 0.45 |
| 2:P:12:VAL:HG23 | 2:P:84:LEU:HB2 | 1.98 | 0.45 |
| 2:P:17:VAL:CG2 | 2:P:34:LYS:HD2 | 2.46 | 0.45 |
| 2:P:60:LYS:N | 2:P:63:ASP:OD2 | 2.50 | 0.45 |
| 2:R:17:VAL:CG1 | 2:R:33:ALA:O | 2.64 | 0.45 |
| 2:R:40:VAL:HG12 | 2:R:61:VAL:HA | 1.99 | 0.45 |
| 1:A:310:GLU:CD | 1:A:310:GLU:N | 2.63 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:214:GLU:HA | 1:A:323:VAL:O | 2.16 | 0.45 |
| 1:A:39:VAL:HG23 | 1:G:517:THR:HG23 | 1.99 | 0.45 |
| 1:B:95:LEU:O | 1:B:98:ALA:HB3 | 2.17 | 0.45 |
| 1:C:205:ILE:HD13 | 1:C:211:GLY:HA2 | 1.97 | 0.45 |
| 1:C:249:ILE:HD13 | 1:C:274:ALA:O | 2.16 | 0.45 |
| 1:C:325:ILE:CG1 | 1:C:330:THR:HG23 | 2.40 | 0.45 |
| 1:D:302:SER:O | 1:D:304:GLU:N | 2.49 | 0.45 |
| 1:D:360:TYR:CE1 | 1:D:364:LYS:HD3 | 2.52 | 0.45 |
| 1:D:9:GLY:HA2 | 1:D:13:ARG:HH12 | 1.82 | 0.45 |
| 1:E:198:GLY:HA3 | 1:E:327:LYS:C | 2.38 | 0.45 |
| 1:F:160:LYS:HE3 | 1:F:164:GLU:OE2 | 2.16 | 0.45 |
| 1:F:266:THR:HG22 | 1:F:273:VAL:N | 2.31 | 0.45 |
| 1:F:326:ASN:ND2 | 1:F:328:ASP:N | 2.65 | 0.45 |
| 1:G:113:PRO:O | 1:G:116:LEU:HB2 | 2.17 | 0.45 |
| 1:G:183:LEU:O | 1:G:382:GLY:HA3 | 2.17 | 0.45 |
| 1:G:478:TYR:CE2 | 1:G:480:ALA:HA | 2.52 | 0.45 |
| 1:H:187:LEU:HD23 | 1:H:187:LEU:C | 2.37 | 0.45 |
| 1:H:233:MET:SD | 1:H:233:MET:N | 2.90 | 0.45 |
| 1:I:298:GLY:HA2 | 1:I:317:LEU:O | 2.17 | 0.45 |
| 1:I:513:LEU:HD12 | 1:I:513:LEU:HA | 1.70 | 0.45 |
| 1:J:55:SER:O | 1:J:58:ARG:HB3 | 2.16 | 0.45 |
| 1:K:183:LEU:HD22 | 1:L:360:TYR:CE2 | 2.51 | 0.45 |
| 1:K:204:PHE:CD2 | 1:K:274:ALA:HB1 | 2.52 | 0.45 |
| 1:K:336:VAL:O | 1:K:336:VAL:HG12 | 2.16 | 0.45 |
| 1:K:448:GLU:HB3 | 1:K:452:ARG:HD2 | 1.99 | 0.45 |
| 1:K:74:VAL:O | 1:K:75:LYS:C | 2.54 | 0.45 |
| 1:K:88:GLY:O | 1:K:89:THR:C | 2.55 | 0.45 |
| 1:L:219:PHE:CB | 1:L:317:LEU:HD23 | 2.47 | 0.45 |
| 1:L:37:ASN:HB3 | 1:L:51:LYS:CG | 2.47 | 0.45 |
| 1:M:209:GLU:HA | 1:M:209:GLU:OE1 | 2.17 | 0.45 |
| 1:M:17:LEU:HA | 1:M:20:VAL:CG1 | 2.47 | 0.45 |
| 1:M:272:LYS:HE3 | 1:M:272:LYS:HB2 | 1.78 | 0.45 |
| 1:H:516:THR:O | 1:N:36:ARG:HB3 | 2.17 | 0.45 |
| 1:N:389:MET:C | 1:N:389:MET:CE | 2.85 | 0.45 |
| 2:O:7:HIS:O | 2:O:8:ASP:CB | 2.60 | 0.45 |
| 2:S:34:LYS:HG3 | 2:S:35:SER:N | 2.29 | 0.45 |
| 2:U:53:GLU:OE1 | 2:U:53:GLU:N | 2.50 | 0.45 |
| 1:A:352:GLN:C | 1:A:365:LEU:HD11 | 2.37 | 0.45 |
| 1:A:365:LEU:O | 1:A:369:VAL:HG23 | 2.16 | 0.45 |
| 1:A:486:GLY:HA3 | 1:A:491:MET:CE | 2.46 | 0.45 |
| 1:A:74:VAL:O | 1:A:77:VAL:CG1 | 2.59 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:293:ALA:HB1 | 1:B:298:GLY:O | 2.17 | 0.45 |
| 1:B:305:ILE:CG2 | 1:B:306:GLY:H | 2.09 | 0.45 |
| 1:B:353:ILE:HG22 | 1:B:354:GLU:N | 2.32 | 0.45 |
| 1:C:158:VAL:O | 1:C:159:GLY:C | 2.55 | 0.45 |
| 1:D:421:ARG:HD3 | 1:D:421:ARG:HA | 1.73 | 0.45 |
| 1:E:385:THR:OG1 | 1:E:388:GLU:HB2 | 2.16 | 0.45 |
| 1:E:449:ALA:O | 1:E:450:PRO:C | 2.53 | 0.45 |
| 1:E:150:ILE:HD13 | 1:E:493:ILE:HA | 1.99 | 0.45 |
| 1:F:227:ILE:CD1 | 1:F:227:ILE:N | 2.78 | 0.45 |
| 1:G:215:LEU:C | 1:G:322:ARG:HG3 | 2.37 | 0.45 |
| 1:F:69:MET:SD | 1:G:41:ASP:HB2 | 2.57 | 0.45 |
| 1:G:486:GLY:CA | 1:G:491:MET:CE | 2.94 | 0.45 |
| 1:J:104:LEU:HA | 1:J:104:LEU:HD12 | 1.75 | 0.45 |
| 1:J:128:VAL:O | 1:J:132:LYS:HG3 | 2.17 | 0.45 |
| 1:J:287:ALA:O | 1:J:288:MET:C | 2.55 | 0.45 |
| 1:J:433:ASN:HD22 | 1:J:434:GLU:N | 2.14 | 0.45 |
| 1:J:64:ASP:C | 1:J:65:LYS:O | 2.51 | 0.45 |
| 1:K:219:PHE:CE1 | 1:K:245:LYS:HD2 | 2.52 | 0.45 |
| 1:K:232:GLU:HA | 1:K:310:GLU:HG3 | 1.99 | 0.45 |
| 1:K:190:VAL:HG21 | 1:K:334:ASP:CG | 2.36 | 0.45 |
| 1:K:186:GLU:OE1 | 1:K:380:LYS:HD2 | 2.17 | 0.45 |
| 1:L:104:LEU:O | 1:L:107:VAL:HG22 | 2.16 | 0.45 |
| 1:L:130:GLU:O | 1:L:133:ALA:HB3 | 2.16 | 0.45 |
| 1:M:191:GLU:HB3 | 1:M:295:LEU:HD11 | 1.98 | 0.45 |
| 1:M:287:ALA:O | 1:M:290:GLN:N | 2.50 | 0.45 |
| 1:M:325:ILE:N | 1:M:325:ILE:CD1 | 2.78 | 0.45 |
| 1:M:411:VAL:CG2 | 1:M:494:LEU:HD12 | 2.42 | 0.45 |
| 1:N:299:THR:N | 1:N:316:ASP:O | 2.32 | 0.45 |
| 2:U:5:PRO:HB2 | 2:U:9:ARG:O | 2.17 | 0.45 |
| 1:A:267:MET:O | 1:A:269:GLY:N | 2.50 | 0.45 |
| 1:A:347:ALA:O | 1:A:350:ARG:HG2 | 2.16 | 0.45 |
| 1:B:117:LYS:HG2 | 1:B:121:ASP:OD2 | 2.17 | 0.45 |
| 1:B:397:GLU:O | 1:B:398:ASP:C | 2.55 | 0.45 |
| 1:C:72:GLN:HA | 1:C:72:GLN:NE2 | 2.31 | 0.45 |
| 1:C:84:ALA:CB | 1:C:506:TYR:HE2 | 2.29 | 0.45 |
| 1:D:203:TYR:CD1 | 1:D:203:TYR:N | 2.80 | 0.45 |
| 1:D:232:GLU:O | 1:D:310:GLU:OE2 | 2.35 | 0.45 |
| 1:E:56:VAL:O | 1:E:57:ALA:C | 2.55 | 0.45 |
| 1:E:66:PHE:O | 1:E:67:GLU:C | 2.55 | 0.45 |
| 1:F:240:VAL:C | 1:F:242:LYS:N | 2.69 | 0.45 |
| 1:F:409:GLU:OE1 | 1:F:501:ARG:NH2 | 2.50 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:478:TYR:CE2 | 1:F:480:ALA:HA | 2.52 | 0.45 |
| 1:G:216:GLU:OE1 | 1:G:216:GLU:HA | 2.17 | 0.45 |
| 1:H:222:LEU:HD22 | 1:H:289:LEU:HD11 | 1.97 | 0.45 |
| 1:I:166:MET:O | 1:I:170:GLY:CA | 2.65 | 0.45 |
| 1:H:384:ALA:O | 1:I:281:PHE:HZ | 1.99 | 0.45 |
| 1:J:37:ASN:HB3 | 1:J:51:LYS:HG2 | 1.99 | 0.45 |
| 1:K:426:LEU:HD23 | 1:K:426:LEU:N | 2.14 | 0.45 |
| 1:L:197:ARG:HG2 | 1:L:277:LYS:O | 2.17 | 0.45 |
| 1:L:37:ASN:N | 1:L:37:ASN:HD22 | 2.12 | 0.45 |
| 1:L:186:GLU:HB2 | 1:L:380:LYS:HB2 | 1.99 | 0.45 |
| 1:M:232:GLU:HA | 1:M:310:GLU:HG2 | 1.99 | 0.45 |
| 1:M:420:ILE:CD1 | 1:M:448:GLU:HG2 | 2.47 | 0.45 |
| 1:N:77:VAL:HG22 | 1:N:506:TYR:HB3 | 1.98 | 0.45 |
| 1:A:112:ASN:ND2 | 1:A:115:ASP:H | 2.15 | 0.44 |
| 1:A:219:PHE:HE2 | 1:A:245:LYS:HB2 | 1.80 | 0.44 |
| 1:A:180:GLY:HA2 | 1:A:380:LYS:HB3 | 1.98 | 0.44 |
| 1:A:112:ASN:N | 1:A:435:ASP:OD2 | 2.40 | 0.44 |
| 1:A:438:VAL:O | 1:A:442:VAL:HG23 | 2.17 | 0.44 |
| 1:A:54:VAL:HG13 | 1:A:55:SER:N | 2.32 | 0.44 |
| 1:B:88:GLY:CA | 4:B:1:ADP:O2B | 2.64 | 0.44 |
| 1:C:148:GLY:HA2 | 1:C:399:ALA:HB1 | 1.99 | 0.44 |
| 1:B:509:SER:CB | 1:C:385:THR:HG23 | 2.47 | 0.44 |
| 1:C:452:ARG:HB2 | 1:C:462:PRO:CB | 2.36 | 0.44 |
| 1:C:493:ILE:C | 1:C:494:LEU:HD23 | 2.37 | 0.44 |
| 1:D:41:ASP:O | 1:D:42:LYS:HG3 | 2.16 | 0.44 |
| 1:D:496:PRO:CG | 1:D:499:VAL:HG13 | 2.47 | 0.44 |
| 1:D:6:VAL:HG12 | 1:D:521:VAL:HG22 | 2.00 | 0.44 |
| 1:D:86:GLY:O | 1:D:87:ASP:HB2 | 2.16 | 0.44 |
| 1:E:368:ARG:O | 1:E:372:LEU:N | 2.46 | 0.44 |
| 1:F:302:SER:O | 1:F:304:GLU:N | 2.50 | 0.44 |
| 1:F:409:GLU:OE2 | 1:F:498:LYS:HA | 2.17 | 0.44 |
| 1:F:84:ALA:HB2 | 1:F:506:TYR:CE2 | 2.51 | 0.44 |
| 1:G:207:LYS:NZ | 1:G:207:LYS:CB | 2.77 | 0.44 |
| 1:G:304:GLU:HB2 | 1:G:305:ILE:HD12 | 1.99 | 0.44 |
| 1:G:346:VAL:HG12 | 1:G:350:ARG:NH2 | 2.31 | 0.44 |
| 1:G:357:THR:HG21 | 1:G:361:ASP:HB2 | 1.98 | 0.44 |
| 1:H:126:ALA:CB | 1:H:426:LEU:HD13 | 2.47 | 0.44 |
| 1:H:265:ASN:OD1 | 1:H:271:VAL:O | 2.34 | 0.44 |
| 1:H:308:GLU:OE2 | 1:H:310:GLU:HG3 | 2.17 | 0.44 |
| 1:H:217:SER:N | 1:H:321:LYS:O | 2.48 | 0.44 |
| 1:I:223:ALA:HB3 | 1:I:251:ALA:CB | 2.41 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:264:VAL:HA | 1:I:267:MET:CG | 2.47 | 0.44 |
| 1:J:305:ILE:O | 1:J:305:ILE:HG22 | 2.16 | 0.44 |
| 1:K:216:GLU:HA | 1:K:216:GLU:OE1 | 2.17 | 0.44 |
| 1:K:102:GLU:HB2 | 1:K:442:VAL:HG13 | 1.98 | 0.44 |
| 1:K:449:ALA:HB3 | 1:K:450:PRO:CD | 2.39 | 0.44 |
| 1:L:324:VAL:C | 1:L:325:ILE:HD12 | 2.36 | 0.44 |
| 1:L:422:VAL:O | 1:L:426:LEU:CD2 | 2.64 | 0.44 |
| 1:L:441:LYS:O | 1:L:442:VAL:C | 2.54 | 0.44 |
| 1:M:222:LEU:HD22 | 1:M:289:LEU:HD11 | 1.99 | 0.44 |
| 1:M:64:ASP:OD1 | 1:M:65:LYS:O | 2.35 | 0.44 |
| 1:N:175:ILE:CD1 | 1:N:175:ILE:N | 2.78 | 0.44 |
| 2:O:64:ILE:O | 2:O:94:ILE:HG23 | 2.17 | 0.44 |
| 2:P:14:ARG:CB | 2:P:14:ARG:NH1 | 2.80 | 0.44 |
| 2:P:67:PHE:C | 2:P:67:PHE:CD1 | 2.90 | 0.44 |
| 1:A:127:ALA:O | 1:A:131:LEU:HG | 2.17 | 0.44 |
| 1:A:153:ASN:C | 1:A:153:ASN:HD22 | 2.20 | 0.44 |
| 1:A:263:VAL:O | 1:A:267:MET:SD | 2.75 | 0.44 |
| 1:A:313:THR:HG22 | 1:A:315:GLU:HG3 | 1.99 | 0.44 |
| 1:A:59:GLU:OE1 | 1:A:59:GLU:HA | 2.17 | 0.44 |
| 1:B:206:ASN:HB2 | 1:B:214:GLU:H | 1.80 | 0.44 |
| 1:B:438:VAL:O | 1:B:442:VAL:HG23 | 2.17 | 0.44 |
| 1:B:74:VAL:O | 1:B:77:VAL:CG1 | 2.59 | 0.44 |
| 1:C:280:GLY:CA | 1:C:284:ARG:HD2 | 2.47 | 0.44 |
| 1:D:325:ILE:HG22 | 1:D:326:ASN:O | 2.17 | 0.44 |
| 1:F:281:PHE:H | 1:F:284:ARG:CD | 2.29 | 0.44 |
| 1:F:325:ILE:CG1 | 1:F:330:THR:HG23 | 2.44 | 0.44 |
| 1:F:358:SER:HA | 1:F:362:ARG:HG3 | 2.00 | 0.44 |
| 1:G:313:THR:HG22 | 1:G:314:LEU:N | 2.31 | 0.44 |
| 1:G:364:LYS:O | 1:G:367:GLU:HB3 | 2.16 | 0.44 |
| 1:G:174:VAL:HG23 | 1:G:370:ALA:CB | 2.48 | 0.44 |
| 1:G:185:ASP:HA | 1:G:380:LYS:O | 2.17 | 0.44 |
| 1:G:72:GLN:HE21 | 1:G:72:GLN:CA | 2.30 | 0.44 |
| 1:H:434:GLU:HA | 1:H:437:ASN:HD22 | 1.81 | 0.44 |
| 1:I:155:ASP:CG | 1:I:158:VAL:HG23 | 2.38 | 0.44 |
| 1:I:194:GLN:HG3 | 1:I:331:THR:HB | 1.98 | 0.44 |
| 1:I:77:VAL:HG11 | 1:I:510:VAL:HB | 1.99 | 0.44 |
| 1:J:164:GLU:O | 1:J:167:ASP:HB3 | 2.16 | 0.44 |
| 1:J:226:LYS:HG3 | 1:J:252:GLU:CB | 2.47 | 0.44 |
| 1:J:317:LEU:N | 1:J:317:LEU:CD1 | 2.80 | 0.44 |
| 1:I:47:PRO:HG3 | 1:J:73:MET:HG3 | 1.99 | 0.44 |
| 1:K:117:LYS:HG2 | 1:K:121:ASP:OD2 | 2.16 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:157:THR:O | 1:K:161:LEU:CD1 | 2.65 | 0.44 |
| 1:K:199:TYR:CZ | 1:K:327:LYS:HA | 2.52 | 0.44 |
| 1:L:101:THR:HG22 | 1:L:105:LYS:HE3 | 1.98 | 0.44 |
| 1:L:247:LEU:HB3 | 1:L:273:VAL:HG11 | 1.99 | 0.44 |
| 1:L:313:THR:HG22 | 1:L:314:LEU:H | 1.83 | 0.44 |
| 1:L:370:ALA:O | 1:L:371:LYS:C | 2.56 | 0.44 |
| 1:L:417:VAL:O | 1:L:418:ALA:C | 2.55 | 0.44 |
| 1:M:106:ALA:HA | 1:M:111:MET:CE | 2.48 | 0.44 |
| 1:M:128:VAL:O | 1:M:132:LYS:HG3 | 2.17 | 0.44 |
| 1:M:349:ILE:O | 1:M:352:GLN:HB2 | 2.17 | 0.44 |
| 1:N:200:LEU:HD13 | 1:N:275:ALA:O | 2.17 | 0.44 |
| 2:O:17:VAL:CG1 | 2:O:33:ALA:O | 2.65 | 0.44 |
| 2:O:48:ILE:HG23 | 2:O:54:VAL:CG2 | 2.42 | 0.44 |
| 2:R:20:LYS:HG2 | 2:R:27:LEU:HD23 | 1.98 | 0.44 |
| 2:S:14:ARG:NH2 | 2:S:69:ASP:OD2 | 2.50 | 0.44 |
| 2:T:14:ARG:CG | 2:T:15:LYS:H | 2.29 | 0.44 |
| 1:A:128:VAL:HG12 | 1:A:132:LYS:HE2 | 1.98 | 0.44 |
| 1:A:208:PRO:C | 1:A:212:ALA:HB3 | 2.38 | 0.44 |
| 1:A:238:GLU:CB | 2:O:23:GLY:O | 2.65 | 0.44 |
| 1:A:417:VAL:O | 1:A:418:ALA:C | 2.56 | 0.44 |
| 1:A:94:VAL:HG12 | 1:A:449:ALA:HB1 | 1.98 | 0.44 |
| 1:B:199:TYR:HE1 | 1:B:327:LYS:HG3 | 1.82 | 0.44 |
| 1:A:509:SER:CB | 1:B:385:THR:HG23 | 2.47 | 0.44 |
| 1:B:417:VAL:O | 1:B:420:ILE:CG2 | 2.58 | 0.44 |
| 1:C:210:THR:O | 1:C:210:THR:HG22 | 2.17 | 0.44 |
| 1:C:216:GLU:O | 1:C:246:PRO:HG3 | 2.16 | 0.44 |
| 1:C:338:GLU:O | 1:C:341:ALA:HB3 | 2.17 | 0.44 |
| 1:C:349:ILE:HG22 | 1:C:349:ILE:O | 2.16 | 0.44 |
| 1:C:147:VAL:CG2 | 1:C:403:THR:HG22 | 2.48 | 0.44 |
| 1:D:209:GLU:O | 1:D:210:THR:CB | 2.65 | 0.44 |
| 1:D:249:ILE:CG2 | 1:D:250:ILE:N | 2.80 | 0.44 |
| 1:D:325:ILE:CG1 | 1:D:330:THR:HG23 | 2.48 | 0.44 |
| 1:E:134:LEU:HD11 | 1:E:425:LYS:NZ | 2.33 | 0.44 |
| 1:E:225:LYS:C | 1:E:252:GLU:HB2 | 2.38 | 0.44 |
| 1:E:436:GLN:O | 1:E:440:ILE:HG13 | 2.17 | 0.44 |
| 1:E:466:ALA:O | 1:E:470:LYS:HG3 | 2.18 | 0.44 |
| 1:E:510:VAL:CG2 | 1:E:511:ALA:H | 2.30 | 0.44 |
| 1:F:302:SER:HB2 | 1:F:305:ILE:CD1 | 2.44 | 0.44 |
| 1:G:368:ARG:CD | 1:G:372:LEU:HD11 | 2.48 | 0.44 |
| 1:G:78:ALA:O | 1:G:89:THR:HG22 | 2.18 | 0.44 |
| 1:H:193:MET:CG | 1:H:194:GLN:H | 2.29 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:40:LEU:HD22 | 1:H:40:LEU:N | 2.32 | 0.44 |
| 1:H:131:LEU:HD12 | 1:H:422:VAL:HG11 | 1.98 | 0.44 |
| 1:H:496:PRO:HB2 | 1:H:499:VAL:HG13 | 1.99 | 0.44 |
| 1:H:95:LEU:O | 1:H:98:ALA:HB3 | 2.17 | 0.44 |
| 1:J:117:LYS:HG2 | 1:J:121:ASP:OD2 | 2.17 | 0.44 |
| 1:J:247:LEU:HD22 | 1:J:248:LEU:N | 2.32 | 0.44 |
| 1:J:325:ILE:N | 1:J:325:ILE:CD1 | 2.80 | 0.44 |
| 1:J:344:GLY:O | 1:J:347:ALA:HB3 | 2.18 | 0.44 |
| 1:K:248:LEU:HD13 | 1:K:248:LEU:C | 2.37 | 0.44 |
| 1:K:214:GLU:HG2 | 1:K:324:VAL:CG1 | 2.47 | 0.44 |
| 1:K:90:THR:O | 1:K:93:THR:HB | 2.17 | 0.44 |
| 1:L:149:THR:HG21 | 1:L:156:GLU:HA | 2.00 | 0.44 |
| 1:L:158:VAL:O | 1:L:159:GLY:C | 2.56 | 0.44 |
| 1:L:308:GLU:CB | 1:L:311:LYS:HD3 | 2.32 | 0.44 |
| 1:L:345:ARG:O | 1:L:348:GLN:HB2 | 2.17 | 0.44 |
| 1:M:200:LEU:N | 1:M:200:LEU:HD12 | 2.32 | 0.44 |
| 1:M:421:ARG:HA | 1:M:421:ARG:NE | 2.32 | 0.44 |
| 1:M:66:PHE:HA | 1:M:520:MET:HE1 | 1.99 | 0.44 |
| 1:M:66:PHE:CD1 | 1:M:520:MET:HE2 | 2.49 | 0.44 |
| 1:N:240:VAL:HA | 1:N:243:ALA:HB3 | 2.00 | 0.44 |
| 2:P:4:ARG:HA | 2:P:5:PRO:HD2 | 1.88 | 0.44 |
| 2:Q:69:ASP:HA | 2:Q:73:VAL:HG21 | 1.99 | 0.44 |
| 2:T:58:ASP:N | 2:T:88:GLU:OE2 | 2.36 | 0.44 |
| 1:A:144:ILE:O | 1:A:147:VAL:HG22 | 2.16 | 0.44 |
| 1:A:24:ALA:O | 1:A:28:LYS:HG3 | 2.18 | 0.44 |
| 1:A:62:LEU:CD1 | 1:A:62:LEU:N | 2.81 | 0.44 |
| 1:B:290:GLN:O | 1:B:294:THR:N | 2.49 | 0.44 |
| 1:C:219:PHE:HE2 | 1:C:245:LYS:HB2 | 1.81 | 0.44 |
| 1:C:270:ILE:HD11 | 2:Q:27:LEU:HD13 | 1.98 | 0.44 |
| 1:D:368:ARG:O | 1:D:372:LEU:N | 2.50 | 0.44 |
| 1:D:417:VAL:CA | 1:D:420:ILE:HG22 | 2.47 | 0.44 |
| 1:D:420:ILE:HD11 | 1:D:470:LYS:CG | 2.47 | 0.44 |
| 1:E:291:ASP:HB2 | 1:E:372:LEU:CD2 | 2.46 | 0.44 |
| 1:E:325:ILE:HG22 | 1:E:326:ASN:N | 2.31 | 0.44 |
| 1:E:86:GLY:O | 1:E:87:ASP:HB2 | 2.18 | 0.44 |
| 1:F:128:VAL:HG12 | 1:F:132:LYS:HE2 | 1.98 | 0.44 |
| 1:F:218:PRO:HA | 1:F:246:PRO:O | 2.18 | 0.44 |
| 1:F:417:VAL:O | 1:F:420:ILE:CG2 | 2.60 | 0.44 |
| 1:F:65:LYS:O | 1:F:69:MET:HG3 | 2.17 | 0.44 |
| 1:G:202:PRO:O | 1:G:205:ILE:HG13 | 2.17 | 0.44 |
| 1:G:221:LEU:HD13 | 1:G:317:LEU:CD2 | 2.47 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:430:ARG:HG2 | 1:G:430:ARG:HH11 | 1.82 | 0.44 |
| 1:G:70:GLY:O | 1:G:74:VAL:HG22 | 2.18 | 0.44 |
| 1:H:443:ALA:O | 1:H:447:MET:HG3 | 2.17 | 0.44 |
| 1:I:175:ILE:N | 1:I:175:ILE:CD1 | 2.78 | 0.44 |
| 1:I:214:GLU:HA | 1:I:324:VAL:HG12 | 1.99 | 0.44 |
| 1:J:231:ARG:O | 1:J:234:LEU:HG | 2.18 | 0.44 |
| 1:K:66:PHE:N | 1:K:69:MET:HG3 | 2.29 | 0.44 |
| 1:L:101:THR:O | 1:L:105:LYS:HG3 | 2.17 | 0.44 |
| 1:L:349:ILE:O | 1:L:352:GLN:HB2 | 2.17 | 0.44 |
| 1:L:421:ARG:NH2 | 1:L:469:VAL:O | 2.48 | 0.44 |
| 1:N:194:GLN:HG3 | 1:N:330:THR:O | 2.18 | 0.44 |
| 1:N:37:ASN:N | 1:N:37:ASN:ND2 | 2.64 | 0.44 |
| 1:N:391:GLU:O | 1:N:394:ALA:HB3 | 2.18 | 0.44 |
| 1:N:420:ILE:HG23 | 1:N:470:LYS:HD3 | 1.99 | 0.44 |
| 1:N:449:ALA:HB3 | 1:N:450:PRO:CD | 2.39 | 0.44 |
| 2:O:37:ARG:N | 2:O:37:ARG:HD2 | 2.32 | 0.44 |
| 2:Q:86:MET:SD | 2:Q:86:MET:N | 2.91 | 0.44 |
| 1:A:219:PHE:HB3 | 1:A:317:LEU:CD1 | 2.44 | 0.44 |
| 1:B:232:GLU:C | 1:B:310:GLU:OE2 | 2.56 | 0.44 |
| 1:B:326:ASN:HD21 | 1:B:328:ASP:HB2 | 1.82 | 0.44 |
| 1:B:357:THR:HB | 1:B:361:ASP:HB2 | 1.98 | 0.44 |
| 1:B:72:GLN:HA | 1:B:72:GLN:NE2 | 2.31 | 0.44 |
| 1:C:327:LYS:HD3 | 1:C:327:LYS:N | 2.32 | 0.44 |
| 1:C:404:ARG:HG3 | 1:C:404:ARG:NH1 | 2.30 | 0.44 |
| 1:D:287:ALA:O | 1:D:290:GLN:NE2 | 2.50 | 0.44 |
| 1:D:77:VAL:CG1 | 1:D:510:VAL:HG21 | 2.47 | 0.44 |
| 1:E:199:TYR:CE2 | 1:E:202:PRO:HA | 2.52 | 0.44 |
| 1:E:479:ASN:O | 1:E:483:GLU:N | 2.50 | 0.44 |
| 1:E:72:GLN:NE2 | 1:E:72:GLN:CA | 2.79 | 0.44 |
| 1:F:23:LEU:C | 1:F:23:LEU:CD1 | 2.86 | 0.44 |
| 1:F:302:SER:C | 1:F:304:GLU:N | 2.70 | 0.44 |
| 1:F:406:ALA:HB1 | 1:F:411:VAL:HG13 | 1.99 | 0.44 |
| 1:G:87:ASP:OD1 | 1:G:88:GLY:N | 2.50 | 0.44 |
| 1:H:230:ILE:CD1 | 1:H:257:GLU:HG2 | 2.48 | 0.44 |
| 1:H:217:SER:CB | 1:H:321:LYS:HA | 2.47 | 0.44 |
| 1:H:178:GLU:O | 1:H:380:LYS:HA | 2.17 | 0.44 |
| 1:H:441:LYS:O | 1:H:442:VAL:C | 2.55 | 0.44 |
| 1:H:475:ASN:ND2 | 1:H:489:ILE:HD12 | 2.32 | 0.44 |
| 1:I:226:LYS:HD2 | 1:I:252:GLU:HG3 | 2.00 | 0.44 |
| 1:J:112:ASN:HA | 1:J:113:PRO:HD3 | 1.70 | 0.44 |
| 1:J:174:VAL:C | 1:J:175:ILE:HD12 | 2.37 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:343:GLN:O | 1:J:346:VAL:HB | 2.18 | 0.44 |
| 1:J:351:GLN:O | 1:J:354:GLU:N | 2.34 | 0.44 |
| 1:J:422:VAL:HG23 | 1:J:423:ALA:N | 2.32 | 0.44 |
| 1:L:221:LEU:HD11 | 1:L:223:ALA:HB2 | 1.98 | 0.44 |
| 1:L:443:ALA:O | 1:L:447:MET:HG3 | 2.16 | 0.44 |
| 1:M:153:ASN:O | 1:M:154:SER:HB2 | 2.17 | 0.44 |
| 1:N:290:GLN:HG3 | 1:N:345:ARG:HE | 1.82 | 0.44 |
| 1:N:40:LEU:HD23 | 1:N:50:THR:HG22 | 1.99 | 0.44 |
| 2:O:14:ARG:HB3 | 2:O:14:ARG:HH11 | 1.82 | 0.44 |
| 2:R:20:LYS:HD2 | 2:R:20:LYS:H | 1.83 | 0.44 |
| 2:S:47:ARG:CD | 2:S:49:LEU:HB2 | 2.48 | 0.44 |
| 2:T:14:ARG:HH11 | 2:T:14:ARG:CB | 2.30 | 0.44 |
| 1:A:143:ALA:O | 1:A:146:GLN:HB2 | 2.17 | 0.44 |
| 1:A:194:GLN:HG3 | 1:A:331:THR:OG1 | 2.18 | 0.44 |
| 1:A:279:PRO:HB2 | 1:A:285:ARG:HA | 1.99 | 0.44 |
| 1:A:519:CYS:SG | 1:A:520:MET:N | 2.91 | 0.44 |
| 1:A:88:GLY:C | 4:A:1:ADP:O2B | 2.56 | 0.44 |
| 1:B:207:LYS:HB3 | 1:B:208:PRO:CD | 2.36 | 0.44 |
| 1:B:348:GLN:HE22 | 1:B:352:GLN:NE2 | 2.14 | 0.44 |
| 1:B:401:HIS:O | 1:B:402:ALA:C | 2.56 | 0.44 |
| 1:B:451:LEU:O | 1:B:454:ILE:HB | 2.18 | 0.44 |
| 1:C:116:LEU:O | 1:C:120:ILE:HG13 | 2.17 | 0.44 |
| 1:D:183:LEU:HD22 | 1:D:384:ALA:HA | 2.00 | 0.44 |
| 1:E:267:MET:O | 1:E:269:GLY:N | 2.50 | 0.44 |
| 1:E:494:LEU:HD23 | 1:E:494:LEU:N | 2.31 | 0.44 |
| 1:F:325:ILE:HG22 | 1:F:326:ASN:O | 2.18 | 0.44 |
| 1:F:95:LEU:HD23 | 1:F:450:PRO:HD3 | 1.98 | 0.44 |
| 1:G:30:THR:HB | 1:G:51:LYS:HG3 | 1.98 | 0.44 |
| 1:H:165:ALA:O | 1:H:168:LYS:HB2 | 2.18 | 0.44 |
| 1:H:199:TYR:HD1 | 1:H:201:SER:H | 1.64 | 0.44 |
| 1:H:450:PRO:O | 1:H:454:ILE:HG12 | 2.17 | 0.44 |
| 1:H:64:ASP:HB3 | 1:H:67:GLU:HB2 | 2.00 | 0.44 |
| 1:I:158:VAL:O | 1:I:162:ILE:HG13 | 2.17 | 0.44 |
| 1:J:152:ALA:O | 1:J:153:ASN:HB3 | 2.18 | 0.44 |
| 1:J:286:LYS:HA | 1:J:286:LYS:CE | 2.42 | 0.44 |
| 1:J:351:GLN:O | 1:J:353:ILE:N | 2.51 | 0.44 |
| 1:K:165:ALA:O | 1:K:168:LYS:HB2 | 2.17 | 0.44 |
| 1:K:233:MET:HE1 | 1:K:309:LEU:HD13 | 1.99 | 0.44 |
| 1:K:314:LEU:O | 1:K:316:ASP:N | 2.51 | 0.44 |
| 1:K:384:ALA:O | 1:L:281:PHE:CZ | 2.69 | 0.44 |
| 1:L:343:GLN:O | 1:L:346:VAL:HB | 2.18 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:512:GLY:HA2 | 1:L:515:ILE:HD12 | 2.00 | 0.44 |
| 1:M:120:ILE:HG22 | 1:M:121:ASP:N | 2.33 | 0.44 |
| 1:M:233:MET:CE | 1:M:309:LEU:HD13 | 2.47 | 0.44 |
| 1:N:130:GLU:OE2 | 1:N:425:LYS:HB3 | 2.18 | 0.44 |
| 1:N:149:THR:CG2 | 1:N:159:GLY:HA3 | 2.45 | 0.44 |
| 1:N:165:ALA:O | 1:N:168:LYS:N | 2.35 | 0.44 |
| 1:N:187:LEU:HD23 | 1:N:187:LEU:C | 2.37 | 0.44 |
| 1:N:221:LEU:HD13 | 1:N:223:ALA:H | 1.82 | 0.44 |
| 1:N:266:THR:O | 1:N:268:ARG:N | 2.50 | 0.44 |
| 1:N:496:PRO:O | 1:N:499:VAL:HG22 | 2.17 | 0.44 |
| 1:M:38:VAL:HG22 | 1:N:519:CYS:HB3 | 2.00 | 0.44 |
| 2:Q:96:GLU:O | 2:Q:97:ALA:C | 2.55 | 0.44 |
| 2:U:47:ARG:HB3 | 2:U:55:LYS:HG2 | 1.99 | 0.44 |
| 2:O:4:ARG:O | 2:U:93:ALA:HB1 | 2.17 | 0.44 |
| 1:A:147:VAL:CG2 | 1:A:403:THR:HG22 | 2.48 | 0.44 |
| 1:A:150:ILE:CG2 | 1:A:151:SER:N | 2.80 | 0.44 |
| 1:B:221:LEU:HD13 | 1:B:317:LEU:CD2 | 2.47 | 0.44 |
| 1:C:194:GLN:NE2 | 1:C:331:THR:OG1 | 2.51 | 0.44 |
| 1:C:199:TYR:CE1 | 1:C:202:PRO:HA | 2.53 | 0.44 |
| 1:D:200:LEU:O | 1:D:202:PRO:CD | 2.66 | 0.44 |
| 1:D:451:LEU:O | 1:D:451:LEU:HD23 | 2.17 | 0.44 |
| 1:F:207:LYS:NZ | 1:F:207:LYS:CB | 2.81 | 0.44 |
| 1:G:176:THR:O | 1:G:378:VAL:HA | 2.18 | 0.44 |
| 1:G:200:LEU:HD12 | 1:G:200:LEU:N | 2.32 | 0.44 |
| 1:G:237:LEU:CD2 | 1:G:237:LEU:C | 2.85 | 0.44 |
| 1:G:309:LEU:N | 1:G:309:LEU:HD12 | 2.33 | 0.44 |
| 1:H:314:LEU:O | 1:H:316:ASP:N | 2.50 | 0.44 |
| 1:H:326:ASN:O | 1:H:327:LYS:C | 2.55 | 0.44 |
| 1:H:356:ALA:C | 1:H:358:SER:H | 2.21 | 0.44 |
| 1:H:455:VAL:HG11 | 1:H:462:PRO:HA | 1.99 | 0.44 |
| 1:I:285:ARG:HG2 | 1:I:285:ARG:HH11 | 1.82 | 0.44 |
| 1:I:351:GLN:O | 1:I:353:ILE:N | 2.51 | 0.44 |
| 1:I:413:ALA:HB1 | 1:I:417:VAL:HB | 1.99 | 0.44 |
| 1:J:122:LYS:O | 1:J:125:THR:HB | 2.17 | 0.44 |
| 1:J:32:GLY:CA | 1:J:454:ILE:HG23 | 2.48 | 0.44 |
| 1:K:343:GLN:O | 1:K:346:VAL:HB | 2.18 | 0.44 |
| 1:K:381:VAL:HB | 1:K:389:MET:CE | 2.47 | 0.44 |
| 1:L:190:VAL:HG21 | 1:L:334:ASP:CG | 2.38 | 0.44 |
| 1:L:221:LEU:HD13 | 1:L:223:ALA:N | 2.33 | 0.44 |
| 1:M:229:ASN:HA | 1:M:257:GLU:CD | 2.38 | 0.44 |
| 1:M:504:LEU:HD22 | 1:M:504:LEU:O | 2.18 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:95:LEU:O | 1:M:96:ALA:C | 2.54 | 0.44 |
| 2:R:11:ILE:HG22 | 2:R:41:LEU:HB2 | 1.98 | 0.44 |
| 2:S:47:ARG:HD3 | 2:S:49:LEU:CG | 2.48 | 0.44 |
| 2:U:58:ASP:N | 2:U:88:GLU:OE2 | 2.44 | 0.44 |
| 1:A:147:VAL:CG2 | 1:A:148:GLY:N | 2.80 | 0.44 |
| 1:A:400:LEU:HD13 | 1:A:400:LEU:C | 2.39 | 0.44 |
| 1:B:309:LEU:CD1 | 1:B:309:LEU:H | 2.30 | 0.44 |
| 1:B:308:GLU:H | 1:B:311:LYS:HB3 | 1.83 | 0.44 |
| 1:C:417:VAL:CA | 1:C:420:ILE:HG22 | 2.47 | 0.44 |
| 1:D:486:GLY:CA | 1:D:491:MET:CE | 2.96 | 0.44 |
| 1:E:204:PHE:O | 1:E:213:VAL:HG22 | 2.18 | 0.44 |
| 1:E:262:LEU:HD11 | 1:E:273:VAL:HB | 2.00 | 0.44 |
| 1:E:344:GLY:C | 1:E:346:VAL:N | 2.71 | 0.44 |
| 1:E:346:VAL:O | 1:E:350:ARG:NH1 | 2.51 | 0.44 |
| 1:F:400:LEU:C | 1:F:400:LEU:HD13 | 2.38 | 0.44 |
| 1:F:417:VAL:C | 1:F:420:ILE:HG22 | 2.37 | 0.44 |
| 1:G:127:ALA:O | 1:G:131:LEU:HG | 2.18 | 0.44 |
| 1:G:220:ILE:H | 1:G:220:ILE:HD12 | 1.80 | 0.44 |
| 1:G:44:PHE:HB2 | 1:G:45:GLY:H | 1.57 | 0.44 |
| 1:H:24:ALA:O | 1:H:28:LYS:HG2 | 2.17 | 0.44 |
| 1:H:321:LYS:HD2 | 1:H:334:ASP:OD2 | 2.17 | 0.44 |
| 1:H:478:TYR:HB2 | 1:H:485:TYR:CD2 | 2.53 | 0.44 |
| 1:H:521:VAL:HB | 1:N:40:LEU:HD13 | 1.99 | 0.44 |
| 1:I:255:GLU:O | 1:I:257:GLU:N | 2.51 | 0.44 |
| 1:I:350:ARG:HE | 1:I:369:VAL:HG11 | 1.82 | 0.44 |
| 1:I:399:ALA:O | 1:I:400:LEU:C | 2.53 | 0.44 |
| 1:I:19:GLY:HA3 | 1:I:67:GLU:O | 2.17 | 0.44 |
| 1:J:77:VAL:HG22 | 1:J:506:TYR:HB3 | 1.99 | 0.44 |
| 1:K:256:GLY:HA2 | 1:K:260:ALA:H | 1.82 | 0.44 |
| 1:L:201:SER:HA | 1:L:202:PRO:HD3 | 1.87 | 0.44 |
| 1:L:218:PRO:HB3 | 1:L:246:PRO:C | 2.38 | 0.44 |
| 1:L:232:GLU:HA | 1:L:310:GLU:HG3 | 1.99 | 0.44 |
| 1:L:354:GLU:HG2 | 1:L:355:GLU:H | 1.82 | 0.44 |
| 1:M:155:ASP:OD1 | 1:M:158:VAL:HG23 | 2.17 | 0.44 |
| 1:M:313:THR:CG2 | 1:M:314:LEU:N | 2.80 | 0.44 |
| 1:M:381:VAL:HG21 | 1:M:393:LYS:CA | 2.38 | 0.44 |
| 1:M:122:LYS:NZ | 1:M:430:ARG:O | 2.39 | 0.44 |
| 1:N:15:LYS:HA | 1:N:15:LYS:HD3 | 1.85 | 0.44 |
| 1:N:88:GLY:O | 1:N:89:THR:C | 2.56 | 0.44 |
| 2:O:20:LYS:HG2 | 2:O:27:LEU:HD21 | 1.99 | 0.44 |
| 2:O:47:ARG:HB3 | 2:O:55:LYS:HG2 | 1.99 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:79:ASP:HB2 | 2:P:81:GLU:OE1 | 2.18 | 0.44 |
| 2:Q:97:ALA:HB3 | 2:R:2:ASN:H | 1.83 | 0.44 |
| 2:T:86:MET:HG3 | 2:T:90:ASP:HB2 | 1.99 | 0.44 |
| 2:U:7:HIS:HB2 | 2:U:46:GLY:O | 2.18 | 0.44 |
| 1:A:199:TYR:OH | 1:A:211:GLY:HA2 | 2.17 | 0.44 |
| 1:A:235:PRO:HG2 | 1:A:236:VAL:HG23 | 1.99 | 0.44 |
| 1:A:345:ARG:O | 1:A:349:ILE:HG13 | 2.18 | 0.44 |
| 1:A:434:GLU:O | 1:A:437:ASN:N | 2.50 | 0.44 |
| 1:A:465:VAL:O | 1:A:466:ALA:C | 2.55 | 0.44 |
| 1:B:165:ALA:O | 1:B:169:VAL:HG22 | 2.17 | 0.44 |
| 1:B:217:SER:N | 1:B:218:PRO:CD | 2.80 | 0.44 |
| 1:B:183:LEU:HD22 | 1:B:384:ALA:HA | 2.00 | 0.44 |
| 1:B:44:PHE:HB2 | 1:B:45:GLY:H | 1.50 | 0.44 |
| 1:C:84:ALA:HB2 | 1:C:506:TYR:CE2 | 2.49 | 0.44 |
| 1:D:176:THR:O | 1:D:378:VAL:HA | 2.18 | 0.44 |
| 1:D:272:LYS:CB | 1:D:272:LYS:NZ | 2.81 | 0.44 |
| 1:D:289:LEU:HD23 | 1:D:292:ILE:HD12 | 1.99 | 0.44 |
| 1:D:391:GLU:O | 1:D:394:ALA:HB3 | 2.18 | 0.44 |
| 1:E:106:ALA:O | 1:E:109:ALA:HB3 | 2.17 | 0.44 |
| 1:E:211:GLY:O | 1:E:325:ILE:O | 2.36 | 0.44 |
| 1:E:302:SER:C | 1:E:304:GLU:N | 2.71 | 0.44 |
| 1:E:325:ILE:N | 1:E:325:ILE:CD1 | 2.79 | 0.44 |
| 1:E:358:SER:HA | 1:E:362:ARG:HG3 | 2.00 | 0.44 |
| 1:F:130:GLU:OE1 | 1:F:130:GLU:HA | 2.18 | 0.44 |
| 1:F:308:GLU:HB2 | 1:F:311:LYS:CB | 2.43 | 0.44 |
| 1:G:145:ALA:O | 1:G:159:GLY:HA3 | 2.18 | 0.44 |
| 1:G:325:ILE:HG22 | 1:G:326:ASN:N | 2.33 | 0.44 |
| 1:H:153:ASN:O | 1:H:154:SER:HB2 | 2.18 | 0.44 |
| 1:H:479:ASN:O | 1:H:483:GLU:N | 2.49 | 0.44 |
| 1:I:478:TYR:HA | 1:I:485:TYR:HA | 1.99 | 0.44 |
| 1:J:262:LEU:HA | 1:J:265:ASN:HB3 | 1.99 | 0.44 |
| 1:L:160:LYS:HG2 | 1:L:164:GLU:OE2 | 2.17 | 0.44 |
| 1:L:308:GLU:OE2 | 1:L:310:GLU:HG3 | 2.18 | 0.44 |
| 1:M:104:LEU:HD12 | 1:M:104:LEU:HA | 1.69 | 0.44 |
| 1:M:140:ASP:O | 1:M:144:ILE:HG12 | 2.18 | 0.44 |
| 1:N:175:ILE:HD13 | 1:N:404:ARG:NH2 | 2.33 | 0.44 |
| 1:N:353:ILE:HA | 1:N:365:LEU:CD1 | 2.48 | 0.44 |
| 2:Q:43:VAL:HG23 | 2:Q:61:VAL:HG22 | 2.00 | 0.44 |
| 2:R:67:PHE:CD1 | 2:R:67:PHE:C | 2.91 | 0.44 |
| 2:R:7:HIS:O | 2:R:7:HIS:ND1 | 2.50 | 0.44 |
| 2:T:68:ASN:ND2 | 2:U:74:LYS:CE | 2.79 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:74:LYS:HE3 | 2:U:68:ASN:ND2 | 2.33 | 0.44 |
| 1:A:219:PHE:HA | 1:A:318:GLY:O | 2.18 | 0.43 |
| 1:A:344:GLY:C | 1:A:346:VAL:N | 2.71 | 0.43 |
| 1:A:430:ARG:HG2 | 1:A:430:ARG:HH11 | 1.82 | 0.43 |
| 1:B:194:GLN:HG2 | 1:B:195:PHE:N | 2.33 | 0.43 |
| 1:B:206:ASN:HB3 | 1:B:214:GLU:H | 1.83 | 0.43 |
| 1:B:219:PHE:CE2 | 1:B:245:LYS:HB2 | 2.52 | 0.43 |
| 1:B:305:ILE:HD11 | 1:C:203:TYR:OH | 2.17 | 0.43 |
| 1:B:350:ARG:HA | 1:B:353:ILE:HD12 | 2.00 | 0.43 |
| 1:B:360:TYR:H | 1:B:363:GLU:HG3 | 1.83 | 0.43 |
| 1:C:283:ASP:O | 1:C:287:ALA:HB2 | 2.18 | 0.43 |
| 1:C:308:GLU:O | 1:C:309:LEU:O | 2.36 | 0.43 |
| 1:C:190:VAL:HB | 1:C:376:VAL:HB | 1.99 | 0.43 |
| 1:C:456:LEU:HD22 | 1:C:462:PRO:HG2 | 2.00 | 0.43 |
| 1:C:8:PHE:N | 1:C:8:PHE:CD1 | 2.85 | 0.43 |
| 1:E:290:GLN:O | 1:E:294:THR:N | 2.50 | 0.43 |
| 1:F:180:GLY:CA | 1:F:380:LYS:HB3 | 2.47 | 0.43 |
| 1:F:518:GLU:HA | 1:F:518:GLU:OE1 | 2.18 | 0.43 |
| 1:G:290:GLN:O | 1:G:294:THR:HG23 | 2.17 | 0.43 |
| 1:G:313:THR:HG22 | 1:G:315:GLU:H | 1.83 | 0.43 |
| 1:G:406:ALA:O | 1:G:410:GLY:N | 2.51 | 0.43 |
| 1:A:39:VAL:HG12 | 1:G:69:MET:CE | 2.48 | 0.43 |
| 1:I:37:ASN:ND2 | 1:I:37:ASN:N | 2.65 | 0.43 |
| 1:J:420:ILE:CD1 | 1:J:448:GLU:HA | 2.47 | 0.43 |
| 1:J:522:THR:OG1 | 1:J:523:ASP:N | 2.51 | 0.43 |
| 1:K:256:GLY:O | 1:K:257:GLU:C | 2.57 | 0.43 |
| 1:K:227:ILE:HD12 | 1:K:309:LEU:HD11 | 1.98 | 0.43 |
| 1:L:389:MET:O | 1:L:389:MET:HE1 | 2.18 | 0.43 |
| 1:L:433:ASN:OD1 | 1:L:435:ASP:HB2 | 2.18 | 0.43 |
| 1:N:256:GLY:O | 1:N:257:GLU:C | 2.55 | 0.43 |
| 1:N:362:ARG:CB | 1:N:362:ARG:NH1 | 2.81 | 0.43 |
| 2:P:68:ASN:O | 2:P:70:GLY:N | 2.50 | 0.43 |
| 2:T:47:ARG:HB3 | 2:T:55:LYS:CG | 2.48 | 0.43 |
| 1:A:200:LEU:O | 1:A:202:PRO:HD2 | 2.18 | 0.43 |
| 1:A:208:PRO:O | 1:A:212:ALA:HB3 | 2.18 | 0.43 |
| 1:A:216:GLU:O | 1:A:246:PRO:HG3 | 2.19 | 0.43 |
| 1:A:213:VAL:HB | 1:A:325:ILE:HD13 | 1.99 | 0.43 |
| 1:B:237:LEU:C | 1:B:237:LEU:CD2 | 2.87 | 0.43 |
| 1:B:474:GLY:C | 1:B:475:ASN:HD22 | 2.20 | 0.43 |
| 1:C:200:LEU:O | 1:C:202:PRO:HD2 | 2.18 | 0.43 |
| 1:C:293:ALA:O | 1:C:294:THR:C | 2.56 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:362:ARG:O | 1:C:366:GLN:OE1 | 2.36 | 0.43 |
| 1:D:325:ILE:HG22 | 1:D:326:ASN:N | 2.32 | 0.43 |
| 1:D:451:LEU:CD2 | 1:D:451:LEU:C | 2.86 | 0.43 |
| 1:D:465:VAL:O | 1:D:466:ALA:C | 2.57 | 0.43 |
| 1:E:284:ARG:HG2 | 1:E:288:MET:HE2 | 2.00 | 0.43 |
| 1:E:9:GLY:HA2 | 1:E:13:ARG:HH12 | 1.82 | 0.43 |
| 1:F:155:ASP:HB3 | 1:F:158:VAL:CG2 | 2.47 | 0.43 |
| 1:F:207:LYS:CB | 1:F:208:PRO:CD | 2.96 | 0.43 |
| 1:F:29:VAL:HG23 | 1:F:30:THR:CG2 | 2.45 | 0.43 |
| 1:G:217:SER:N | 1:G:218:PRO:CD | 2.82 | 0.43 |
| 1:G:284:ARG:O | 1:G:287:ALA:HB3 | 2.18 | 0.43 |
| 1:G:413:ALA:HB1 | 1:G:417:VAL:HG11 | 2.01 | 0.43 |
| 1:H:287:ALA:O | 1:H:288:MET:C | 2.56 | 0.43 |
| 1:I:215:LEU:CB | 1:I:218:PRO:HG2 | 2.46 | 0.43 |
| 1:I:38:VAL:HG22 | 1:J:519:CYS:HB3 | 1.99 | 0.43 |
| 1:J:301:ILE:O | 1:J:301:ILE:HG22 | 2.17 | 0.43 |
| 1:J:345:ARG:O | 1:J:348:GLN:HB2 | 2.17 | 0.43 |
| 1:J:131:LEU:HD12 | 1:J:422:VAL:HG11 | 2.00 | 0.43 |
| 1:K:248:LEU:CD1 | 1:K:250:ILE:HG13 | 2.47 | 0.43 |
| 1:K:362:ARG:NH1 | 1:K:362:ARG:CB | 2.81 | 0.43 |
| 1:K:413:ALA:HB3 | 1:K:417:VAL:HB | 1.98 | 0.43 |
| 1:J:49:ILE:HD11 | 1:K:73:MET:HE2 | 2.00 | 0.43 |
| 1:M:203:TYR:HD1 | 1:M:203:TYR:H | 1.66 | 0.43 |
| 1:M:448:GLU:HB3 | 1:M:452:ARG:HD2 | 1.99 | 0.43 |
| 1:M:80:LYS:O | 1:M:83:ASP:HB2 | 2.18 | 0.43 |
| 1:N:165:ALA:O | 1:N:168:LYS:HB2 | 2.18 | 0.43 |
| 1:N:313:THR:CG2 | 1:N:314:LEU:N | 2.81 | 0.43 |
| 1:N:317:LEU:CD1 | 1:N:317:LEU:N | 2.81 | 0.43 |
| 1:N:513:LEU:HA | 1:N:513:LEU:HD12 | 1.73 | 0.43 |
| 2:P:20:LYS:HA | 2:P:28:THR:HG23 | 1.99 | 0.43 |
| 2:P:47:ARG:HG2 | 2:P:48:ILE:N | 2.33 | 0.43 |
| 2:R:31:ALA:O | 2:R:32:ALA:HB3 | 2.18 | 0.43 |
| 2:T:7:HIS:HB3 | 2:T:45:ASN:HD22 | 1.82 | 0.43 |
| 1:A:248:LEU:HD13 | 1:A:248:LEU:C | 2.38 | 0.43 |
| 1:A:321:LYS:HB2 | 1:A:333:ILE:HB | 1.99 | 0.43 |
| 1:B:116:LEU:O | 1:B:120:ILE:HG13 | 2.19 | 0.43 |
| 1:B:249:ILE:HB | 1:B:275:ALA:HB1 | 1.99 | 0.43 |
| 1:C:266:THR:HA | 1:C:271:VAL:O | 2.18 | 0.43 |
| 1:C:303:GLU:C | 1:C:303:GLU:OE1 | 2.57 | 0.43 |
| 1:C:346:VAL:O | 1:C:349:ILE:HB | 2.18 | 0.43 |
| 1:D:246:PRO:HA | 1:D:272:LYS:O | 2.19 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:325:ILE:CG1 | 1:E:330:THR:HG23 | 2.45 | 0.43 |
| 1:F:112:ASN:HA | 1:F:113:PRO:HD3 | 1.73 | 0.43 |
| 1:F:150:ILE:HG23 | 1:F:151:SER:N | 2.32 | 0.43 |
| 1:G:285:ARG:O | 1:G:288:MET:N | 2.48 | 0.43 |
| 1:G:295:LEU:HD23 | 1:G:335:GLY:O | 2.18 | 0.43 |
| 1:G:111:MET:CE | 1:G:438:VAL:HG21 | 2.48 | 0.43 |
| 1:G:456:LEU:HD12 | 1:G:456:LEU:HA | 1.84 | 0.43 |
| 1:H:32:GLY:HA2 | 1:H:454:ILE:HG23 | 2.01 | 0.43 |
| 1:I:259:LEU:HD23 | 1:I:260:ALA:N | 2.33 | 0.43 |
| 1:I:290:GLN:HG3 | 1:I:345:ARG:HE | 1.83 | 0.43 |
| 1:I:186:GLU:O | 1:I:379:ILE:HA | 2.18 | 0.43 |
| 1:J:259:LEU:HD23 | 1:J:259:LEU:C | 2.38 | 0.43 |
| 1:J:287:ALA:O | 1:J:290:GLN:HB3 | 2.17 | 0.43 |
| 1:K:120:ILE:O | 1:K:121:ASP:C | 2.57 | 0.43 |
| 1:K:226:LYS:HD2 | 1:K:252:GLU:HG3 | 2.00 | 0.43 |
| 1:K:227:ILE:O | 1:K:254:VAL:HA | 2.17 | 0.43 |
| 1:K:232:GLU:CB | 1:K:309:LEU:HD12 | 2.49 | 0.43 |
| 1:K:296:THR:HB | 1:K:319:GLN:H | 1.82 | 0.43 |
| 1:K:353:ILE:HG12 | 1:K:365:LEU:CB | 2.48 | 0.43 |
| 1:L:293:ALA:HB2 | 1:L:300:VAL:HG13 | 1.99 | 0.43 |
| 1:L:433:ASN:HD22 | 1:L:434:GLU:N | 2.15 | 0.43 |
| 1:N:21:ASN:HA | 1:N:21:ASN:HD22 | 1.59 | 0.43 |
| 1:N:385:THR:HG23 | 1:N:388:GLU:HB3 | 1.99 | 0.43 |
| 2:O:13:LYS:O | 2:O:13:LYS:HG3 | 2.17 | 0.43 |
| 2:S:97:ALA:O | 2:T:1:MET:HA | 2.18 | 0.43 |
| 1:A:233:MET:HE2 | 1:A:233:MET:O | 2.19 | 0.43 |
| 1:A:279:PRO:CB | 1:A:288:MET:HE3 | 2.49 | 0.43 |
| 1:B:153:ASN:C | 1:B:153:ASN:HD22 | 2.20 | 0.43 |
| 1:C:103:GLY:O | 1:C:107:VAL:HG23 | 2.18 | 0.43 |
| 1:C:302:SER:CB | 1:C:305:ILE:HB | 2.48 | 0.43 |
| 1:C:315:GLU:OE1 | 1:C:316:ASP:N | 2.51 | 0.43 |
| 1:C:451:LEU:CD2 | 1:C:451:LEU:C | 2.86 | 0.43 |
| 1:C:451:LEU:O | 1:C:451:LEU:HD23 | 2.19 | 0.43 |
| 1:D:128:VAL:CG1 | 1:D:132:LYS:HE2 | 2.48 | 0.43 |
| 1:D:232:GLU:O | 1:D:233:MET:CB | 2.67 | 0.43 |
| 1:D:272:LYS:HB2 | 1:D:272:LYS:HZ2 | 1.82 | 0.43 |
| 1:F:27:VAL:HG13 | 1:F:53:GLY:HA2 | 2.00 | 0.43 |
| 1:F:309:LEU:O | 1:F:310:GLU:C | 2.56 | 0.43 |
| 1:F:417:VAL:CA | 1:F:420:ILE:HG22 | 2.48 | 0.43 |
| 1:G:134:LEU:CD1 | 1:G:134:LEU:H | 2.32 | 0.43 |
| 1:G:313:THR:HG22 | 1:G:315:GLU:HG3 | 1.99 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:361:ASP:C | 1:G:363:GLU:H | 2.22 | 0.43 |
| 1:H:314:LEU:CA | 1:H:317:LEU:HD13 | 2.41 | 0.43 |
| 1:H:420:ILE:CD1 | 1:H:448:GLU:HA | 2.48 | 0.43 |
| 1:I:478:TYR:HB2 | 1:I:485:TYR:CD2 | 2.52 | 0.43 |
| 1:J:248:LEU:HD13 | 1:J:248:LEU:C | 2.38 | 0.43 |
| 1:J:321:LYS:HD2 | 1:J:334:ASP:OD2 | 2.18 | 0.43 |
| 1:J:88:GLY:O | 1:J:89:THR:C | 2.56 | 0.43 |
| 1:K:200:LEU:CD1 | 1:K:200:LEU:N | 2.82 | 0.43 |
| 1:K:325:ILE:N | 1:K:325:ILE:CD1 | 2.80 | 0.43 |
| 1:K:178:GLU:O | 1:K:380:LYS:HA | 2.18 | 0.43 |
| 1:L:149:THR:HG22 | 1:L:156:GLU:HA | 1.99 | 0.43 |
| 1:L:152:ALA:CB | 1:L:158:VAL:HG11 | 2.48 | 0.43 |
| 1:M:303:GLU:C | 1:M:305:ILE:H | 2.19 | 0.43 |
| 1:M:461:GLU:HB3 | 1:M:464:VAL:HB | 2.00 | 0.43 |
| 1:L:47:PRO:HG3 | 1:M:73:MET:CG | 2.48 | 0.43 |
| 1:N:104:LEU:HD12 | 1:N:104:LEU:HA | 1.72 | 0.43 |
| 1:N:202:PRO:C | 1:N:204:PHE:H | 2.22 | 0.43 |
| 1:N:227:ILE:O | 1:N:254:VAL:HA | 2.18 | 0.43 |
| 1:N:259:LEU:HD23 | 1:N:259:LEU:C | 2.38 | 0.43 |
| 1:N:323:VAL:HG23 | 1:N:332:ILE:HG22 | 2.00 | 0.43 |
| 1:N:351:GLN:O | 1:N:354:GLU:HB3 | 2.19 | 0.43 |
| 1:N:364:LYS:HD2 | 1:N:367:GLU:OE1 | 2.17 | 0.43 |
| 1:N:420:ILE:HG13 | 1:N:451:LEU:HD22 | 2.01 | 0.43 |
| 2:Q:93:ALA:HB1 | 2:R:4:ARG:O | 2.17 | 0.43 |
| 2:S:84:LEU:CD1 | 2:S:84:LEU:N | 2.81 | 0.43 |
| 2:T:5:PRO:HD3 | 2:T:42:ALA:HB1 | 2.01 | 0.43 |
| 1:A:451:LEU:C | 1:A:451:LEU:HD23 | 2.39 | 0.43 |
| 1:A:6:VAL:HG23 | 1:A:6:VAL:O | 2.18 | 0.43 |
| 1:B:325:ILE:CD1 | 1:B:325:ILE:N | 2.77 | 0.43 |
| 1:B:339:GLU:HG3 | 1:B:342:ILE:HD12 | 1.99 | 0.43 |
| 1:B:428:ASP:C | 1:B:430:ARG:NH1 | 2.71 | 0.43 |
| 1:C:122:LYS:HE2 | 1:C:429:LEU:HD11 | 1.99 | 0.43 |
| 1:C:365:LEU:C | 1:C:367:GLU:N | 2.71 | 0.43 |
| 1:C:519:CYS:SG | 1:C:520:MET:N | 2.92 | 0.43 |
| 1:C:65:LYS:O | 1:C:69:MET:HG3 | 2.18 | 0.43 |
| 1:D:207:LYS:HB2 | 1:D:207:LYS:NZ | 2.34 | 0.43 |
| 1:D:30:THR:HB | 1:D:51:LYS:CG | 2.47 | 0.43 |
| 1:D:348:GLN:NE2 | 1:D:352:GLN:NE2 | 2.66 | 0.43 |
| 1:D:381:VAL:HG13 | 1:D:392:LYS:CG | 2.48 | 0.43 |
| 1:D:411:VAL:HG12 | 1:D:496:PRO:CA | 2.35 | 0.43 |
| 1:E:164:GLU:O | 1:E:167:ASP:HB3 | 2.18 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:201:SER:HB3 | 1:E:259:LEU:HD22 | 2.00 | 0.43 |
| 1:E:73:MET:O | 1:E:74:VAL:C | 2.56 | 0.43 |
| 1:F:222:LEU:CD1 | 1:F:222:LEU:N | 2.78 | 0.43 |
| 1:F:265:ASN:HB3 | 1:F:271:VAL:CG2 | 2.48 | 0.43 |
| 1:F:279:PRO:HD2 | 1:F:285:ARG:CB | 2.48 | 0.43 |
| 1:F:499:VAL:CG2 | 1:F:500:THR:H | 2.31 | 0.43 |
| 1:G:240:VAL:C | 1:G:242:LYS:N | 2.68 | 0.43 |
| 1:H:149:THR:HG21 | 1:H:156:GLU:HA | 1.99 | 0.43 |
| 1:H:81:ALA:HA | 1:H:506:TYR:CD2 | 2.54 | 0.43 |
| 1:I:104:LEU:HD12 | 1:I:104:LEU:HA | 1.80 | 0.43 |
| 1:I:385:THR:HG23 | 1:I:388:GLU:N | 2.30 | 0.43 |
| 1:I:472:GLY:HA3 | 1:I:476:TYR:CD2 | 2.54 | 0.43 |
| 1:I:97:GLN:O | 1:I:98:ALA:C | 2.57 | 0.43 |
| 1:J:192:GLY:C | 1:J:376:VAL:HG23 | 2.38 | 0.43 |
| 1:J:266:THR:O | 1:J:268:ARG:N | 2.51 | 0.43 |
| 1:J:282:GLY:O | 1:J:285:ARG:HG2 | 2.19 | 0.43 |
| 1:J:414:GLY:N | 1:J:494:LEU:HA | 2.33 | 0.43 |
| 1:K:186:GLU:HB2 | 1:K:380:LYS:HB2 | 2.00 | 0.43 |
| 1:K:202:PRO:C | 1:K:204:PHE:H | 2.22 | 0.43 |
| 1:L:302:SER:HB2 | 1:L:305:ILE:CG1 | 2.48 | 0.43 |
| 1:L:38:VAL:HG12 | 1:L:39:VAL:N | 2.33 | 0.43 |
| 1:M:184:GLN:HA | 1:M:184:GLN:OE1 | 2.18 | 0.43 |
| 1:M:221:LEU:HD13 | 1:M:223:ALA:N | 2.34 | 0.43 |
| 1:N:37:ASN:H | 1:N:37:ASN:HD22 | 1.65 | 0.43 |
| 2:O:14:ARG:HB2 | 2:O:14:ARG:NH1 | 2.33 | 0.43 |
| 2:Q:58:ASP:N | 2:Q:88:GLU:OE2 | 2.47 | 0.43 |
| 2:T:76:GLU:O | 2:T:83:VAL:HG22 | 2.17 | 0.43 |
| 2:U:44:GLY:O | 2:U:57:LEU:HD12 | 2.19 | 0.43 |
| 2:U:84:LEU:N | 2:U:84:LEU:CD1 | 2.81 | 0.43 |
| 1:A:284:ARG:HG2 | 1:A:288:MET:CE | 2.48 | 0.43 |
| 1:A:360:TYR:H | 1:A:363:GLU:CG | 2.32 | 0.43 |
| 1:B:229:ASN:C | 1:B:231:ARG:N | 2.70 | 0.43 |
| 1:B:239:ALA:HB1 | 1:B:314:LEU:HB3 | 2.00 | 0.43 |
| 1:B:279:PRO:CG | 1:B:288:MET:HE3 | 2.46 | 0.43 |
| 1:C:281:PHE:O | 1:C:284:ARG:HB3 | 2.19 | 0.43 |
| 1:C:309:LEU:O | 1:C:311:LYS:N | 2.51 | 0.43 |
| 1:C:185:ASP:HA | 1:C:380:LYS:O | 2.19 | 0.43 |
| 1:E:237:LEU:C | 1:E:237:LEU:CD2 | 2.87 | 0.43 |
| 1:F:165:ALA:O | 1:F:169:VAL:HG22 | 2.19 | 0.43 |
| 1:F:179:ASP:OD1 | 1:F:389:MET:HG3 | 2.18 | 0.43 |
| 1:F:229:ASN:O | 1:F:231:ARG:N | 2.51 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:326:ASN:OD1 | 1:F:329:THR:N | 2.51 | 0.43 |
| 1:F:348:GLN:NE2 | 1:F:352:GLN:HE21 | 2.17 | 0.43 |
| 1:F:183:LEU:HD22 | 1:F:384:ALA:HA | 2.01 | 0.43 |
| 1:H:121:ASP:O | 1:H:125:THR:OG1 | 2.32 | 0.43 |
| 1:I:233:MET:N | 1:I:233:MET:SD | 2.91 | 0.43 |
| 1:I:290:GLN:OE1 | 1:I:290:GLN:HA | 2.18 | 0.43 |
| 1:J:288:MET:HE3 | 1:J:288:MET:HA | 2.01 | 0.43 |
| 1:J:69:MET:O | 1:J:70:GLY:C | 2.57 | 0.43 |
| 1:J:8:PHE:O | 1:J:9:GLY:C | 2.57 | 0.43 |
| 1:L:398:ASP:O | 1:L:401:HIS:N | 2.51 | 0.43 |
| 1:L:413:ALA:HB1 | 1:L:417:VAL:CB | 2.48 | 0.43 |
| 1:M:247:LEU:HD13 | 1:M:248:LEU:N | 2.33 | 0.43 |
| 1:M:472:GLY:HA3 | 1:M:476:TYR:CD2 | 2.54 | 0.43 |
| 1:N:255:GLU:O | 1:N:256:GLY:C | 2.56 | 0.43 |
| 2:O:76:GLU:O | 2:O:83:VAL:HG22 | 2.18 | 0.43 |
| 1:C:270:ILE:HD11 | 2:Q:27:LEU:CD1 | 2.49 | 0.43 |
| 2:T:37:ARG:N | 2:T:37:ARG:HD2 | 2.34 | 0.43 |
| 2:U:13:LYS:O | 2:U:13:LYS:HG3 | 2.19 | 0.43 |
| 1:A:272:LYS:NZ | 1:A:272:LYS:HB2 | 2.34 | 0.43 |
| 1:A:38:VAL:HG12 | 1:A:39:VAL:N | 2.34 | 0.43 |
| 1:B:436:GLN:O | 1:B:440:ILE:HG13 | 2.18 | 0.43 |
| 1:B:510:VAL:HG23 | 1:B:511:ALA:H | 1.82 | 0.43 |
| 1:B:5:ASP:HB2 | 1:B:524:LEU:CD2 | 2.46 | 0.43 |
| 1:C:140:ASP:OD1 | 1:C:142:LYS:HB3 | 2.18 | 0.43 |
| 1:C:237:LEU:HD22 | 2:Q:26:VAL:CG2 | 2.42 | 0.43 |
| 1:D:177:VAL:HG11 | 1:D:397:GLU:CG | 2.49 | 0.43 |
| 1:D:299:THR:N | 1:D:316:ASP:O | 2.52 | 0.43 |
| 1:D:219:PHE:CB | 1:D:317:LEU:HD13 | 2.45 | 0.43 |
| 1:D:355:GLU:O | 1:D:362:ARG:NH2 | 2.52 | 0.43 |
| 1:D:417:VAL:O | 1:D:420:ILE:CG2 | 2.59 | 0.43 |
| 1:E:207:LYS:CB | 1:E:208:PRO:CD | 2.93 | 0.43 |
| 1:E:266:THR:HA | 1:E:271:VAL:O | 2.18 | 0.43 |
| 1:D:519:CYS:HB3 | 1:E:38:VAL:HG22 | 1.99 | 0.43 |
| 1:E:451:LEU:C | 1:E:451:LEU:HD23 | 2.39 | 0.43 |
| 1:F:200:LEU:N | 1:F:200:LEU:CD1 | 2.82 | 0.43 |
| 1:F:262:LEU:HA | 1:F:265:ASN:HD22 | 1.82 | 0.43 |
| 1:F:362:ARG:HA | 1:F:365:LEU:HD13 | 2.01 | 0.43 |
| 1:G:183:LEU:CD2 | 1:G:384:ALA:HA | 2.49 | 0.43 |
| 1:G:228:SER:HA | 1:G:255:GLU:CG | 2.48 | 0.43 |
| 1:G:281:PHE:CG | 1:G:282:GLY:N | 2.86 | 0.43 |
| 1:G:280:GLY:CA | 1:G:284:ARG:HD2 | 2.49 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:279:PRO:HD2 | 1:G:285:ARG:CB | 2.49 | 0.43 |
| 1:G:384:ALA:N | 1:G:388:GLU:OE1 | 2.50 | 0.43 |
| 1:G:31:LEU:HD23 | 1:G:453:GLN:HB3 | 2.00 | 0.43 |
| 1:H:336:VAL:HG12 | 1:H:336:VAL:O | 2.18 | 0.43 |
| 1:I:27:VAL:HG11 | 1:I:93:THR:HG21 | 2.01 | 0.43 |
| 1:I:318:GLY:O | 1:I:319:GLN:CG | 2.67 | 0.43 |
| 1:I:353:ILE:HG22 | 1:I:353:ILE:O | 2.18 | 0.43 |
| 1:J:120:ILE:O | 1:J:121:ASP:C | 2.56 | 0.43 |
| 1:K:135:SER:HA | 1:K:412:VAL:CG1 | 2.48 | 0.43 |
| 1:K:15:LYS:HD3 | 1:K:15:LYS:HA | 1.88 | 0.43 |
| 1:K:323:VAL:HG23 | 1:K:331:THR:O | 2.18 | 0.43 |
| 1:K:323:VAL:HG13 | 1:K:323:VAL:O | 2.18 | 0.43 |
| 1:L:171:LYS:HD3 | 1:L:407:VAL:HG11 | 2.01 | 0.43 |
| 1:L:326:ASN:O | 1:L:328:ASP:N | 2.51 | 0.43 |
| 1:L:353:ILE:HA | 1:L:365:LEU:HD13 | 2.01 | 0.43 |
| 1:M:202:PRO:C | 1:M:204:PHE:N | 2.72 | 0.43 |
| 1:M:291:ASP:OD1 | 1:M:368:ARG:NH2 | 2.51 | 0.43 |
| 1:M:364:LYS:O | 1:M:365:LEU:C | 2.56 | 0.43 |
| 1:N:479:ASN:O | 1:N:483:GLU:N | 2.51 | 0.43 |
| 1:N:56:VAL:O | 1:N:57:ALA:C | 2.55 | 0.43 |
| 2:O:55:LYS:N | 2:O:55:LYS:CE | 2.67 | 0.43 |
| 2:R:14:ARG:HH11 | 2:R:14:ARG:HB3 | 1.82 | 0.43 |
| 2:S:68:ASN:HD22 | 2:T:74:LYS:HE3 | 1.83 | 0.43 |
| 2:U:43:VAL:HG13 | 2:U:57:LEU:HD12 | 2.01 | 0.43 |
| 1:A:176:THR:OG1 | 1:A:378:VAL:HG22 | 2.18 | 0.43 |
| 1:A:397:GLU:O | 1:A:398:ASP:C | 2.55 | 0.43 |
| 1:A:95:LEU:HD13 | 1:A:504:LEU:HD23 | 2.01 | 0.43 |
| 1:B:206:ASN:CB | 1:B:213:VAL:HA | 2.49 | 0.43 |
| 1:B:220:ILE:HG23 | 1:B:248:LEU:HD12 | 2.01 | 0.43 |
| 1:B:39:VAL:HA | 1:B:48:THR:O | 2.18 | 0.43 |
| 1:C:222:LEU:HD22 | 1:C:293:ALA:HB2 | 2.01 | 0.43 |
| 1:C:279:PRO:HD2 | 1:C:285:ARG:CB | 2.49 | 0.43 |
| 1:C:346:VAL:HA | 1:C:349:ILE:HD12 | 2.00 | 0.43 |
| 1:C:496:PRO:HG2 | 1:C:499:VAL:CG1 | 2.49 | 0.43 |
| 1:D:136:VAL:HA | 1:D:137:PRO:HD3 | 1.79 | 0.43 |
| 1:D:302:SER:HB2 | 1:D:305:ILE:CB | 2.46 | 0.43 |
| 1:D:349:ILE:HG12 | 1:D:352:GLN:HE22 | 1.82 | 0.43 |
| 1:D:479:ASN:O | 1:D:483:GLU:N | 2.51 | 0.43 |
| 1:E:456:LEU:HD22 | 1:E:462:PRO:HG2 | 1.99 | 0.43 |
| 1:F:233:MET:CE | 1:F:237:LEU:HB2 | 2.49 | 0.43 |
| 1:F:240:VAL:O | 1:F:241:ALA:C | 2.57 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:249:ILE:HB | 1:F:275:ALA:HB1 | 2.00 | 0.43 |
| 1:F:520:MET:HB3 | 1:F:520:MET:HE2 | 1.94 | 0.43 |
| 1:G:215:LEU:O | 1:G:322:ARG:HG3 | 2.18 | 0.43 |
| 1:H:157:THR:O | 1:H:161:LEU:CD1 | 2.64 | 0.43 |
| 1:H:202:PRO:C | 1:H:204:PHE:H | 2.21 | 0.43 |
| 1:H:247:LEU:HB3 | 1:H:273:VAL:HG11 | 2.00 | 0.43 |
| 1:H:249:ILE:HD12 | 1:H:275:ALA:HB2 | 2.00 | 0.43 |
| 1:H:69:MET:O | 1:H:70:GLY:C | 2.56 | 0.43 |
| 1:H:384:ALA:O | 1:I:281:PHE:CZ | 2.71 | 0.43 |
| 1:I:401:HIS:O | 1:I:402:ALA:C | 2.57 | 0.43 |
| 1:J:231:ARG:HH11 | 1:J:231:ARG:HB3 | 1.83 | 0.43 |
| 1:J:311:LYS:HD2 | 1:J:311:LYS:N | 2.34 | 0.43 |
| 1:K:418:ALA:O | 1:K:421:ARG:HB3 | 2.19 | 0.43 |
| 1:K:496:PRO:O | 1:K:499:VAL:HG22 | 2.18 | 0.43 |
| 1:L:318:GLY:O | 1:L:319:GLN:HG3 | 2.18 | 0.43 |
| 1:L:385:THR:HG23 | 1:L:388:GLU:N | 2.31 | 0.43 |
| 1:L:440:ILE:O | 1:L:443:ALA:HB3 | 2.18 | 0.43 |
| 1:L:37:ASN:HB3 | 1:L:51:LYS:HG3 | 2.00 | 0.43 |
| 1:M:193:MET:CG | 1:M:194:GLN:N | 2.81 | 0.43 |
| 1:M:221:LEU:HD11 | 1:M:223:ALA:HB2 | 2.00 | 0.43 |
| 1:N:112:ASN:C | 1:N:112:ASN:OD1 | 2.57 | 0.43 |
| 1:N:220:ILE:HG23 | 1:N:248:LEU:HD12 | 2.01 | 0.43 |
| 1:N:302:SER:HB2 | 1:N:305:ILE:CG1 | 2.48 | 0.43 |
| 1:N:214:GLU:HG2 | 1:N:324:VAL:CG1 | 2.48 | 0.43 |
| 1:N:81:ALA:HA | 1:N:506:TYR:CD2 | 2.54 | 0.43 |
| 2:P:4:ARG:O | 2:P:5:PRO:O | 2.37 | 0.43 |
| 2:T:20:LYS:HA | 2:T:28:THR:HG23 | 2.01 | 0.43 |
| 2:T:47:ARG:HD3 | 2:T:49:LEU:HB2 | 2.01 | 0.43 |
| 2:T:73:VAL:O | 2:T:74:LYS:HD3 | 2.19 | 0.43 |
| 1:A:401:HIS:O | 1:A:404:ARG:HB2 | 2.18 | 0.43 |
| 1:C:200:LEU:H | 1:C:200:LEU:HD12 | 1.84 | 0.43 |
| 1:C:249:ILE:HG22 | 1:C:250:ILE:N | 2.34 | 0.43 |
| 1:C:254:VAL:HG12 | 1:C:259:LEU:HG | 2.01 | 0.43 |
| 1:C:289:LEU:O | 1:C:290:GLN:C | 2.57 | 0.43 |
| 1:C:302:SER:C | 1:C:304:GLU:N | 2.72 | 0.43 |
| 1:C:350:ARG:HA | 1:C:353:ILE:HD12 | 2.00 | 0.43 |
| 1:C:488:MET:HE3 | 1:C:493:ILE:HB | 1.99 | 0.43 |
| 1:D:401:HIS:O | 1:D:404:ARG:HB2 | 2.19 | 0.43 |
| 1:D:486:GLY:HA3 | 1:D:491:MET:HE2 | 2.00 | 0.43 |
| 1:E:293:ALA:O | 1:E:294:THR:C | 2.56 | 0.43 |
| 1:E:321:LYS:HD2 | 1:E:333:ILE:CG2 | 2.42 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:519:CYS:SG | 1:E:520:MET:N | 2.92 | 0.43 |
| 1:F:241:ALA:HB3 | 2:T:25:ILE:HD12 | 2.01 | 0.43 |
| 1:F:482:THR:OG1 | 1:F:484:GLU:HG2 | 2.19 | 0.43 |
| 1:G:215:LEU:O | 1:G:322:ARG:HA | 2.19 | 0.43 |
| 1:G:7:LYS:HD2 | 1:G:66:PHE:CD2 | 2.53 | 0.43 |
| 1:H:169:VAL:CG1 | 1:H:173:GLY:HA3 | 2.42 | 0.43 |
| 1:H:80:LYS:O | 1:H:83:ASP:HB2 | 2.19 | 0.43 |
| 1:I:109:ALA:HB3 | 1:I:111:MET:CE | 2.49 | 0.43 |
| 1:I:130:GLU:HG3 | 1:I:426:LEU:HD22 | 2.01 | 0.43 |
| 1:I:391:GLU:O | 1:I:394:ALA:HB3 | 2.19 | 0.43 |
| 1:I:487:ASN:O | 1:I:491:MET:HG3 | 2.19 | 0.43 |
| 1:J:109:ALA:HB3 | 1:J:111:MET:CE | 2.48 | 0.43 |
| 1:J:221:LEU:CD1 | 1:J:221:LEU:C | 2.85 | 0.43 |
| 1:J:383:ALA:HB3 | 1:J:389:MET:HA | 2.00 | 0.43 |
| 1:J:411:VAL:HG21 | 1:J:494:LEU:HD12 | 2.00 | 0.43 |
| 1:J:72:GLN:NE2 | 1:J:72:GLN:HA | 2.34 | 0.43 |
| 1:L:130:GLU:HG3 | 1:L:426:LEU:HD22 | 2.01 | 0.43 |
| 1:L:249:ILE:CG2 | 1:L:250:ILE:N | 2.81 | 0.43 |
| 1:L:272:LYS:HE3 | 1:L:272:LYS:HB2 | 1.87 | 0.43 |
| 1:L:286:LYS:CE | 1:L:286:LYS:HA | 2.45 | 0.43 |
| 1:L:34:LYS:HB2 | 1:L:458:CYS:HG | 1.79 | 0.43 |
| 1:M:138:CYS:SG | 1:M:144:ILE:HD13 | 2.59 | 0.43 |
| 1:M:328:ASP:OD1 | 1:M:328:ASP:N | 2.52 | 0.43 |
| 1:M:351:GLN:O | 1:M:354:GLU:CB | 2.67 | 0.43 |
| 1:L:41:ASP:HB2 | 1:M:69:MET:HE2 | 2.00 | 0.43 |
| 1:N:112:ASN:OD1 | 1:N:114:MET:N | 2.52 | 0.43 |
| 1:N:221:LEU:HD22 | 1:N:222:LEU:N | 2.33 | 0.43 |
| 1:N:228:SER:O | 1:N:257:GLU:HB3 | 2.19 | 0.43 |
| 1:N:351:GLN:O | 1:N:354:GLU:CB | 2.67 | 0.43 |
| 1:N:401:HIS:O | 1:N:404:ARG:N | 2.52 | 0.43 |
| 2:S:47:ARG:HD3 | 2:S:49:LEU:HB2 | 2.01 | 0.43 |
| 2:S:67:PHE:HE1 | 2:S:69:ASP:HB2 | 1.84 | 0.43 |
| 2:T:40:VAL:CG2 | 2:T:63:ASP:HB2 | 2.49 | 0.43 |
| 2:T:50:GLU:OE1 | 2:U:50:GLU:HA | 2.18 | 0.43 |
| 2:T:59:VAL:HG23 | 2:T:59:VAL:O | 2.18 | 0.43 |
| 1:A:267:MET:C | 1:A:269:GLY:N | 2.71 | 0.43 |
| 1:A:220:ILE:N | 1:A:318:GLY:O | 2.48 | 0.43 |
| 1:A:456:LEU:HD13 | 1:A:462:PRO:HG2 | 1.98 | 0.43 |
| 1:B:213:VAL:O | 1:B:324:VAL:HA | 2.18 | 0.43 |
| 1:B:220:ILE:CD1 | 1:B:220:ILE:N | 2.81 | 0.43 |
| 1:B:239:ALA:HB1 | 1:B:314:LEU:HD23 | 2.01 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:266:THR:HA | 1:B:271:VAL:O | 2.19 | 0.43 |
| 1:B:76:GLU:HA | 1:B:79:SER:HB3 | 2.01 | 0.43 |
| 1:C:456:LEU:C | 1:C:458:CYS:H | 2.21 | 0.43 |
| 1:C:73:MET:O | 1:C:74:VAL:C | 2.57 | 0.43 |
| 1:D:130:GLU:O | 1:D:133:ALA:HB3 | 2.19 | 0.43 |
| 1:D:322:ARG:CB | 1:D:333:ILE:HD12 | 2.29 | 0.43 |
| 1:D:456:LEU:C | 1:D:458:CYS:H | 2.23 | 0.43 |
| 1:E:438:VAL:O | 1:E:442:VAL:HG23 | 2.19 | 0.43 |
| 1:F:222:LEU:CD2 | 1:F:293:ALA:HB2 | 2.47 | 0.43 |
| 1:G:84:ALA:HB2 | 1:G:506:TYR:CE2 | 2.51 | 0.43 |
| 1:H:349:ILE:O | 1:H:352:GLN:HB2 | 2.17 | 0.43 |
| 1:H:356:ALA:HB1 | 1:H:362:ARG:NE | 2.26 | 0.43 |
| 1:I:203:TYR:HB2 | 1:I:263:VAL:HG13 | 2.00 | 0.43 |
| 1:H:49:ILE:HD11 | 1:I:73:MET:HE3 | 2.01 | 0.43 |
| 1:J:124:VAL:HG13 | 1:J:504:LEU:HD11 | 1.99 | 0.43 |
| 1:J:227:ILE:O | 1:J:254:VAL:HA | 2.19 | 0.43 |
| 1:K:233:MET:HE2 | 1:K:233:MET:CA | 2.46 | 0.43 |
| 1:L:414:GLY:HA2 | 1:L:495:ASP:OD2 | 2.19 | 0.43 |
| 1:M:101:THR:O | 1:M:105:LYS:HG3 | 2.18 | 0.43 |
| 1:M:15:LYS:HD3 | 1:M:15:LYS:HA | 1.83 | 0.43 |
| 1:M:351:GLN:O | 1:M:354:GLU:HB3 | 2.19 | 0.43 |
| 1:M:354:GLU:O | 1:M:355:GLU:C | 2.56 | 0.43 |
| 1:M:391:GLU:OE1 | 1:M:395:ARG:HD3 | 2.18 | 0.43 |
| 1:M:90:THR:O | 1:M:94:VAL:HG23 | 2.18 | 0.43 |
| 1:N:302:SER:HB2 | 1:N:305:ILE:HG13 | 2.00 | 0.43 |
| 1:N:343:GLN:O | 1:N:346:VAL:HB | 2.19 | 0.43 |
| 1:N:385:THR:HG22 | 1:N:388:GLU:HB3 | 2.01 | 0.43 |
| 2:P:5:PRO:HD3 | 2:P:42:ALA:CB | 2.48 | 0.43 |
| 2:O:94:ILE:N | 2:P:4:ARG:O | 2.51 | 0.43 |
| 2:R:12:VAL:HG12 | 2:R:40:VAL:HA | 2.01 | 0.43 |
| 2:S:14:ARG:CB | 2:S:14:ARG:NH1 | 2.82 | 0.43 |
| 2:U:27:LEU:O | 2:U:27:LEU:HD23 | 2.19 | 0.43 |
| 2:U:65:VAL:CG1 | 2:U:94:ILE:HG12 | 2.35 | 0.43 |
| 1:A:155:ASP:OD1 | 1:A:157:THR:HB | 2.19 | 0.42 |
| 1:A:214:GLU:O | 1:A:322:ARG:HD3 | 2.19 | 0.42 |
| 1:A:353:ILE:HG22 | 1:A:354:GLU:N | 2.34 | 0.42 |
| 1:A:87:ASP:OD1 | 1:A:88:GLY:N | 2.51 | 0.42 |
| 1:B:362:ARG:HA | 1:B:365:LEU:HD13 | 2.01 | 0.42 |
| 1:B:368:ARG:HG2 | 1:B:372:LEU:CG | 2.46 | 0.42 |
| 1:B:385:THR:OG1 | 1:B:388:GLU:HB2 | 2.18 | 0.42 |
| 1:B:488:MET:CE | 1:B:493:ILE:HG21 | 2.49 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:59:GLU:OE1 | 1:B:59:GLU:HA | 2.19 | 0.42 |
| 1:C:222:LEU:HD22 | 1:C:300:VAL:HG22 | 1.99 | 0.42 |
| 1:C:250:ILE:O | 1:C:251:ALA:HB2 | 2.19 | 0.42 |
| 1:C:289:LEU:N | 1:C:290:GLN:OE1 | 2.45 | 0.42 |
| 1:D:249:ILE:HB | 1:D:275:ALA:HB1 | 1.96 | 0.42 |
| 1:D:259:LEU:O | 1:D:263:VAL:N | 2.48 | 0.42 |
| 1:D:409:GLU:HG2 | 1:D:409:GLU:O | 2.18 | 0.42 |
| 1:D:95:LEU:HD13 | 1:D:504:LEU:HD23 | 2.01 | 0.42 |
| 1:E:267:MET:C | 1:E:269:GLY:H | 2.23 | 0.42 |
| 1:E:309:LEU:O | 1:E:310:GLU:C | 2.57 | 0.42 |
| 1:F:150:ILE:HD11 | 4:F:1:ADP:C8 | 2.54 | 0.42 |
| 1:F:219:PHE:HD1 | 1:F:319:GLN:HE21 | 1.66 | 0.42 |
| 1:F:279:PRO:CB | 1:F:288:MET:HE1 | 2.48 | 0.42 |
| 1:F:291:ASP:O | 1:F:295:LEU:HB2 | 2.18 | 0.42 |
| 1:F:353:ILE:O | 1:F:355:GLU:N | 2.52 | 0.42 |
| 1:F:456:LEU:HA | 1:F:456:LEU:HD12 | 1.86 | 0.42 |
| 1:G:114:MET:O | 1:G:118:ARG:HG3 | 2.19 | 0.42 |
| 1:G:14:VAL:O | 1:G:15:LYS:C | 2.57 | 0.42 |
| 1:G:211:GLY:O | 1:G:325:ILE:O | 2.37 | 0.42 |
| 1:G:233:MET:HE2 | 1:G:237:LEU:HB2 | 2.01 | 0.42 |
| 1:G:479:ASN:HB3 | 1:G:482:THR:OG1 | 2.19 | 0.42 |
| 1:H:158:VAL:C | 1:H:160:LYS:N | 2.71 | 0.42 |
| 1:H:205:ILE:HD13 | 1:H:211:GLY:CA | 2.42 | 0.42 |
| 1:H:362:ARG:HB3 | 1:H:362:ARG:HH11 | 1.84 | 0.42 |
| 1:H:364:LYS:O | 1:H:365:LEU:C | 2.57 | 0.42 |
| 1:H:389:MET:HE1 | 1:H:393:LYS:HB2 | 2.00 | 0.42 |
| 1:I:226:LYS:HG3 | 1:I:252:GLU:HB3 | 2.01 | 0.42 |
| 1:I:472:GLY:HA3 | 1:I:476:TYR:HD2 | 1.84 | 0.42 |
| 1:J:266:THR:HG22 | 1:J:273:VAL:H | 1.84 | 0.42 |
| 1:K:17:LEU:HA | 1:K:20:VAL:CG1 | 2.49 | 0.42 |
| 1:K:200:LEU:HD11 | 1:K:276:VAL:HA | 1.99 | 0.42 |
| 1:M:107:VAL:HG11 | 1:M:515:ILE:HG23 | 2.00 | 0.42 |
| 1:M:402:ALA:O | 1:M:405:ALA:HB3 | 2.19 | 0.42 |
| 1:M:432:GLN:N | 1:M:432:GLN:OE1 | 2.52 | 0.42 |
| 1:M:465:VAL:HG11 | 1:M:478:TYR:CD2 | 2.54 | 0.42 |
| 1:N:508:ALA:O | 1:N:509:SER:C | 2.56 | 0.42 |
| 2:S:3:ILE:HD12 | 2:S:3:ILE:H | 1.83 | 0.42 |
| 2:T:3:ILE:N | 2:T:3:ILE:HD12 | 2.34 | 0.42 |
| 1:B:277:LYS:HD3 | 1:B:285:ARG:NH2 | 2.20 | 0.42 |
| 1:B:27:VAL:HG13 | 1:B:53:GLY:HA2 | 2.00 | 0.42 |
| 1:B:292:ILE:O | 1:B:295:LEU:HB3 | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:449:ALA:O | 1:B:450:PRO:C | 2.57 | 0.42 |
| 1:C:128:VAL:O | 1:C:129:GLU:C | 2.57 | 0.42 |
| 1:C:232:GLU:O | 1:C:310:GLU:OE2 | 2.37 | 0.42 |
| 1:C:261:THR:O | 1:C:265:ASN:ND2 | 2.52 | 0.42 |
| 1:C:288:MET:HG2 | 1:C:368:ARG:HE | 1.83 | 0.42 |
| 1:C:178:GLU:O | 1:C:380:LYS:HA | 2.18 | 0.42 |
| 1:C:433:ASN:ND2 | 1:C:435:ASP:HB2 | 2.31 | 0.42 |
| 1:D:293:ALA:O | 1:D:297:GLY:N | 2.52 | 0.42 |
| 1:E:266:THR:HG22 | 1:E:273:VAL:N | 2.29 | 0.42 |
| 1:E:302:SER:CB | 1:E:305:ILE:HB | 2.47 | 0.42 |
| 1:E:41:ASP:O | 1:E:42:LYS:CG | 2.67 | 0.42 |
| 1:E:487:ASN:OD1 | 1:E:489:ILE:N | 2.52 | 0.42 |
| 1:E:88:GLY:O | 1:E:91:THR:HB | 2.19 | 0.42 |
| 1:F:150:ILE:HD11 | 4:F:1:ADP:N7 | 2.34 | 0.42 |
| 1:G:245:LYS:HE2 | 1:G:245:LYS:CA | 2.38 | 0.42 |
| 1:H:349:ILE:O | 1:H:350:ARG:C | 2.58 | 0.42 |
| 1:I:354:GLU:HG3 | 1:I:355:GLU:N | 2.33 | 0.42 |
| 1:J:326:ASN:ND2 | 1:J:328:ASP:H | 2.17 | 0.42 |
| 1:K:107:VAL:CG2 | 1:K:108:ALA:H | 2.32 | 0.42 |
| 1:K:194:GLN:CG | 1:K:331:THR:HB | 2.48 | 0.42 |
| 1:K:350:ARG:HE | 1:K:369:VAL:CG1 | 2.33 | 0.42 |
| 1:K:192:GLY:C | 1:K:376:VAL:HG23 | 2.39 | 0.42 |
| 1:K:420:ILE:HG13 | 1:K:451:LEU:HD22 | 2.01 | 0.42 |
| 1:L:172:GLU:N | 1:L:172:GLU:OE1 | 2.52 | 0.42 |
| 1:L:299:THR:OG1 | 1:L:316:ASP:HA | 2.19 | 0.42 |
| 1:L:339:GLU:O | 1:L:340:ALA:C | 2.58 | 0.42 |
| 1:L:420:ILE:HG23 | 1:L:470:LYS:HD3 | 2.01 | 0.42 |
| 1:L:95:LEU:O | 1:L:96:ALA:C | 2.56 | 0.42 |
| 1:M:197:ARG:HG2 | 1:M:277:LYS:O | 2.19 | 0.42 |
| 1:M:400:LEU:O | 1:M:400:LEU:HD23 | 2.19 | 0.42 |
| 1:M:90:THR:O | 1:M:93:THR:HB | 2.19 | 0.42 |
| 1:N:420:ILE:CG2 | 1:N:470:LYS:HD3 | 2.50 | 0.42 |
| 1:N:57:ALA:O | 1:N:58:ARG:C | 2.58 | 0.42 |
| 1:A:14:VAL:O | 1:A:18:ARG:HG3 | 2.19 | 0.42 |
| 1:A:219:PHE:HD1 | 1:A:319:GLN:NE2 | 2.03 | 0.42 |
| 1:A:325:ILE:N | 1:A:325:ILE:CD1 | 2.79 | 0.42 |
| 1:B:266:THR:HG22 | 1:B:273:VAL:N | 2.31 | 0.42 |
| 1:B:456:LEU:HD13 | 1:B:462:PRO:HG2 | 2.00 | 0.42 |
| 1:B:494:LEU:N | 1:B:494:LEU:HD23 | 2.34 | 0.42 |
| 1:C:205:ILE:HG12 | 1:C:211:GLY:HA2 | 2.01 | 0.42 |
| 1:C:230:ILE:C | 1:C:232:GLU:N | 2.71 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:509:SER:HB3 | 1:C:385:THR:HG23 | 2.01 | 0.42 |
| 1:C:305:ILE:HG21 | 1:D:263:VAL:HG11 | 2.01 | 0.42 |
| 1:D:302:SER:C | 1:D:304:GLU:H | 2.23 | 0.42 |
| 1:E:136:VAL:HA | 1:E:137:PRO:HD3 | 1.86 | 0.42 |
| 1:E:235:PRO:HG2 | 1:E:236:VAL:HG23 | 2.01 | 0.42 |
| 1:F:203:TYR:H | 1:F:203:TYR:HD1 | 1.65 | 0.42 |
| 1:F:206:ASN:HB3 | 1:F:214:GLU:N | 2.33 | 0.42 |
| 1:F:455:VAL:HG11 | 1:F:462:PRO:HA | 2.02 | 0.42 |
| 1:G:40:LEU:HD13 | 1:G:59:GLU:HG3 | 2.01 | 0.42 |
| 1:G:411:VAL:HG12 | 1:G:496:PRO:CA | 2.39 | 0.42 |
| 1:H:221:LEU:CD1 | 1:H:223:ALA:H | 2.33 | 0.42 |
| 1:I:17:LEU:HA | 1:I:20:VAL:CG1 | 2.49 | 0.42 |
| 1:J:218:PRO:CB | 1:J:246:PRO:HB2 | 2.49 | 0.42 |
| 1:J:415:GLY:H | 1:J:417:VAL:CG2 | 2.26 | 0.42 |
| 1:J:420:ILE:CD1 | 1:J:448:GLU:HG2 | 2.50 | 0.42 |
| 1:K:130:GLU:HG3 | 1:K:426:LEU:HD22 | 2.01 | 0.42 |
| 1:K:399:ALA:O | 1:K:400:LEU:C | 2.58 | 0.42 |
| 1:L:149:THR:H | 1:L:159:GLY:HA3 | 1.83 | 0.42 |
| 1:L:24:ALA:O | 1:L:28:LYS:HG2 | 2.20 | 0.42 |
| 1:L:325:ILE:N | 1:L:325:ILE:CD1 | 2.82 | 0.42 |
| 1:L:77:VAL:HG22 | 1:L:506:TYR:HB3 | 2.01 | 0.42 |
| 1:M:233:MET:O | 1:M:234:LEU:C | 2.57 | 0.42 |
| 1:M:258:ALA:O | 1:M:261:THR:OG1 | 2.36 | 0.42 |
| 1:M:37:ASN:HB3 | 1:M:51:LYS:CG | 2.49 | 0.42 |
| 1:M:66:PHE:HA | 1:M:520:MET:CE | 2.49 | 0.42 |
| 1:N:290:GLN:HB3 | 1:N:345:ARG:HH21 | 1.84 | 0.42 |
| 1:N:501:ARG:NH1 | 1:N:505:GLN:OE1 | 2.51 | 0.42 |
| 1:N:72:GLN:HE21 | 1:N:72:GLN:HA | 1.84 | 0.42 |
| 2:O:20:LYS:CG | 2:O:27:LEU:HD23 | 2.49 | 0.42 |
| 2:T:34:LYS:HG3 | 2:T:35:SER:N | 2.26 | 0.42 |
| 2:T:40:VAL:HG21 | 2:T:63:ASP:HB2 | 2.00 | 0.42 |
| 1:A:220:ILE:CD1 | 1:A:220:ILE:H | 2.31 | 0.42 |
| 1:A:262:LEU:O | 1:A:266:THR:HG23 | 2.19 | 0.42 |
| 1:A:23:LEU:HD23 | 1:A:60:ILE:HB | 2.01 | 0.42 |
| 1:B:224:ASP:HB2 | 1:B:303:GLU:CB | 2.42 | 0.42 |
| 1:C:42:LYS:HE2 | 1:C:48:THR:HB | 2.00 | 0.42 |
| 1:D:278:ALA:CB | 1:D:279:PRO:CD | 2.95 | 0.42 |
| 1:E:256:GLY:HA2 | 1:E:259:LEU:HB2 | 2.01 | 0.42 |
| 1:E:38:VAL:HG12 | 1:E:39:VAL:N | 2.34 | 0.42 |
| 1:E:5:ASP:HB2 | 1:E:524:LEU:CD2 | 2.47 | 0.42 |
| 1:F:309:LEU:HD12 | 1:F:309:LEU:N | 2.34 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:7:LYS:HD2 | 1:F:66:PHE:CD2 | 2.55 | 0.42 |
| 1:G:299:THR:N | 1:G:316:ASP:O | 2.52 | 0.42 |
| 1:G:54:VAL:O | 1:G:58:ARG:HG3 | 2.19 | 0.42 |
| 1:G:59:GLU:HA | 1:G:59:GLU:OE1 | 2.19 | 0.42 |
| 1:H:112:ASN:HA | 1:H:113:PRO:HD3 | 1.73 | 0.42 |
| 1:I:184:GLN:HA | 1:I:184:GLN:OE1 | 2.19 | 0.42 |
| 1:I:187:LEU:HD23 | 1:I:188:ASP:N | 2.34 | 0.42 |
| 1:I:414:GLY:N | 1:I:494:LEU:HA | 2.33 | 0.42 |
| 1:I:95:LEU:O | 1:I:96:ALA:C | 2.58 | 0.42 |
| 1:J:248:LEU:HD22 | 1:J:249:ILE:N | 2.32 | 0.42 |
| 1:K:164:GLU:O | 1:K:167:ASP:HB3 | 2.18 | 0.42 |
| 1:L:178:GLU:O | 1:L:380:LYS:HA | 2.19 | 0.42 |
| 1:L:412:VAL:O | 1:L:494:LEU:HB2 | 2.20 | 0.42 |
| 1:L:74:VAL:O | 1:L:75:LYS:C | 2.57 | 0.42 |
| 2:S:7:HIS:O | 2:S:8:ASP:CB | 2.57 | 0.42 |
| 1:A:247:LEU:HD13 | 1:A:248:LEU:O | 2.18 | 0.42 |
| 1:A:302:SER:HB2 | 1:A:305:ILE:CB | 2.48 | 0.42 |
| 1:A:221:LEU:HD13 | 1:A:317:LEU:CD2 | 2.49 | 0.42 |
| 1:A:7:LYS:HD2 | 1:A:66:PHE:CD2 | 2.55 | 0.42 |
| 1:B:235:PRO:O | 1:B:239:ALA:HB2 | 2.20 | 0.42 |
| 1:B:29:VAL:HG23 | 1:B:30:THR:CG2 | 2.47 | 0.42 |
| 1:C:131:LEU:HD23 | 1:C:422:VAL:HG11 | 2.00 | 0.42 |
| 1:D:291:ASP:OD1 | 1:D:292:ILE:N | 2.52 | 0.42 |
| 1:D:352:GLN:C | 1:D:365:LEU:HD11 | 2.39 | 0.42 |
| 1:D:401:HIS:O | 1:D:404:ARG:N | 2.52 | 0.42 |
| 1:E:193:MET:O | 1:E:331:THR:HG23 | 2.19 | 0.42 |
| 1:E:265:ASN:HB3 | 1:E:271:VAL:CG2 | 2.47 | 0.42 |
| 1:E:199:TYR:CE1 | 1:E:327:LYS:HG3 | 2.54 | 0.42 |
| 1:E:349:ILE:CG2 | 1:E:365:LEU:HD21 | 2.50 | 0.42 |
| 1:E:183:LEU:HD22 | 1:E:384:ALA:HA | 2.02 | 0.42 |
| 1:E:405:ALA:HA | 1:E:408:GLU:HG2 | 2.01 | 0.42 |
| 1:E:450:PRO:O | 1:E:454:ILE:HG13 | 2.18 | 0.42 |
| 1:E:54:VAL:HG13 | 1:E:55:SER:N | 2.35 | 0.42 |
| 1:E:80:LYS:HD2 | 1:E:506:TYR:CZ | 2.54 | 0.42 |
| 1:F:194:GLN:HG3 | 1:F:331:THR:OG1 | 2.20 | 0.42 |
| 1:F:216:GLU:HA | 1:F:216:GLU:OE1 | 2.19 | 0.42 |
| 1:F:150:ILE:HG21 | 1:F:494:LEU:O | 2.18 | 0.42 |
| 1:G:203:TYR:CD1 | 1:G:203:TYR:N | 2.87 | 0.42 |
| 1:H:128:VAL:O | 1:H:132:LYS:HG3 | 2.19 | 0.42 |
| 1:H:149:THR:H | 1:H:159:GLY:HA3 | 1.84 | 0.42 |
| 1:H:40:LEU:HD23 | 1:H:50:THR:HG22 | 2.00 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:200:LEU:N | 1:I:200:LEU:HD12 | 2.35 | 0.42 |
| 1:I:323:VAL:O | 1:I:323:VAL:HG13 | 2.20 | 0.42 |
| 1:H:37:ASN:O | 1:I:517:THR:HA | 2.20 | 0.42 |
| 1:I:520:MET:HB3 | 1:I:520:MET:HE2 | 1.84 | 0.42 |
| 1:J:155:ASP:CG | 1:J:158:VAL:HG23 | 2.39 | 0.42 |
| 1:J:172:GLU:OE1 | 1:J:172:GLU:N | 2.53 | 0.42 |
| 1:K:221:LEU:CD1 | 1:K:221:LEU:C | 2.87 | 0.42 |
| 1:K:236:VAL:HG23 | 1:K:237:LEU:H | 1.85 | 0.42 |
| 1:K:414:GLY:N | 1:K:494:LEU:HA | 2.35 | 0.42 |
| 1:M:218:PRO:CG | 1:M:246:PRO:HB2 | 2.48 | 0.42 |
| 1:M:222:LEU:HD11 | 1:M:293:ALA:HA | 2.02 | 0.42 |
| 1:M:386:GLU:HG2 | 1:M:390:LYS:HE2 | 2.01 | 0.42 |
| 1:M:433:ASN:HD22 | 1:M:434:GLU:N | 2.15 | 0.42 |
| 1:N:126:ALA:HB1 | 1:N:426:LEU:HD13 | 2.00 | 0.42 |
| 1:N:130:GLU:HB3 | 1:N:422:VAL:HG12 | 2.01 | 0.42 |
| 1:N:149:THR:HG21 | 1:N:156:GLU:HA | 1.99 | 0.42 |
| 1:N:354:GLU:CG | 1:N:355:GLU:N | 2.83 | 0.42 |
| 1:N:185:ASP:HA | 1:N:380:LYS:O | 2.20 | 0.42 |
| 2:O:4:ARG:HA | 2:O:5:PRO:HD2 | 1.86 | 0.42 |
| 2:Q:17:VAL:CG1 | 2:Q:34:LYS:HA | 2.49 | 0.42 |
| 2:R:78:ILE:CD1 | 2:R:78:ILE:N | 2.82 | 0.42 |
| 2:U:43:VAL:HG23 | 2:U:61:VAL:HG22 | 2.02 | 0.42 |
| 1:A:278:ALA:O | 1:A:279:PRO:O | 2.37 | 0.42 |
| 1:A:350:ARG:HD3 | 1:A:350:ARG:HA | 1.83 | 0.42 |
| 1:A:41:ASP:O | 1:A:42:LYS:CG | 2.67 | 0.42 |
| 1:B:259:LEU:O | 1:B:260:ALA:C | 2.57 | 0.42 |
| 1:B:314:LEU:C | 1:B:314:LEU:HD12 | 2.39 | 0.42 |
| 1:C:263:VAL:HG12 | 1:C:267:MET:SD | 2.59 | 0.42 |
| 1:C:296:THR:HG22 | 1:C:335:GLY:CA | 2.42 | 0.42 |
| 1:C:430:ARG:NH1 | 1:C:430:ARG:HG2 | 2.35 | 0.42 |
| 1:C:5:ASP:O | 1:C:66:PHE:HZ | 2.02 | 0.42 |
| 1:D:147:VAL:CA | 1:D:150:ILE:HG22 | 2.50 | 0.42 |
| 1:D:206:ASN:HB3 | 1:D:214:GLU:H | 1.85 | 0.42 |
| 1:D:288:MET:O | 1:D:289:LEU:HG | 2.20 | 0.42 |
| 1:D:361:ASP:C | 1:D:363:GLU:H | 2.22 | 0.42 |
| 1:E:113:PRO:O | 1:E:116:LEU:HB2 | 2.20 | 0.42 |
| 1:E:288:MET:O | 1:E:289:LEU:HG | 2.19 | 0.42 |
| 1:E:434:GLU:HA | 1:E:437:ASN:HD22 | 1.85 | 0.42 |
| 1:F:116:LEU:O | 1:F:120:ILE:HG13 | 2.19 | 0.42 |
| 1:F:349:ILE:HG23 | 1:F:365:LEU:HD21 | 2.00 | 0.42 |
| 1:F:72:GLN:NE2 | 1:F:72:GLN:HA | 2.34 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:206:ASN:HB3 | 1:G:214:GLU:N | 2.33 | 0.42 |
| 1:G:180:GLY:HA2 | 1:G:380:LYS:HB3 | 2.00 | 0.42 |
| 1:G:177:VAL:CG1 | 1:G:397:GLU:HG2 | 2.48 | 0.42 |
| 1:H:200:LEU:HD12 | 1:H:200:LEU:N | 2.34 | 0.42 |
| 1:H:253:ASP:OD2 | 1:H:277:LYS:HD3 | 2.19 | 0.42 |
| 1:H:313:THR:CG2 | 1:H:314:LEU:N | 2.83 | 0.42 |
| 1:H:361:ASP:O | 1:H:365:LEU:HG | 2.19 | 0.42 |
| 1:H:66:PHE:HD1 | 1:H:520:MET:HE2 | 1.83 | 0.42 |
| 1:I:112:ASN:OD1 | 1:I:114:MET:N | 2.52 | 0.42 |
| 1:I:130:GLU:O | 1:I:133:ALA:HB3 | 2.19 | 0.42 |
| 1:I:233:MET:O | 1:I:234:LEU:C | 2.58 | 0.42 |
| 1:I:277:LYS:HZ2 | 1:I:277:LYS:HB2 | 1.83 | 0.42 |
| 1:J:419:LEU:O | 1:J:422:VAL:HG22 | 2.20 | 0.42 |
| 1:J:95:LEU:O | 1:J:96:ALA:C | 2.58 | 0.42 |
| 1:K:266:THR:CG2 | 1:K:273:VAL:H | 2.32 | 0.42 |
| 1:K:419:LEU:HD21 | 1:K:500:THR:HG23 | 2.00 | 0.42 |
| 1:K:419:LEU:HA | 1:K:422:VAL:HG22 | 2.01 | 0.42 |
| 1:K:433:ASN:ND2 | 1:K:434:GLU:N | 2.67 | 0.42 |
| 1:L:381:VAL:HB | 1:L:389:MET:HE3 | 2.02 | 0.42 |
| 1:L:171:LYS:HD3 | 1:L:407:VAL:CG1 | 2.49 | 0.42 |
| 1:L:419:LEU:O | 1:L:422:VAL:HG22 | 2.20 | 0.42 |
| 1:L:66:PHE:HA | 1:L:520:MET:CE | 2.49 | 0.42 |
| 1:N:104:LEU:O | 1:N:107:VAL:HG22 | 2.19 | 0.42 |
| 1:N:476:TYR:HA | 1:N:486:GLY:O | 2.19 | 0.42 |
| 1:N:19:GLY:HA3 | 1:N:67:GLU:O | 2.20 | 0.42 |
| 2:O:5:PRO:HG3 | 2:O:43:VAL:C | 2.39 | 0.42 |
| 2:P:47:ARG:HD2 | 2:P:55:LYS:HD2 | 2.01 | 0.42 |
| 1:A:200:LEU:H | 1:A:200:LEU:HD12 | 1.85 | 0.42 |
| 1:A:236:VAL:O | 1:A:239:ALA:HB3 | 2.20 | 0.42 |
| 1:A:252:GLU:O | 1:A:277:LYS:HE2 | 2.20 | 0.42 |
| 1:A:456:LEU:HA | 1:A:456:LEU:HD12 | 1.86 | 0.42 |
| 1:B:134:LEU:HD11 | 1:B:425:LYS:HZ1 | 1.82 | 0.42 |
| 1:B:207:LYS:HZ2 | 1:B:207:LYS:HB2 | 1.83 | 0.42 |
| 1:C:220:ILE:N | 1:C:220:ILE:CD1 | 2.82 | 0.42 |
| 1:C:301:ILE:HG12 | 1:C:307:MET:CE | 2.50 | 0.42 |
| 1:C:411:VAL:HG12 | 1:C:496:PRO:CA | 2.43 | 0.42 |
| 1:D:496:PRO:O | 1:D:497:THR:C | 2.56 | 0.42 |
| 1:E:339:GLU:HA | 1:E:342:ILE:CB | 2.48 | 0.42 |
| 1:E:357:THR:O | 1:E:359:ASP:N | 2.53 | 0.42 |
| 1:F:128:VAL:CG1 | 1:F:132:LYS:HE2 | 2.49 | 0.42 |
| 1:F:88:GLY:HA2 | 4:F:1:ADP:O2B | 2.20 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:339:GLU:O | 1:G:343:GLN:OE1 | 2.36 | 0.42 |
| 1:G:348:GLN:NE2 | 1:G:352:GLN:HE21 | 2.15 | 0.42 |
| 1:G:473:ASP:O | 1:G:474:GLY:C | 2.58 | 0.42 |
| 1:H:432:GLN:N | 1:H:432:GLN:OE1 | 2.53 | 0.42 |
| 1:I:165:ALA:O | 1:I:168:LYS:HB2 | 2.20 | 0.42 |
| 1:I:433:ASN:ND2 | 1:I:434:GLU:N | 2.68 | 0.42 |
| 1:J:140:ASP:O | 1:J:144:ILE:HG12 | 2.19 | 0.42 |
| 1:K:230:ILE:O | 1:K:231:ARG:C | 2.58 | 0.42 |
| 1:K:37:ASN:HB3 | 1:K:51:LYS:CG | 2.50 | 0.42 |
| 1:K:37:ASN:ND2 | 1:K:37:ASN:H | 2.18 | 0.42 |
| 1:K:77:VAL:HG11 | 1:K:510:VAL:HB | 2.00 | 0.42 |
| 1:L:349:ILE:HA | 1:L:352:GLN:NE2 | 2.35 | 0.42 |
| 1:L:478:TYR:HB2 | 1:L:485:TYR:CE2 | 2.55 | 0.42 |
| 1:M:203:TYR:CD1 | 1:M:203:TYR:N | 2.88 | 0.42 |
| 1:M:353:ILE:HA | 1:M:365:LEU:HD12 | 2.00 | 0.42 |
| 1:N:232:GLU:OE1 | 1:N:232:GLU:N | 2.37 | 0.42 |
| 1:N:272:LYS:HE3 | 1:N:272:LYS:HB2 | 1.68 | 0.42 |
| 1:N:348:GLN:O | 1:N:351:GLN:HB3 | 2.19 | 0.42 |
| 1:N:349:ILE:O | 1:N:350:ARG:C | 2.58 | 0.42 |
| 1:N:30:THR:HB | 1:N:51:LYS:O | 2.19 | 0.42 |
| 2:S:41:LEU:O | 2:S:61:VAL:HG13 | 2.19 | 0.42 |
| 2:S:7:HIS:ND1 | 2:S:7:HIS:O | 2.52 | 0.42 |
| 2:T:44:GLY:O | 2:T:45:ASN:C | 2.58 | 0.42 |
| 2:U:20:LYS:HG2 | 2:U:27:LEU:HD23 | 2.00 | 0.42 |
| 2:U:31:ALA:O | 2:U:32:ALA:HB3 | 2.20 | 0.42 |
| 1:A:147:VAL:HA | 1:A:150:ILE:HG22 | 2.01 | 0.42 |
| 1:A:241:ALA:HA | 1:A:271:VAL:HG12 | 2.01 | 0.42 |
| 1:A:290:GLN:O | 1:A:294:THR:HG23 | 2.19 | 0.42 |
| 1:A:409:GLU:OE1 | 1:A:501:ARG:NH2 | 2.52 | 0.42 |
| 1:B:267:MET:C | 1:B:269:GLY:H | 2.21 | 0.42 |
| 1:B:272:LYS:NZ | 1:B:272:LYS:CB | 2.83 | 0.42 |
| 1:C:195:PHE:CE1 | 1:C:330:THR:HB | 2.55 | 0.42 |
| 1:C:417:VAL:HA | 1:C:420:ILE:CG2 | 2.49 | 0.42 |
| 1:D:349:ILE:HA | 1:D:352:GLN:HE21 | 1.76 | 0.42 |
| 1:D:368:ARG:O | 1:D:369:VAL:C | 2.58 | 0.42 |
| 1:D:433:ASN:OD1 | 1:D:436:GLN:HB2 | 2.20 | 0.42 |
| 1:D:434:GLU:HA | 1:D:437:ASN:HD22 | 1.85 | 0.42 |
| 1:E:326:ASN:HD21 | 1:E:328:ASP:HB2 | 1.83 | 0.42 |
| 1:E:345:ARG:O | 1:E:349:ILE:HG13 | 2.19 | 0.42 |
| 1:E:441:LYS:HA | 1:E:441:LYS:HD2 | 1.80 | 0.42 |
| 1:E:475:ASN:ND2 | 1:E:475:ASN:N | 2.67 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:7:LYS:HD2 | 1:E:66:PHE:CD2 | 2.55 | 0.42 |
| 1:F:23:LEU:HD23 | 1:F:60:ILE:HB | 2.02 | 0.42 |
| 1:F:302:SER:O | 1:F:305:ILE:N | 2.50 | 0.42 |
| 1:F:185:ASP:HA | 1:F:380:LYS:O | 2.20 | 0.42 |
| 1:G:273:VAL:O | 1:G:274:ALA:HB2 | 2.20 | 0.42 |
| 1:G:279:PRO:CB | 1:G:285:ARG:HA | 2.47 | 0.42 |
| 1:G:430:ARG:HG2 | 1:G:430:ARG:NH1 | 2.35 | 0.42 |
| 1:H:130:GLU:O | 1:H:133:ALA:HB3 | 2.19 | 0.42 |
| 1:I:44:PHE:CD1 | 1:I:44:PHE:N | 2.88 | 0.42 |
| 1:J:455:VAL:CG1 | 1:J:460:GLU:HB2 | 2.48 | 0.42 |
| 1:K:112:ASN:OD1 | 1:K:114:MET:N | 2.52 | 0.42 |
| 1:K:226:LYS:HG3 | 1:K:252:GLU:CB | 2.48 | 0.42 |
| 1:L:152:ALA:HB1 | 1:L:158:VAL:HG21 | 2.02 | 0.42 |
| 1:L:270:ILE:HG22 | 1:L:271:VAL:N | 2.34 | 0.42 |
| 1:L:349:ILE:O | 1:L:350:ARG:C | 2.57 | 0.42 |
| 1:M:152:ALA:O | 1:M:153:ASN:HB3 | 2.20 | 0.42 |
| 1:M:192:GLY:C | 1:M:376:VAL:HG23 | 2.39 | 0.42 |
| 1:M:218:PRO:HB3 | 1:M:246:PRO:O | 2.19 | 0.42 |
| 1:M:402:ALA:O | 1:M:406:ALA:N | 2.40 | 0.42 |
| 1:N:354:GLU:HG2 | 1:N:355:GLU:H | 1.85 | 0.42 |
| 1:N:44:PHE:N | 1:N:44:PHE:CD1 | 2.87 | 0.42 |
| 1:N:475:ASN:ND2 | 1:N:489:ILE:HD12 | 2.35 | 0.42 |
| 2:Q:7:HIS:HB3 | 2:Q:45:ASN:HD22 | 1.85 | 0.42 |
| 2:T:9:ARG:NH1 | 2:T:86:MET:HA | 2.35 | 0.42 |
| 2:U:8:ASP:OD2 | 2:U:87:SER:HB2 | 2.20 | 0.42 |
| 1:A:222:LEU:HD22 | 1:A:293:ALA:HB2 | 2.02 | 0.42 |
| 1:A:451:LEU:O | 1:A:454:ILE:HB | 2.19 | 0.42 |
| 1:B:227:ILE:CD1 | 1:B:227:ILE:N | 2.79 | 0.42 |
| 1:B:246:PRO:HB3 | 1:B:272:LYS:HZ2 | 1.84 | 0.42 |
| 1:B:357:THR:HB | 1:B:361:ASP:CB | 2.49 | 0.42 |
| 1:B:456:LEU:HD13 | 1:B:462:PRO:HG3 | 1.99 | 0.42 |
| 1:C:117:LYS:HG2 | 1:C:121:ASP:OD2 | 2.19 | 0.42 |
| 1:C:206:ASN:HB2 | 1:C:214:GLU:H | 1.84 | 0.42 |
| 1:C:278:ALA:CB | 1:C:279:PRO:CD | 2.87 | 0.42 |
| 1:C:301:ILE:O | 1:C:303:GLU:N | 2.47 | 0.42 |
| 1:D:147:VAL:C | 1:D:150:ILE:HG22 | 2.41 | 0.42 |
| 1:E:218:PRO:HA | 1:E:246:PRO:O | 2.20 | 0.42 |
| 1:F:177:VAL:CG1 | 1:F:397:GLU:CG | 2.97 | 0.42 |
| 1:E:517:THR:HG23 | 1:F:39:VAL:HG23 | 2.01 | 0.42 |
| 1:G:158:VAL:O | 1:G:159:GLY:C | 2.58 | 0.42 |
| 1:G:177:VAL:HG22 | 1:G:393:LYS:HG3 | 2.01 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:208:PRO:HB2 | 1:G:212:ALA:HB3 | 2.01 | 0.42 |
| 1:G:349:ILE:HG22 | 1:G:349:ILE:O | 2.19 | 0.42 |
| 1:G:383:ALA:HB3 | 1:G:389:MET:HE1 | 2.00 | 0.42 |
| 1:G:451:LEU:CD2 | 1:G:451:LEU:C | 2.89 | 0.42 |
| 1:G:496:PRO:O | 1:G:497:THR:C | 2.58 | 0.42 |
| 1:I:158:VAL:O | 1:I:159:GLY:C | 2.56 | 0.42 |
| 1:I:233:MET:HB3 | 1:I:237:LEU:HB2 | 2.01 | 0.42 |
| 1:J:359:ASP:O | 1:J:363:GLU:CB | 2.68 | 0.42 |
| 1:J:345:ARG:HH22 | 1:J:368:ARG:HH22 | 1.67 | 0.42 |
| 1:J:384:ALA:O | 1:K:281:PHE:CZ | 2.72 | 0.42 |
| 1:K:354:GLU:CG | 1:K:355:GLU:N | 2.83 | 0.42 |
| 1:L:345:ARG:HA | 1:L:348:GLN:HE21 | 1.84 | 0.42 |
| 1:L:453:GLN:O | 1:L:456:LEU:HB3 | 2.20 | 0.42 |
| 1:L:7:LYS:HG3 | 1:L:66:PHE:CZ | 2.54 | 0.42 |
| 1:L:19:GLY:HA3 | 1:L:67:GLU:O | 2.19 | 0.42 |
| 1:M:201:SER:HA | 1:M:202:PRO:HD3 | 1.90 | 0.42 |
| 1:N:17:LEU:HA | 1:N:20:VAL:CG1 | 2.50 | 0.42 |
| 1:N:214:GLU:HG2 | 1:N:324:VAL:HG12 | 2.00 | 0.42 |
| 1:N:323:VAL:CG2 | 1:N:332:ILE:HG22 | 2.49 | 0.42 |
| 1:N:38:VAL:HG12 | 1:N:39:VAL:N | 2.34 | 0.42 |
| 2:P:14:ARG:CB | 2:P:14:ARG:HH11 | 2.33 | 0.42 |
| 2:P:55:LYS:N | 2:P:55:LYS:HE2 | 2.23 | 0.42 |
| 2:Q:20:LYS:HA | 2:Q:28:THR:CG2 | 2.50 | 0.42 |
| 2:Q:11:ILE:CB | 2:Q:42:ALA:HB3 | 2.42 | 0.42 |
| 2:Q:46:GLY:HA3 | 2:Q:55:LYS:O | 2.19 | 0.42 |
| 2:R:47:ARG:HD3 | 2:R:49:LEU:CD1 | 2.43 | 0.42 |
| 2:U:16:GLU:CB | 2:U:19:THR:OG1 | 2.67 | 0.42 |
| 1:G:270:ILE:HD11 | 2:U:27:LEU:HD13 | 2.00 | 0.42 |
| 2:U:7:HIS:ND1 | 2:U:7:HIS:O | 2.53 | 0.42 |
| 1:A:168:LYS:O | 1:A:170:GLY:N | 2.53 | 0.42 |
| 1:A:295:LEU:C | 1:A:295:LEU:CD2 | 2.88 | 0.42 |
| 1:B:479:ASN:O | 1:B:483:GLU:N | 2.53 | 0.42 |
| 1:C:232:GLU:O | 1:C:233:MET:CB | 2.66 | 0.42 |
| 1:C:233:MET:HE2 | 1:C:233:MET:O | 2.20 | 0.42 |
| 1:C:293:ALA:O | 1:C:296:THR:N | 2.53 | 0.42 |
| 1:C:7:LYS:HD2 | 1:C:66:PHE:CD2 | 2.55 | 0.42 |
| 1:D:202:PRO:HG2 | 1:D:203:TYR:CE1 | 2.54 | 0.42 |
| 1:D:262:LEU:HD11 | 1:D:273:VAL:HB | 2.01 | 0.42 |
| 1:D:279:PRO:HB2 | 1:D:285:ARG:HA | 2.02 | 0.42 |
| 1:D:296:THR:HA | 1:D:335:GLY:HA3 | 2.02 | 0.42 |
| 1:E:234:LEU:HA | 1:E:237:LEU:HB3 | 2.01 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:240:VAL:C | 1:E:242:LYS:N | 2.73 | 0.42 |
| 1:E:325:ILE:HG22 | 1:E:326:ASN:O | 2.20 | 0.42 |
| 1:E:404:ARG:NH1 | 1:E:404:ARG:HG3 | 2.34 | 0.42 |
| 1:F:194:GLN:HG2 | 1:F:195:PHE:N | 2.34 | 0.42 |
| 1:F:259:LEU:O | 1:F:263:VAL:N | 2.50 | 0.42 |
| 1:F:30:THR:HB | 1:F:51:LYS:CG | 2.46 | 0.42 |
| 1:G:161:LEU:HD12 | 1:G:161:LEU:HA | 1.82 | 0.42 |
| 1:G:301:ILE:HG12 | 1:G:307:MET:CE | 2.50 | 0.42 |
| 1:H:389:MET:CE | 1:H:389:MET:C | 2.87 | 0.42 |
| 1:H:130:GLU:HB3 | 1:H:422:VAL:HG12 | 2.02 | 0.42 |
| 1:H:81:ALA:O | 1:H:82:ASN:C | 2.57 | 0.42 |
| 1:I:420:ILE:CD1 | 1:I:448:GLU:HG2 | 2.50 | 0.42 |
| 1:J:228:SER:O | 1:J:258:ALA:N | 2.53 | 0.42 |
| 1:J:449:ALA:CB | 1:J:450:PRO:HD3 | 2.35 | 0.42 |
| 1:J:513:LEU:HA | 1:J:513:LEU:HD12 | 1.65 | 0.42 |
| 1:L:193:MET:CG | 1:L:194:GLN:N | 2.81 | 0.42 |
| 1:K:37:ASN:O | 1:L:517:THR:HA | 2.19 | 0.42 |
| 1:M:283:ASP:O | 1:M:286:LYS:HB2 | 2.20 | 0.42 |
| 1:M:56:VAL:O | 1:M:57:ALA:C | 2.58 | 0.42 |
| 1:M:64:ASP:C | 1:M:65:LYS:O | 2.52 | 0.42 |
| 1:N:232:GLU:HA | 1:N:310:GLU:CG | 2.50 | 0.42 |
| 2:T:96:GLU:O | 2:T:97:ALA:C | 2.57 | 0.42 |
| 2:T:93:ALA:HB1 | 2:U:4:ARG:O | 2.20 | 0.42 |
| 1:A:200:LEU:N | 1:A:200:LEU:CD1 | 2.82 | 0.41 |
| 1:A:291:ASP:O | 1:A:295:LEU:HB2 | 2.20 | 0.41 |
| 1:A:66:PHE:HD1 | 1:A:520:MET:HE2 | 1.84 | 0.41 |
| 1:C:10:ASN:O | 1:C:11:ASP:C | 2.58 | 0.41 |
| 1:C:486:GLY:HA3 | 1:C:491:MET:HE2 | 2.00 | 0.41 |
| 1:D:255:GLU:O | 1:D:259:LEU:HG | 2.20 | 0.41 |
| 1:D:487:ASN:C | 1:D:487:ASN:OD1 | 2.59 | 0.41 |
| 1:E:199:TYR:CE1 | 1:E:202:PRO:HA | 2.54 | 0.41 |
| 1:E:215:LEU:O | 1:E:322:ARG:HA | 2.20 | 0.41 |
| 1:E:235:PRO:CG | 1:E:236:VAL:H | 2.28 | 0.41 |
| 1:E:249:ILE:N | 1:E:249:ILE:CD1 | 2.79 | 0.41 |
| 1:E:252:GLU:O | 1:E:277:LYS:HE2 | 2.20 | 0.41 |
| 1:E:305:ILE:HD12 | 1:E:305:ILE:H | 1.82 | 0.41 |
| 1:E:430:ARG:NH1 | 1:E:430:ARG:HG2 | 2.35 | 0.41 |
| 1:F:309:LEU:H | 1:F:309:LEU:CD1 | 2.31 | 0.41 |
| 1:F:115:ASP:HB3 | 1:F:436:GLN:HG3 | 2.02 | 0.41 |
| 1:G:354:GLU:HG3 | 1:G:354:GLU:O | 2.20 | 0.41 |
| 1:G:368:ARG:HG2 | 1:G:372:LEU:CG | 2.49 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:37:ASN:HB3 | 1:H:51:LYS:CG | 2.50 | 0.41 |
| 1:H:81:ALA:HA | 1:H:506:TYR:CE2 | 2.55 | 0.41 |
| 1:I:455:VAL:HG12 | 1:I:460:GLU:O | 2.20 | 0.41 |
| 1:I:411:VAL:HA | 1:I:497:THR:H | 1.83 | 0.41 |
| 1:I:496:PRO:O | 1:I:499:VAL:HG22 | 2.20 | 0.41 |
| 1:J:104:LEU:O | 1:J:107:VAL:HG22 | 2.19 | 0.41 |
| 1:J:520:MET:HE2 | 1:J:520:MET:HB3 | 1.88 | 0.41 |
| 1:K:286:LYS:CE | 1:K:286:LYS:HA | 2.47 | 0.41 |
| 1:L:146:GLN:HE21 | 1:L:150:ILE:HD11 | 1.85 | 0.41 |
| 1:L:236:VAL:HG23 | 1:L:237:LEU:H | 1.83 | 0.41 |
| 1:L:313:THR:CG2 | 1:L:314:LEU:H | 2.32 | 0.41 |
| 1:L:81:ALA:HA | 1:L:506:TYR:CE2 | 2.54 | 0.41 |
| 1:M:172:GLU:N | 1:M:172:GLU:OE1 | 2.52 | 0.41 |
| 1:M:256:GLY:O | 1:M:257:GLU:C | 2.59 | 0.41 |
| 1:M:37:ASN:ND2 | 1:M:37:ASN:H | 2.19 | 0.41 |
| 1:M:406:ALA:O | 1:M:410:GLY:N | 2.52 | 0.41 |
| 1:M:417:VAL:O | 1:M:418:ALA:C | 2.59 | 0.41 |
| 1:M:449:ALA:HB3 | 1:M:450:PRO:CD | 2.32 | 0.41 |
| 1:N:112:ASN:HA | 1:N:113:PRO:HD3 | 1.79 | 0.41 |
| 1:N:236:VAL:HG23 | 1:N:237:LEU:N | 2.34 | 0.41 |
| 2:T:5:PRO:CD | 2:T:42:ALA:HB1 | 2.50 | 0.41 |
| 1:A:313:THR:HB | 1:A:315:GLU:CD | 2.40 | 0.41 |
| 1:A:430:ARG:HG2 | 1:A:430:ARG:NH1 | 2.35 | 0.41 |
| 1:A:494:LEU:HD23 | 1:A:494:LEU:N | 2.35 | 0.41 |
| 1:A:499:VAL:CG2 | 1:A:500:THR:H | 2.33 | 0.41 |
| 1:B:215:LEU:O | 1:B:322:ARG:HA | 2.20 | 0.41 |
| 1:B:28:LYS:C | 1:B:30:THR:N | 2.74 | 0.41 |
| 1:B:361:ASP:C | 1:B:363:GLU:H | 2.24 | 0.41 |
| 1:B:451:LEU:HD23 | 1:B:451:LEU:C | 2.40 | 0.41 |
| 1:B:6:VAL:HG12 | 1:B:521:VAL:HG13 | 2.01 | 0.41 |
| 1:C:209:GLU:N | 1:C:209:GLU:CD | 2.73 | 0.41 |
| 1:C:293:ALA:O | 1:C:297:GLY:N | 2.53 | 0.41 |
| 1:E:428:ASP:C | 1:E:430:ARG:NH1 | 2.74 | 0.41 |
| 1:E:84:ALA:HB2 | 1:E:506:TYR:CE2 | 2.51 | 0.41 |
| 1:F:215:LEU:O | 1:F:322:ARG:HA | 2.20 | 0.41 |
| 1:G:150:ILE:CG2 | 1:G:151:SER:N | 2.83 | 0.41 |
| 1:G:304:GLU:C | 1:G:305:ILE:HD12 | 2.40 | 0.41 |
| 1:H:130:GLU:HG3 | 1:H:426:LEU:CD2 | 2.49 | 0.41 |
| 1:H:149:THR:N | 1:H:159:GLY:HA3 | 2.35 | 0.41 |
| 1:H:233:MET:CE | 1:H:233:MET:CA | 2.98 | 0.41 |
| 1:I:228:SER:CB | 1:I:255:GLU:HB2 | 2.51 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:201:SER:HA | 1:J:202:PRO:HD3 | 1.91 | 0.41 |
| 1:J:7:LYS:HG3 | 1:J:66:PHE:CZ | 2.54 | 0.41 |
| 1:K:217:SER:HB3 | 1:K:321:LYS:HA | 2.02 | 0.41 |
| 1:K:464:VAL:O | 1:K:467:ASN:HB3 | 2.20 | 0.41 |
| 1:L:414:GLY:N | 1:L:494:LEU:HA | 2.35 | 0.41 |
| 1:F:464:VAL:CG2 | 1:L:464:VAL:HA | 2.51 | 0.41 |
| 1:L:513:LEU:HA | 1:L:513:LEU:HD12 | 1.71 | 0.41 |
| 1:M:191:GLU:HB3 | 1:M:295:LEU:CD1 | 2.50 | 0.41 |
| 1:N:383:ALA:HB3 | 1:N:389:MET:HA | 2.02 | 0.41 |
| 1:N:81:ALA:HA | 1:N:506:TYR:CE2 | 2.55 | 0.41 |
| 2:O:45:ASN:HB2 | 2:O:46:GLY:H | 1.73 | 0.41 |
| 2:Q:34:LYS:HG3 | 2:Q:35:SER:N | 2.33 | 0.41 |
| 2:T:86:MET:N | 2:T:86:MET:SD | 2.94 | 0.41 |
| 1:A:124:VAL:HG13 | 1:A:504:LEU:HD12 | 2.02 | 0.41 |
| 1:A:293:ALA:O | 1:A:296:THR:N | 2.53 | 0.41 |
| 1:B:305:ILE:CG2 | 1:B:306:GLY:N | 2.70 | 0.41 |
| 1:B:178:GLU:O | 1:B:380:LYS:HA | 2.21 | 0.41 |
| 1:C:240:VAL:CG1 | 1:C:245:LYS:O | 2.68 | 0.41 |
| 1:C:240:VAL:HG12 | 1:C:245:LYS:O | 2.20 | 0.41 |
| 1:C:252:GLU:HG3 | 1:C:285:ARG:NH1 | 2.35 | 0.41 |
| 1:C:355:GLU:HB3 | 1:C:361:ASP:OD2 | 2.20 | 0.41 |
| 1:C:372:LEU:O | 1:C:373:ALA:HB2 | 2.20 | 0.41 |
| 1:D:206:ASN:CB | 1:D:213:VAL:HA | 2.50 | 0.41 |
| 1:D:293:ALA:HB1 | 1:D:298:GLY:O | 2.19 | 0.41 |
| 1:E:223:ALA:HB3 | 1:E:251:ALA:HB2 | 2.02 | 0.41 |
| 1:E:349:ILE:HG21 | 1:E:369:VAL:CG2 | 2.47 | 0.41 |
| 1:E:350:ARG:O | 1:E:353:ILE:HB | 2.20 | 0.41 |
| 1:F:477:GLY:HA3 | 1:F:488:MET:CG | 2.50 | 0.41 |
| 1:F:4:LYS:HG3 | 1:G:59:GLU:O | 2.20 | 0.41 |
| 1:A:39:VAL:HG12 | 1:G:69:MET:HE3 | 2.02 | 0.41 |
| 1:H:272:LYS:HB2 | 1:H:272:LYS:HE3 | 1.82 | 0.41 |
| 1:H:385:THR:HG23 | 1:H:388:GLU:CB | 2.50 | 0.41 |
| 1:I:23:LEU:O | 1:I:27:VAL:HG12 | 2.21 | 0.41 |
| 1:I:232:GLU:HB3 | 1:I:309:LEU:HD12 | 2.01 | 0.41 |
| 1:I:322:ARG:HB2 | 1:I:333:ILE:HB | 2.02 | 0.41 |
| 1:I:455:VAL:HG11 | 1:I:462:PRO:HA | 2.03 | 0.41 |
| 1:I:510:VAL:HG13 | 1:I:511:ALA:N | 2.35 | 0.41 |
| 1:J:434:GLU:O | 1:J:438:VAL:HG23 | 2.19 | 0.41 |
| 1:J:43:SER:HB2 | 1:J:44:PHE:CD1 | 2.55 | 0.41 |
| 1:K:301:ILE:HD12 | 1:K:301:ILE:H | 1.79 | 0.41 |
| 1:K:231:ARG:HG2 | 1:K:310:GLU:OE2 | 2.19 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:464:VAL:HG22 | 1:K:464:VAL:HA | 2.01 | 0.41 |
| 1:K:81:ALA:HA | 1:K:506:TYR:CD2 | 2.55 | 0.41 |
| 1:K:99:ILE:O | 1:K:100:ILE:C | 2.58 | 0.41 |
| 1:L:235:PRO:HG3 | 1:L:310:GLU:CA | 2.35 | 0.41 |
| 1:L:247:LEU:CD1 | 1:L:247:LEU:C | 2.88 | 0.41 |
| 1:L:179:ASP:OD2 | 1:L:390:LYS:HG2 | 2.20 | 0.41 |
| 1:M:228:SER:O | 1:M:258:ALA:HB2 | 2.21 | 0.41 |
| 1:M:296:THR:HB | 1:M:319:GLN:N | 2.34 | 0.41 |
| 1:M:290:GLN:HB3 | 1:M:345:ARG:HH21 | 1.85 | 0.41 |
| 1:N:194:GLN:CG | 1:N:195:PHE:N | 2.82 | 0.41 |
| 2:O:8:ASP:OD1 | 2:O:87:SER:HB2 | 2.21 | 0.41 |
| 2:P:22:ALA:O | 2:P:26:VAL:HB | 2.20 | 0.41 |
| 2:P:14:ARG:CD | 2:P:35:SER:HB3 | 2.49 | 0.41 |
| 2:Q:7:HIS:C | 2:Q:9:ARG:H | 2.23 | 0.41 |
| 2:S:20:LYS:CG | 2:S:27:LEU:HD23 | 2.50 | 0.41 |
| 2:T:13:LYS:O | 2:T:13:LYS:HG3 | 2.19 | 0.41 |
| 2:T:77:LYS:C | 2:T:78:ILE:HD12 | 2.41 | 0.41 |
| 2:O:4:ARG:HB2 | 2:U:96:GLU:OE1 | 2.20 | 0.41 |
| 1:A:100:ILE:O | 1:A:101:THR:C | 2.59 | 0.41 |
| 1:A:235:PRO:CG | 1:A:236:VAL:H | 2.29 | 0.41 |
| 1:A:287:ALA:O | 1:A:290:GLN:NE2 | 2.51 | 0.41 |
| 1:A:509:SER:OG | 1:B:385:THR:HG23 | 2.20 | 0.41 |
| 1:C:216:GLU:HA | 1:C:216:GLU:OE1 | 2.20 | 0.41 |
| 1:C:348:GLN:O | 1:C:348:GLN:NE2 | 2.54 | 0.41 |
| 1:C:134:LEU:HD11 | 1:C:425:LYS:NZ | 2.35 | 0.41 |
| 1:D:118:ARG:O | 1:D:119:GLY:C | 2.59 | 0.41 |
| 1:D:144:ILE:O | 1:D:147:VAL:HG22 | 2.19 | 0.41 |
| 1:D:195:PHE:C | 1:D:195:PHE:CD1 | 2.93 | 0.41 |
| 1:D:281:PHE:H | 1:D:284:ARG:HD2 | 1.85 | 0.41 |
| 1:D:350:ARG:HD3 | 1:D:350:ARG:HA | 1.82 | 0.41 |
| 1:E:158:VAL:O | 1:E:159:GLY:C | 2.59 | 0.41 |
| 1:E:281:PHE:HE2 | 1:E:283:ASP:OD2 | 2.04 | 0.41 |
| 1:E:289:LEU:HD23 | 1:E:292:ILE:HD12 | 2.01 | 0.41 |
| 1:E:288:MET:HG2 | 1:E:368:ARG:HE | 1.85 | 0.41 |
| 1:E:397:GLU:O | 1:E:398:ASP:C | 2.58 | 0.41 |
| 1:E:421:ARG:HA | 1:E:421:ARG:HD3 | 1.76 | 0.41 |
| 1:E:41:ASP:O | 1:E:42:LYS:HG3 | 2.20 | 0.41 |
| 1:E:456:LEU:HD13 | 1:E:462:PRO:HG3 | 2.02 | 0.41 |
| 1:E:72:GLN:HE21 | 1:E:72:GLN:HA | 1.84 | 0.41 |
| 1:F:234:LEU:N | 1:F:235:PRO:CD | 2.78 | 0.41 |
| 1:G:160:LYS:HE3 | 1:G:164:GLU:OE2 | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:325:ILE:CD1 | 1:G:325:ILE:N | 2.78 | 0.41 |
| 1:G:443:ALA:O | 1:G:447:MET:HG3 | 2.20 | 0.41 |
| 1:H:352:GLN:O | 1:H:355:GLU:OE1 | 2.38 | 0.41 |
| 1:H:385:THR:HG23 | 1:H:388:GLU:N | 2.35 | 0.41 |
| 1:I:120:ILE:O | 1:I:123:ALA:N | 2.53 | 0.41 |
| 1:I:254:VAL:O | 1:I:259:LEU:HD12 | 2.21 | 0.41 |
| 1:J:155:ASP:OD1 | 1:J:158:VAL:HG23 | 2.20 | 0.41 |
| 1:J:204:PHE:CD2 | 1:J:274:ALA:HB1 | 2.55 | 0.41 |
| 1:K:115:ASP:O | 1:K:118:ARG:HB3 | 2.21 | 0.41 |
| 1:K:342:ILE:O | 1:K:346:VAL:HG23 | 2.20 | 0.41 |
| 1:L:115:ASP:O | 1:L:116:LEU:C | 2.58 | 0.41 |
| 1:M:166:MET:O | 1:M:170:GLY:CA | 2.68 | 0.41 |
| 1:M:508:ALA:O | 1:M:509:SER:C | 2.58 | 0.41 |
| 1:N:227:ILE:HD12 | 1:N:309:LEU:HD11 | 2.02 | 0.41 |
| 1:N:472:GLY:HA3 | 1:N:476:TYR:CD2 | 2.55 | 0.41 |
| 1:M:37:ASN:O | 1:N:517:THR:HA | 2.20 | 0.41 |
| 2:O:7:HIS:HA | 2:O:45:ASN:N | 2.36 | 0.41 |
| 2:Q:55:LYS:CE | 2:Q:55:LYS:N | 2.63 | 0.41 |
| 2:T:13:LYS:HB3 | 2:T:41:LEU:HD11 | 2.02 | 0.41 |
| 1:A:23:LEU:CD1 | 1:A:23:LEU:C | 2.89 | 0.41 |
| 1:A:290:GLN:NE2 | 1:A:345:ARG:HH12 | 2.18 | 0.41 |
| 1:A:487:ASN:OD1 | 1:A:489:ILE:N | 2.53 | 0.41 |
| 1:B:265:ASN:HB3 | 1:B:271:VAL:HG22 | 2.03 | 0.41 |
| 1:A:509:SER:HB3 | 1:B:385:THR:HG23 | 2.02 | 0.41 |
| 1:B:486:GLY:CA | 1:B:491:MET:CE | 2.98 | 0.41 |
| 1:C:295:LEU:C | 1:C:295:LEU:CD2 | 2.89 | 0.41 |
| 1:C:327:LYS:HB2 | 1:C:327:LYS:HE2 | 1.92 | 0.41 |
| 1:D:301:ILE:HG22 | 1:D:301:ILE:O | 2.21 | 0.41 |
| 1:D:353:ILE:HG22 | 1:D:354:GLU:N | 2.36 | 0.41 |
| 1:D:355:GLU:HG2 | 1:D:361:ASP:OD2 | 2.20 | 0.41 |
| 1:E:124:VAL:HG22 | 1:E:504:LEU:HD11 | 2.02 | 0.41 |
| 1:E:147:VAL:C | 1:E:150:ILE:HG22 | 2.41 | 0.41 |
| 1:E:252:GLU:HA | 1:E:285:ARG:HH12 | 1.81 | 0.41 |
| 1:E:350:ARG:HA | 1:E:350:ARG:HD3 | 1.95 | 0.41 |
| 1:E:8:PHE:HE2 | 1:F:26:ALA:HA | 1.85 | 0.41 |
| 1:G:13:ARG:O | 1:G:16:MET:HB3 | 2.21 | 0.41 |
| 1:G:168:LYS:O | 1:G:170:GLY:N | 2.52 | 0.41 |
| 1:G:229:ASN:C | 1:G:231:ARG:N | 2.73 | 0.41 |
| 1:G:293:ALA:O | 1:G:297:GLY:N | 2.52 | 0.41 |
| 1:G:298:GLY:HA2 | 1:G:316:ASP:O | 2.19 | 0.41 |
| 1:H:287:ALA:O | 1:H:290:GLN:HB3 | 2.20 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:366:GLN:O | 1:H:369:VAL:HB | 2.20 | 0.41 |
| 1:H:56:VAL:O | 1:H:57:ALA:C | 2.58 | 0.41 |
| 1:I:199:TYR:HD1 | 1:I:201:SER:H | 1.67 | 0.41 |
| 1:I:230:ILE:HD12 | 1:I:257:GLU:HG2 | 2.03 | 0.41 |
| 1:I:350:ARG:HE | 1:I:369:VAL:CG1 | 2.33 | 0.41 |
| 1:J:215:LEU:CB | 1:J:218:PRO:HG2 | 2.37 | 0.41 |
| 1:J:131:LEU:CD1 | 1:J:422:VAL:HG11 | 2.50 | 0.41 |
| 1:K:313:THR:CG2 | 1:K:314:LEU:H | 2.31 | 0.41 |
| 1:K:349:ILE:O | 1:K:353:ILE:HG13 | 2.20 | 0.41 |
| 1:L:106:ALA:O | 1:L:107:VAL:C | 2.59 | 0.41 |
| 1:L:226:LYS:HA | 1:L:252:GLU:HB2 | 2.02 | 0.41 |
| 1:M:326:ASN:ND2 | 1:M:328:ASP:OD1 | 2.54 | 0.41 |
| 1:M:77:VAL:HG11 | 1:M:510:VAL:HB | 2.01 | 0.41 |
| 1:N:290:GLN:CG | 1:N:345:ARG:HH21 | 2.34 | 0.41 |
| 1:N:350:ARG:HE | 1:N:369:VAL:HG11 | 1.86 | 0.41 |
| 2:Q:20:LYS:HA | 2:Q:28:THR:HG23 | 2.01 | 0.41 |
| 2:Q:79:ASP:HB2 | 2:Q:81:GLU:OE1 | 2.20 | 0.41 |
| 1:A:184:GLN:N | 1:A:184:GLN:OE1 | 2.49 | 0.41 |
| 1:A:205:ILE:HA | 1:A:213:VAL:HG22 | 2.02 | 0.41 |
| 1:A:432:GLN:NE2 | 1:A:436:GLN:HE22 | 2.18 | 0.41 |
| 1:A:88:GLY:HA2 | 4:A:1:ADP:O2B | 2.21 | 0.41 |
| 1:B:400:LEU:O | 1:B:404:ARG:HG2 | 2.21 | 0.41 |
| 1:C:237:LEU:CD2 | 1:C:237:LEU:C | 2.89 | 0.41 |
| 1:C:258:ALA:O | 1:C:261:THR:HG23 | 2.20 | 0.41 |
| 1:C:433:ASN:OD1 | 1:C:436:GLN:HB2 | 2.20 | 0.41 |
| 1:D:6:VAL:HG12 | 1:D:521:VAL:HG13 | 2.02 | 0.41 |
| 1:E:153:ASN:O | 1:E:154:SER:HB2 | 2.20 | 0.41 |
| 1:E:195:PHE:CD1 | 1:E:195:PHE:C | 2.93 | 0.41 |
| 1:E:386:GLU:C | 1:E:388:GLU:H | 2.23 | 0.41 |
| 1:E:413:ALA:HB3 | 1:E:417:VAL:HG13 | 2.02 | 0.41 |
| 1:F:199:TYR:CE1 | 1:F:202:PRO:HA | 2.55 | 0.41 |
| 1:F:233:MET:HE2 | 1:F:237:LEU:HB2 | 2.02 | 0.41 |
| 1:F:233:MET:CE | 1:F:233:MET:O | 2.68 | 0.41 |
| 1:F:281:PHE:CG | 1:F:282:GLY:N | 2.89 | 0.41 |
| 1:F:461:GLU:OE2 | 1:L:452:ARG:NH2 | 2.52 | 0.41 |
| 1:F:519:CYS:O | 1:G:38:VAL:HA | 2.21 | 0.41 |
| 1:F:88:GLY:CA | 4:F:1:ADP:O2B | 2.69 | 0.41 |
| 1:G:235:PRO:CG | 1:G:236:VAL:H | 2.32 | 0.41 |
| 1:G:357:THR:CB | 1:G:361:ASP:HB2 | 2.50 | 0.41 |
| 1:G:95:LEU:HD13 | 1:G:504:LEU:HD23 | 2.03 | 0.41 |
| 1:H:318:GLY:O | 1:H:319:GLN:HG3 | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:37:ASN:ND2 | 1:H:37:ASN:N | 2.69 | 0.41 |
| 1:I:166:MET:HA | 1:I:170:GLY:O | 2.21 | 0.41 |
| 1:I:172:GLU:N | 1:I:172:GLU:OE1 | 2.53 | 0.41 |
| 1:I:233:MET:CA | 1:I:233:MET:HE3 | 2.50 | 0.41 |
| 1:I:186:GLU:HB2 | 1:I:380:LYS:HB2 | 2.01 | 0.41 |
| 1:J:219:PHE:HE1 | 1:J:245:LYS:HB2 | 1.86 | 0.41 |
| 1:J:285:ARG:O | 1:J:288:MET:HB2 | 2.20 | 0.41 |
| 1:K:109:ALA:HB3 | 1:K:111:MET:CE | 2.50 | 0.41 |
| 1:K:305:ILE:CG2 | 1:K:307:MET:HG3 | 2.50 | 0.41 |
| 1:K:5:ASP:HB2 | 1:K:524:LEU:CD2 | 2.42 | 0.41 |
| 1:K:66:PHE:CD1 | 1:K:69:MET:HE3 | 2.56 | 0.41 |
| 1:L:216:GLU:OE1 | 1:L:216:GLU:HA | 2.20 | 0.41 |
| 1:L:351:GLN:HG2 | 1:L:354:GLU:CD | 2.40 | 0.41 |
| 1:L:353:ILE:HD11 | 1:L:369:VAL:HG21 | 2.02 | 0.41 |
| 1:M:130:GLU:O | 1:M:133:ALA:HB3 | 2.19 | 0.41 |
| 1:N:215:LEU:HB3 | 1:N:218:PRO:CG | 2.46 | 0.41 |
| 1:N:364:LYS:O | 1:N:365:LEU:C | 2.59 | 0.41 |
| 1:N:399:ALA:O | 1:N:400:LEU:C | 2.59 | 0.41 |
| 2:O:27:LEU:CD2 | 2:O:27:LEU:O | 2.68 | 0.41 |
| 2:P:50:GLU:O | 2:P:50:GLU:HG2 | 2.21 | 0.41 |
| 2:P:55:LYS:HA | 2:P:56:PRO:HD2 | 1.88 | 0.41 |
| 2:Q:71:TYR:C | 2:Q:73:VAL:N | 2.74 | 0.41 |
| 2:U:11:ILE:HG22 | 2:U:41:LEU:HD12 | 2.02 | 0.41 |
| 1:A:174:VAL:HG23 | 1:A:370:ALA:CB | 2.51 | 0.41 |
| 1:A:216:GLU:OE1 | 1:A:216:GLU:HA | 2.21 | 0.41 |
| 1:A:283:ASP:O | 1:A:287:ALA:CB | 2.68 | 0.41 |
| 1:A:195:PHE:CE1 | 1:A:330:THR:HB | 2.56 | 0.41 |
| 1:A:321:LYS:HG3 | 1:A:334:ASP:HB3 | 2.03 | 0.41 |
| 1:A:385:THR:HG21 | 1:G:510:VAL:HG13 | 2.01 | 0.41 |
| 1:A:489:ILE:CD1 | 1:A:494:LEU:HD22 | 2.50 | 0.41 |
| 1:B:124:VAL:O | 1:B:128:VAL:HG23 | 2.21 | 0.41 |
| 1:B:258:ALA:O | 1:B:261:THR:HG23 | 2.20 | 0.41 |
| 1:B:428:ASP:HA | 1:B:430:ARG:HH12 | 1.84 | 0.41 |
| 1:B:509:SER:OG | 1:C:385:THR:HG23 | 2.21 | 0.41 |
| 1:D:153:ASN:HD22 | 1:D:153:ASN:C | 2.24 | 0.41 |
| 1:D:213:VAL:HB | 1:D:325:ILE:HD13 | 2.01 | 0.41 |
| 1:D:247:LEU:HB3 | 1:D:273:VAL:CG1 | 2.50 | 0.41 |
| 1:D:28:LYS:C | 1:D:30:THR:N | 2.74 | 0.41 |
| 1:D:24:ALA:O | 1:D:28:LYS:HG3 | 2.20 | 0.41 |
| 1:D:344:GLY:C | 1:D:346:VAL:N | 2.74 | 0.41 |
| 1:D:456:LEU:HD22 | 1:D:462:PRO:HG2 | 2.03 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:466:ALA:O | 1:D:470:LYS:HG3 | 2.21 | 0.41 |
| 1:F:174:VAL:HG12 | 1:F:175:ILE:N | 2.35 | 0.41 |
| 1:F:214:GLU:CB | 1:F:322:ARG:HD3 | 2.31 | 0.41 |
| 1:F:326:ASN:CG | 1:F:329:THR:H | 2.24 | 0.41 |
| 1:F:438:VAL:O | 1:F:442:VAL:HG23 | 2.20 | 0.41 |
| 1:G:134:LEU:N | 1:G:134:LEU:CD1 | 2.83 | 0.41 |
| 1:G:218:PRO:HD2 | 1:G:320:ALA:O | 2.21 | 0.41 |
| 1:H:166:MET:HE2 | 1:H:171:LYS:CA | 2.40 | 0.41 |
| 1:H:251:ALA:O | 1:H:252:GLU:C | 2.58 | 0.41 |
| 1:H:262:LEU:O | 1:H:265:ASN:HB3 | 2.20 | 0.41 |
| 1:H:88:GLY:O | 1:H:89:THR:C | 2.59 | 0.41 |
| 1:I:202:PRO:C | 1:I:204:PHE:N | 2.74 | 0.41 |
| 1:I:40:LEU:HD23 | 1:I:50:THR:HG22 | 2.03 | 0.41 |
| 1:I:64:ASP:C | 1:I:65:LYS:O | 2.54 | 0.41 |
| 1:J:478:TYR:CZ | 1:J:483:GLU:HA | 2.55 | 0.41 |
| 1:K:193:MET:CG | 1:K:194:GLN:N | 2.84 | 0.41 |
| 1:K:232:GLU:HA | 1:K:310:GLU:HG2 | 2.03 | 0.41 |
| 1:K:338:GLU:O | 1:K:341:ALA:HB3 | 2.21 | 0.41 |
| 1:L:165:ALA:O | 1:L:168:LYS:HB2 | 2.21 | 0.41 |
| 1:F:464:VAL:HG22 | 1:L:464:VAL:HA | 2.03 | 0.41 |
| 1:M:254:VAL:O | 1:M:259:LEU:HD12 | 2.21 | 0.41 |
| 1:M:65:LYS:O | 1:M:66:PHE:CB | 2.43 | 0.41 |
| 1:N:218:PRO:HB3 | 1:N:246:PRO:HB2 | 2.02 | 0.41 |
| 1:N:353:ILE:HG12 | 1:N:365:LEU:HB3 | 2.03 | 0.41 |
| 2:O:78:ILE:CD1 | 2:O:78:ILE:N | 2.83 | 0.41 |
| 2:O:12:VAL:CG2 | 2:O:84:LEU:HB2 | 2.48 | 0.41 |
| 2:S:59:VAL:O | 2:S:59:VAL:HG23 | 2.21 | 0.41 |
| 1:A:518:GLU:OE1 | 1:A:518:GLU:HA | 2.21 | 0.41 |
| 1:B:161:LEU:HD12 | 1:B:161:LEU:HA | 1.74 | 0.41 |
| 1:B:14:VAL:O | 1:B:18:ARG:HG3 | 2.21 | 0.41 |
| 1:B:209:GLU:O | 1:B:210:THR:HB | 2.21 | 0.41 |
| 1:B:284:ARG:O | 1:B:287:ALA:N | 2.54 | 0.41 |
| 1:C:176:THR:O | 1:C:378:VAL:HA | 2.21 | 0.41 |
| 1:C:428:ASP:HA | 1:C:430:ARG:HH12 | 1.86 | 0.41 |
| 1:C:455:VAL:HG12 | 1:C:460:GLU:O | 2.21 | 0.41 |
| 1:C:479:ASN:O | 1:C:483:GLU:N | 2.54 | 0.41 |
| 1:C:499:VAL:CG2 | 1:C:500:THR:H | 2.33 | 0.41 |
| 1:D:143:ALA:O | 1:D:146:GLN:HB2 | 2.21 | 0.41 |
| 1:D:62:LEU:HB2 | 1:D:68:ASN:HA | 2.02 | 0.41 |
| 1:E:199:TYR:HE2 | 1:E:205:ILE:HG12 | 1.85 | 0.41 |
| 1:E:200:LEU:HD22 | 1:E:254:VAL:HB | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:401:HIS:O | 1:E:402:ALA:C | 2.58 | 0.41 |
| 1:E:30:THR:HB | 1:E:51:LYS:HG3 | 2.02 | 0.41 |
| 1:F:134:LEU:HD12 | 1:F:134:LEU:H | 1.81 | 0.41 |
| 1:F:200:LEU:O | 1:F:202:PRO:HD2 | 2.20 | 0.41 |
| 1:G:249:ILE:N | 1:G:249:ILE:CD1 | 2.77 | 0.41 |
| 1:G:309:LEU:H | 1:G:309:LEU:CD1 | 2.33 | 0.41 |
| 1:G:314:LEU:C | 1:G:314:LEU:HD12 | 2.41 | 0.41 |
| 1:G:479:ASN:O | 1:G:483:GLU:N | 2.51 | 0.41 |
| 1:H:355:GLU:O | 1:H:357:THR:N | 2.54 | 0.41 |
| 1:H:510:VAL:HG13 | 1:H:511:ALA:N | 2.35 | 0.41 |
| 1:I:270:ILE:HG23 | 1:J:229:ASN:ND2 | 2.35 | 0.41 |
| 1:J:305:ILE:CG2 | 1:J:307:MET:HG3 | 2.51 | 0.41 |
| 1:J:95:LEU:O | 1:J:98:ALA:HB3 | 2.21 | 0.41 |
| 1:K:231:ARG:O | 1:K:233:MET:N | 2.54 | 0.41 |
| 1:K:287:ALA:O | 1:K:290:GLN:N | 2.54 | 0.41 |
| 1:K:37:ASN:HB3 | 1:K:51:LYS:HG2 | 2.02 | 0.41 |
| 1:L:262:LEU:O | 1:L:266:THR:HG23 | 2.21 | 0.41 |
| 1:L:420:ILE:CD1 | 1:L:448:GLU:HG2 | 2.51 | 0.41 |
| 1:L:461:GLU:HB3 | 1:L:464:VAL:HB | 2.02 | 0.41 |
| 1:M:105:LYS:O | 1:M:109:ALA:N | 2.53 | 0.41 |
| 1:M:293:ALA:HB2 | 1:M:300:VAL:HG13 | 2.02 | 0.41 |
| 1:M:313:THR:HB | 1:M:315:GLU:HG2 | 2.02 | 0.41 |
| 1:M:419:LEU:N | 1:M:419:LEU:HD22 | 2.35 | 0.41 |
| 1:M:420:ILE:HD13 | 1:M:448:GLU:HG2 | 2.03 | 0.41 |
| 1:M:476:TYR:HA | 1:M:486:GLY:O | 2.20 | 0.41 |
| 1:N:366:GLN:O | 1:N:369:VAL:HB | 2.20 | 0.41 |
| 2:Q:14:ARG:CG | 2:Q:35:SER:HB3 | 2.51 | 0.41 |
| 2:Q:74:LYS:O | 2:Q:84:LEU:HA | 2.21 | 0.41 |
| 2:S:22:ALA:O | 2:S:26:VAL:HB | 2.21 | 0.41 |
| 1:A:168:LYS:C | 1:A:170:GLY:N | 2.74 | 0.41 |
| 1:A:252:GLU:O | 1:A:253:ASP:CB | 2.62 | 0.41 |
| 1:A:496:PRO:O | 1:A:499:VAL:HG22 | 2.20 | 0.41 |
| 1:B:13:ARG:O | 1:B:16:MET:HB3 | 2.21 | 0.41 |
| 1:B:230:ILE:O | 1:B:232:GLU:N | 2.53 | 0.41 |
| 1:B:237:LEU:CD2 | 1:B:238:GLU:N | 2.84 | 0.41 |
| 1:B:329:THR:HG22 | 1:B:330:THR:N | 2.36 | 0.41 |
| 1:C:128:VAL:CG1 | 1:C:132:LYS:HE2 | 2.51 | 0.41 |
| 1:C:23:LEU:O | 1:C:24:ALA:C | 2.59 | 0.41 |
| 1:C:359:ASP:C | 1:C:361:ASP:H | 2.22 | 0.41 |
| 1:C:429:LEU:HG | 1:C:440:ILE:HD13 | 2.02 | 0.41 |
| 1:C:95:LEU:HD23 | 1:C:450:PRO:HD3 | 2.02 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:161:LEU:HA | 1:D:161:LEU:HD12 | 1.85 | 0.41 |
| 1:D:222:LEU:N | 1:D:222:LEU:CD1 | 2.82 | 0.41 |
| 1:D:285:ARG:CG | 1:D:286:LYS:H | 2.30 | 0.41 |
| 1:E:329:THR:HG22 | 1:E:330:THR:N | 2.35 | 0.41 |
| 1:E:183:LEU:CD2 | 1:E:384:ALA:HA | 2.51 | 0.41 |
| 1:E:62:LEU:HB2 | 1:E:68:ASN:HA | 2.03 | 0.41 |
| 1:F:114:MET:O | 1:F:118:ARG:HG3 | 2.21 | 0.41 |
| 1:F:249:ILE:HG22 | 1:F:250:ILE:N | 2.35 | 0.41 |
| 1:F:385:THR:OG1 | 1:F:388:GLU:HB2 | 2.21 | 0.41 |
| 1:F:456:LEU:HD13 | 1:F:462:PRO:HG3 | 2.02 | 0.41 |
| 1:G:100:ILE:O | 1:G:101:THR:C | 2.59 | 0.41 |
| 1:G:485:TYR:N | 1:G:485:TYR:CD1 | 2.89 | 0.41 |
| 1:H:107:VAL:HG11 | 1:H:515:ILE:HG23 | 2.02 | 0.41 |
| 1:H:187:LEU:HD23 | 1:H:188:ASP:N | 2.36 | 0.41 |
| 1:H:342:ILE:O | 1:H:346:VAL:HG23 | 2.21 | 0.41 |
| 1:H:478:TYR:HB2 | 1:H:485:TYR:CE2 | 2.56 | 0.41 |
| 1:H:31:LEU:HD22 | 1:H:94:VAL:HG21 | 2.03 | 0.41 |
| 1:I:49:ILE:HD11 | 1:J:73:MET:HE3 | 2.03 | 0.41 |
| 1:J:158:VAL:C | 1:J:160:LYS:N | 2.74 | 0.41 |
| 1:J:21:ASN:HA | 1:J:21:ASN:HD22 | 1.60 | 0.41 |
| 1:J:455:VAL:HG11 | 1:J:461:GLU:O | 2.20 | 0.41 |
| 1:K:146:GLN:HE21 | 1:K:150:ILE:HD11 | 1.86 | 0.41 |
| 1:K:186:GLU:O | 1:K:379:ILE:HA | 2.21 | 0.41 |
| 1:K:77:VAL:HG22 | 1:K:506:TYR:HB3 | 2.02 | 0.41 |
| 1:L:190:VAL:CG2 | 1:L:191:GLU:N | 2.84 | 0.41 |
| 1:L:202:PRO:O | 1:L:204:PHE:N | 2.53 | 0.41 |
| 1:L:303:GLU:C | 1:L:305:ILE:N | 2.74 | 0.41 |
| 1:L:44:PHE:CD1 | 1:L:44:PHE:N | 2.88 | 0.41 |
| 1:K:49:ILE:HD11 | 1:L:73:MET:HE2 | 2.01 | 0.41 |
| 1:M:222:LEU:HD13 | 1:M:293:ALA:HB2 | 2.02 | 0.41 |
| 1:M:218:PRO:CB | 1:M:246:PRO:HB2 | 2.51 | 0.41 |
| 1:N:107:VAL:HG11 | 1:N:515:ILE:HG23 | 2.02 | 0.41 |
| 1:N:326:ASN:OD1 | 1:N:329:THR:N | 2.53 | 0.41 |
| 1:N:126:ALA:CB | 1:N:426:LEU:HD13 | 2.50 | 0.41 |
| 2:P:14:ARG:CG | 2:P:35:SER:HB3 | 2.50 | 0.41 |
| 2:T:74:LYS:O | 2:T:84:LEU:HA | 2.20 | 0.41 |
| 1:A:284:ARG:O | 1:A:287:ALA:N | 2.54 | 0.41 |
| 1:A:302:SER:C | 1:A:304:GLU:N | 2.74 | 0.41 |
| 1:A:214:GLU:CB | 1:A:322:ARG:HD3 | 2.43 | 0.41 |
| 1:A:323:VAL:HA | 1:A:331:THR:O | 2.21 | 0.41 |
| 1:A:150:ILE:HD11 | 1:A:493:ILE:HG23 | 2.03 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:164:GLU:O | 1:B:167:ASP:HB3 | 2.19 | 0.41 |
| 1:B:398:ASP:O | 1:B:401:HIS:HB2 | 2.21 | 0.41 |
| 1:B:80:LYS:HD2 | 1:B:506:TYR:CZ | 2.55 | 0.41 |
| 1:C:150:ILE:HD11 | 4:C:1:ADP:N7 | 2.35 | 0.41 |
| 1:C:199:TYR:CE2 | 1:C:205:ILE:HG12 | 2.56 | 0.41 |
| 1:D:199:TYR:O | 1:D:199:TYR:HD1 | 2.04 | 0.41 |
| 1:D:187:LEU:HD12 | 1:D:378:VAL:O | 2.21 | 0.41 |
| 1:E:177:VAL:CG1 | 1:E:397:GLU:HG2 | 2.50 | 0.41 |
| 1:E:344:GLY:C | 1:E:346:VAL:H | 2.25 | 0.41 |
| 1:G:252:GLU:OE1 | 1:G:252:GLU:N | 2.54 | 0.41 |
| 1:G:258:ALA:O | 1:G:261:THR:HG23 | 2.21 | 0.41 |
| 1:G:30:THR:HB | 1:G:51:LYS:CG | 2.51 | 0.41 |
| 1:H:21:ASN:HD22 | 1:H:21:ASN:HA | 1.65 | 0.41 |
| 1:H:228:SER:HA | 1:H:255:GLU:HB2 | 2.02 | 0.41 |
| 1:H:330:THR:HG22 | 1:H:331:THR:N | 2.35 | 0.41 |
| 1:H:401:HIS:O | 1:H:402:ALA:C | 2.59 | 0.41 |
| 1:I:229:ASN:ND2 | 1:I:231:ARG:HH12 | 2.19 | 0.41 |
| 1:I:389:MET:C | 1:I:389:MET:CE | 2.90 | 0.41 |
| 1:I:95:LEU:O | 1:I:98:ALA:HB3 | 2.20 | 0.41 |
| 1:J:233:MET:O | 1:J:237:LEU:N | 2.44 | 0.41 |
| 1:J:359:ASP:CA | 1:J:362:ARG:HH12 | 2.28 | 0.41 |
| 1:J:479:ASN:O | 1:J:483:GLU:N | 2.53 | 0.41 |
| 1:K:158:VAL:C | 1:K:160:LYS:N | 2.74 | 0.41 |
| 1:K:64:ASP:C | 1:K:65:LYS:O | 2.59 | 0.41 |
| 1:M:224:ASP:CG | 1:M:224:ASP:O | 2.59 | 0.41 |
| 1:M:38:VAL:HG12 | 1:M:39:VAL:N | 2.36 | 0.41 |
| 1:M:487:ASN:OD1 | 1:M:489:ILE:HB | 2.21 | 0.41 |
| 2:Q:20:LYS:H | 2:Q:20:LYS:CD | 2.25 | 0.41 |
| 2:Q:96:GLU:OE1 | 2:R:4:ARG:HB2 | 2.21 | 0.41 |
| 2:S:43:VAL:CG1 | 2:S:57:LEU:HD12 | 2.51 | 0.41 |
| 2:S:4:ARG:HA | 2:S:5:PRO:HD2 | 1.90 | 0.41 |
| 1:A:290:GLN:O | 1:A:291:ASP:C | 2.60 | 0.41 |
| 1:A:357:THR:CB | 1:A:361:ASP:HB2 | 2.51 | 0.41 |
| 1:A:77:VAL:HG22 | 1:A:78:ALA:N | 2.36 | 0.41 |
| 1:B:267:MET:C | 1:B:269:GLY:N | 2.75 | 0.41 |
| 1:B:289:LEU:HD23 | 1:B:292:ILE:HD12 | 2.03 | 0.41 |
| 1:B:510:VAL:CG2 | 1:B:511:ALA:H | 2.34 | 0.41 |
| 1:C:223:ALA:HB3 | 1:C:251:ALA:CB | 2.49 | 0.41 |
| 1:C:473:ASP:O | 1:C:474:GLY:C | 2.59 | 0.41 |
| 1:D:155:ASP:OD1 | 1:D:157:THR:HB | 2.21 | 0.41 |
| 1:D:224:ASP:OD1 | 1:D:301:ILE:O | 2.39 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:441:LYS:HA | 1:D:441:LYS:HD2 | 1.86 | 0.41 |
| 1:E:149:THR:OG1 | 1:E:156:GLU:HA | 2.21 | 0.41 |
| 1:E:293:ALA:O | 1:E:295:LEU:N | 2.54 | 0.41 |
| 1:E:69:MET:SD | 1:E:522:THR:HB | 2.61 | 0.41 |
| 1:F:155:ASP:HB3 | 1:F:158:VAL:HG21 | 2.03 | 0.41 |
| 1:F:284:ARG:CG | 1:F:288:MET:HE2 | 2.49 | 0.41 |
| 1:F:290:GLN:O | 1:F:294:THR:HG23 | 2.21 | 0.41 |
| 1:F:314:LEU:HD12 | 1:F:315:GLU:CA | 2.50 | 0.41 |
| 1:F:455:VAL:O | 1:F:458:CYS:HB2 | 2.20 | 0.41 |
| 1:G:124:VAL:O | 1:G:125:THR:C | 2.57 | 0.41 |
| 1:G:194:GLN:O | 1:G:371:LYS:NZ | 2.49 | 0.41 |
| 1:G:199:TYR:O | 1:G:199:TYR:HD1 | 2.04 | 0.41 |
| 1:G:21:ASN:O | 1:G:22:VAL:C | 2.58 | 0.41 |
| 1:G:403:THR:OG1 | 1:G:404:ARG:N | 2.54 | 0.41 |
| 1:G:42:LYS:HE2 | 1:G:48:THR:HB | 2.03 | 0.41 |
| 1:G:455:VAL:HG11 | 1:G:462:PRO:HA | 2.03 | 0.41 |
| 1:H:172:GLU:OE1 | 1:H:172:GLU:N | 2.54 | 0.41 |
| 1:H:257:GLU:O | 1:H:261:THR:CG2 | 2.69 | 0.41 |
| 1:H:345:ARG:O | 1:H:348:GLN:HB2 | 2.21 | 0.41 |
| 1:H:183:LEU:HD22 | 1:I:360:TYR:CE2 | 2.57 | 0.41 |
| 1:I:449:ALA:CB | 1:I:450:PRO:CD | 2.97 | 0.41 |
| 1:I:507:ALA:O | 1:I:510:VAL:HG12 | 2.21 | 0.41 |
| 1:J:112:ASN:OD1 | 1:J:114:MET:N | 2.54 | 0.41 |
| 1:J:290:GLN:OE1 | 1:J:290:GLN:HA | 2.20 | 0.41 |
| 1:J:419:LEU:HD21 | 1:J:500:THR:HG23 | 2.02 | 0.41 |
| 1:K:290:GLN:OE1 | 1:K:293:ALA:HB3 | 2.21 | 0.41 |
| 1:K:296:THR:OG1 | 1:K:318:GLY:HA3 | 2.21 | 0.41 |
| 1:K:389:MET:HE1 | 1:K:393:LYS:HB2 | 2.02 | 0.41 |
| 1:L:129:GLU:O | 1:L:130:GLU:C | 2.59 | 0.41 |
| 1:L:305:ILE:CG2 | 1:L:307:MET:HG3 | 2.51 | 0.41 |
| 1:L:364:LYS:O | 1:L:365:LEU:C | 2.59 | 0.41 |
| 1:L:420:ILE:HG13 | 1:L:451:LEU:HD22 | 2.03 | 0.41 |
| 1:L:434:GLU:O | 1:L:438:VAL:HG23 | 2.20 | 0.41 |
| 1:M:224:ASP:HB3 | 1:M:302:SER:HA | 2.03 | 0.41 |
| 1:M:472:GLY:HA3 | 1:M:476:TYR:HD2 | 1.86 | 0.41 |
| 1:N:472:GLY:HA3 | 1:N:476:TYR:HD2 | 1.86 | 0.41 |
| 2:O:93:ALA:HB1 | 2:P:4:ARG:O | 2.21 | 0.41 |
| 2:S:73:VAL:HG13 | 2:S:86:MET:HE3 | 2.03 | 0.41 |
| 2:U:14:ARG:CG | 2:U:15:LYS:N | 2.79 | 0.41 |
| 2:U:3:ILE:CD1 | 2:U:3:ILE:H | 2.33 | 0.41 |
| 1:A:309:LEU:H | 1:A:309:LEU:CD1 | 2.34 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:368:ARG:HG2 | 1:A:372:LEU:CG | 2.49 | 0.40 |
| 1:A:368:ARG:O | 1:A:372:LEU:N | 2.53 | 0.40 |
| 1:A:177:VAL:CG2 | 1:A:393:LYS:HG3 | 2.51 | 0.40 |
| 1:A:411:VAL:HG12 | 1:A:496:PRO:CA | 2.38 | 0.40 |
| 1:B:478:TYR:CE2 | 1:B:480:ALA:HA | 2.56 | 0.40 |
| 1:B:520:MET:HE2 | 1:B:520:MET:HB3 | 1.90 | 0.40 |
| 1:B:54:VAL:HG13 | 1:B:55:SER:N | 2.36 | 0.40 |
| 1:C:130:GLU:O | 1:C:134:LEU:HD13 | 2.21 | 0.40 |
| 1:C:153:ASN:O | 1:C:154:SER:CB | 2.67 | 0.40 |
| 1:C:199:TYR:OH | 1:C:205:ILE:HD11 | 2.21 | 0.40 |
| 1:C:366:GLN:HA | 1:C:369:VAL:HB | 2.03 | 0.40 |
| 1:C:31:LEU:HD23 | 1:C:453:GLN:HB3 | 2.02 | 0.40 |
| 1:D:360:TYR:H | 1:D:363:GLU:CD | 2.24 | 0.40 |
| 1:E:255:GLU:N | 1:E:255:GLU:OE1 | 2.54 | 0.40 |
| 1:E:320:ALA:HA | 1:E:334:ASP:O | 2.21 | 0.40 |
| 1:D:509:SER:CB | 1:E:385:THR:HG23 | 2.51 | 0.40 |
| 1:F:206:ASN:H | 1:F:213:VAL:HA | 1.85 | 0.40 |
| 1:F:254:VAL:HG12 | 1:F:259:LEU:HG | 2.03 | 0.40 |
| 1:G:128:VAL:CG1 | 1:G:132:LYS:HE2 | 2.51 | 0.40 |
| 1:G:284:ARG:HG2 | 1:G:288:MET:CE | 2.50 | 0.40 |
| 1:G:358:SER:HA | 1:G:362:ARG:CD | 2.51 | 0.40 |
| 1:G:433:ASN:ND2 | 1:G:435:ASP:HB2 | 2.33 | 0.40 |
| 1:H:248:LEU:HD13 | 1:H:248:LEU:C | 2.41 | 0.40 |
| 1:H:290:GLN:O | 1:H:291:ASP:C | 2.58 | 0.40 |
| 1:H:301:ILE:CD1 | 1:H:301:ILE:H | 2.34 | 0.40 |
| 1:I:225:LYS:HE2 | 1:I:309:LEU:CD1 | 2.50 | 0.40 |
| 1:I:320:ALA:HB1 | 1:I:333:ILE:O | 2.21 | 0.40 |
| 1:I:188:ASP:O | 1:I:378:VAL:HG22 | 2.21 | 0.40 |
| 1:I:443:ALA:O | 1:I:446:ALA:HB3 | 2.21 | 0.40 |
| 1:J:166:MET:HE2 | 1:J:166:MET:HB3 | 1.93 | 0.40 |
| 1:J:191:GLU:HB3 | 1:J:295:LEU:CD1 | 2.51 | 0.40 |
| 1:I:41:ASP:HB2 | 1:J:69:MET:HE2 | 2.03 | 0.40 |
| 1:K:106:ALA:O | 1:K:107:VAL:C | 2.59 | 0.40 |
| 1:K:227:ILE:CD1 | 1:K:309:LEU:HD11 | 2.51 | 0.40 |
| 1:L:46:ALA:CB | 1:M:76:GLU:OE1 | 2.69 | 0.40 |
| 1:L:501:ARG:O | 1:L:502:SER:C | 2.59 | 0.40 |
| 1:M:190:VAL:O | 1:M:191:GLU:C | 2.59 | 0.40 |
| 1:M:379:ILE:HG22 | 1:M:380:LYS:N | 2.36 | 0.40 |
| 1:M:395:ARG:O | 1:M:398:ASP:HB2 | 2.22 | 0.40 |
| 1:N:303:GLU:C | 1:N:305:ILE:H | 2.24 | 0.40 |
| 1:N:27:VAL:HG23 | 1:N:53:GLY:HA2 | 2.01 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:S:78:ILE:N | 2:S:78:ILE:CD1 | 2.83 | 0.40 |
| 2:T:17:VAL:HG13 | 2:T:34:LYS:CA | 2.50 | 0.40 |
| 2:T:20:LYS:CB | 2:T:27:LEU:HG | 2.50 | 0.40 |
| 2:T:27:LEU:O | 2:T:27:LEU:HD23 | 2.20 | 0.40 |
| 2:T:17:VAL:HG11 | 2:T:33:ALA:O | 2.21 | 0.40 |
| 2:U:50:GLU:O | 2:U:52:GLY:N | 2.53 | 0.40 |
| 1:A:153:ASN:ND2 | 1:A:153:ASN:O | 2.54 | 0.40 |
| 1:B:267:MET:O | 1:B:269:GLY:N | 2.54 | 0.40 |
| 1:B:27:VAL:HG12 | 1:B:90:THR:HG23 | 2.03 | 0.40 |
| 1:C:118:ARG:O | 1:C:119:GLY:C | 2.57 | 0.40 |
| 1:C:199:TYR:HE2 | 1:C:205:ILE:HG12 | 1.86 | 0.40 |
| 1:C:357:THR:HB | 1:C:361:ASP:HB2 | 2.03 | 0.40 |
| 1:C:361:ASP:C | 1:C:363:GLU:H | 2.25 | 0.40 |
| 1:D:18:ARG:O | 1:D:22:VAL:HG23 | 2.21 | 0.40 |
| 1:D:217:SER:N | 1:D:218:PRO:CD | 2.83 | 0.40 |
| 1:D:279:PRO:CD | 1:D:285:ARG:HA | 2.51 | 0.40 |
| 1:D:409:GLU:OE1 | 1:D:501:ARG:NH2 | 2.55 | 0.40 |
| 1:E:195:PHE:HD1 | 1:E:195:PHE:C | 2.24 | 0.40 |
| 1:E:219:PHE:CB | 1:E:247:LEU:HD22 | 2.49 | 0.40 |
| 1:E:434:GLU:O | 1:E:437:ASN:N | 2.53 | 0.40 |
| 1:F:13:ARG:HD2 | 1:F:104:LEU:HD22 | 2.02 | 0.40 |
| 1:F:21:ASN:O | 1:F:22:VAL:C | 2.58 | 0.40 |
| 1:F:43:SER:O | 1:F:44:PHE:O | 2.39 | 0.40 |
| 1:G:406:ALA:HB2 | 1:G:496:PRO:HB3 | 2.03 | 0.40 |
| 1:G:85:ALA:HB2 | 1:G:498:LYS:HE2 | 2.04 | 0.40 |
| 1:H:106:ALA:O | 1:H:109:ALA:N | 2.49 | 0.40 |
| 1:H:158:VAL:O | 1:H:159:GLY:C | 2.60 | 0.40 |
| 1:H:221:LEU:CD1 | 1:H:223:ALA:N | 2.83 | 0.40 |
| 1:I:344:GLY:O | 1:I:345:ARG:C | 2.60 | 0.40 |
| 1:I:90:THR:O | 1:I:94:VAL:HG23 | 2.21 | 0.40 |
| 1:J:24:ALA:HA | 1:J:27:VAL:HG12 | 2.02 | 0.40 |
| 1:J:501:ARG:O | 1:J:502:SER:C | 2.60 | 0.40 |
| 1:K:106:ALA:HA | 1:K:111:MET:CE | 2.51 | 0.40 |
| 1:K:106:ALA:HA | 1:K:111:MET:HE1 | 2.02 | 0.40 |
| 1:K:158:VAL:O | 1:K:159:GLY:C | 2.60 | 0.40 |
| 1:K:272:LYS:HE3 | 1:K:272:LYS:HB2 | 1.79 | 0.40 |
| 1:K:286:LYS:NZ | 1:K:304:GLU:OE2 | 2.47 | 0.40 |
| 1:K:131:LEU:HD12 | 1:K:422:VAL:HG11 | 2.02 | 0.40 |
| 1:L:104:LEU:HA | 1:L:104:LEU:HD12 | 1.80 | 0.40 |
| 1:L:10:ASN:O | 1:L:12:ALA:N | 2.54 | 0.40 |
| 1:L:308:GLU:CG | 1:L:309:LEU:N | 2.75 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:443:ALA:O | 1:L:446:ALA:HB3 | 2.21 | 0.40 |
| 1:M:317:LEU:HD12 | 1:M:317:LEU:N | 2.37 | 0.40 |
| 1:N:24:ALA:HA | 1:N:27:VAL:HG12 | 2.02 | 0.40 |
| 1:N:288:MET:HA | 1:N:288:MET:HE2 | 2.01 | 0.40 |
| 1:N:301:ILE:HG22 | 1:N:301:ILE:O | 2.21 | 0.40 |
| 1:N:313:THR:HG22 | 1:N:314:LEU:H | 1.86 | 0.40 |
| 1:N:419:LEU:HD21 | 1:N:500:THR:CG2 | 2.52 | 0.40 |
| 1:N:76:GLU:O | 1:N:80:LYS:HG3 | 2.21 | 0.40 |
| 2:P:72:GLY:O | 2:P:74:LYS:HE2 | 2.22 | 0.40 |
| 2:U:3:ILE:N | 2:U:3:ILE:HD12 | 2.36 | 0.40 |
| 2:U:7:HIS:C | 2:U:9:ARG:H | 2.25 | 0.40 |
| 1:A:128:VAL:CG1 | 1:A:132:LYS:HE2 | 2.51 | 0.40 |
| 1:A:153:ASN:O | 1:A:154:SER:CB | 2.69 | 0.40 |
| 1:A:278:ALA:CB | 1:A:279:PRO:CD | 2.94 | 0.40 |
| 1:A:284:ARG:CG | 1:A:288:MET:HE1 | 2.51 | 0.40 |
| 1:A:308:GLU:O | 1:A:311:LYS:HB3 | 2.21 | 0.40 |
| 1:A:358:SER:HA | 1:A:362:ARG:CD | 2.51 | 0.40 |
| 1:B:253:ASP:CG | 1:B:254:VAL:N | 2.72 | 0.40 |
| 1:B:441:LYS:HA | 1:B:441:LYS:HD2 | 1.87 | 0.40 |
| 1:B:443:ALA:O | 1:B:447:MET:HG3 | 2.22 | 0.40 |
| 1:C:32:GLY:N | 4:C:1:ADP:O1A | 2.29 | 0.40 |
| 1:C:339:GLU:HA | 1:C:342:ILE:HB | 2.04 | 0.40 |
| 1:C:59:GLU:OE1 | 1:C:59:GLU:HA | 2.21 | 0.40 |
| 1:D:281:PHE:H | 1:D:284:ARG:CD | 2.34 | 0.40 |
| 1:D:329:THR:HG22 | 1:D:330:THR:N | 2.36 | 0.40 |
| 1:D:364:LYS:O | 1:D:367:GLU:HB3 | 2.21 | 0.40 |
| 1:E:134:LEU:H | 1:E:134:LEU:CD1 | 2.34 | 0.40 |
| 1:E:230:ILE:O | 1:E:232:GLU:N | 2.55 | 0.40 |
| 1:E:362:ARG:O | 1:E:366:GLN:OE1 | 2.39 | 0.40 |
| 1:F:10:ASN:O | 1:F:11:ASP:C | 2.59 | 0.40 |
| 1:F:205:ILE:HG12 | 1:F:211:GLY:HA2 | 2.02 | 0.40 |
| 1:F:322:ARG:CB | 1:F:333:ILE:HD12 | 2.18 | 0.40 |
| 1:F:349:ILE:HG22 | 1:F:349:ILE:O | 2.20 | 0.40 |
| 1:F:178:GLU:O | 1:F:380:LYS:HA | 2.22 | 0.40 |
| 1:G:254:VAL:HG12 | 1:G:259:LEU:HG | 2.04 | 0.40 |
| 1:G:288:MET:O | 1:G:289:LEU:HD23 | 2.22 | 0.40 |
| 1:G:309:LEU:O | 1:G:310:GLU:C | 2.60 | 0.40 |
| 1:H:226:LYS:HG3 | 1:H:252:GLU:CB | 2.47 | 0.40 |
| 1:H:221:LEU:N | 1:H:248:LEU:O | 2.53 | 0.40 |
| 1:H:194:GLN:CG | 1:H:331:THR:HB | 2.41 | 0.40 |
| 1:I:140:ASP:C | 1:I:142:LYS:N | 2.75 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:353:ILE:HD11 | 1:I:369:VAL:CG2 | 2.50 | 0.40 |
| 1:I:379:ILE:HG22 | 1:I:380:LYS:N | 2.36 | 0.40 |
| 1:I:475:ASN:ND2 | 1:I:489:ILE:HD12 | 2.36 | 0.40 |
| 1:J:124:VAL:O | 1:J:125:THR:C | 2.60 | 0.40 |
| 1:J:231:ARG:HG2 | 1:J:310:GLU:OE2 | 2.21 | 0.40 |
| 1:J:194:GLN:HG3 | 1:J:331:THR:HB | 2.02 | 0.40 |
| 1:D:461:GLU:OE2 | 1:J:452:ARG:NH2 | 2.54 | 0.40 |
| 1:J:66:PHE:HA | 1:J:520:MET:CE | 2.51 | 0.40 |
| 1:K:257:GLU:O | 1:K:261:THR:HG23 | 2.21 | 0.40 |
| 1:K:501:ARG:O | 1:K:505:GLN:HG3 | 2.20 | 0.40 |
| 1:L:389:MET:CE | 1:L:389:MET:C | 2.90 | 0.40 |
| 1:L:404:ARG:O | 1:L:407:VAL:HB | 2.21 | 0.40 |
| 1:M:322:ARG:HB3 | 1:M:333:ILE:HD12 | 2.03 | 0.40 |
| 1:N:381:VAL:HB | 1:N:389:MET:CE | 2.52 | 0.40 |
| 1:N:66:PHE:CD1 | 1:N:520:MET:HE2 | 2.55 | 0.40 |
| 2:P:86:MET:SD | 2:P:86:MET:N | 2.94 | 0.40 |
| 2:Q:3:ILE:HD13 | 2:Q:11:ILE:CD1 | 2.51 | 0.40 |
| 2:T:7:HIS:O | 2:T:7:HIS:ND1 | 2.55 | 0.40 |
| 2:T:9:ARG:HA | 2:T:9:ARG:HD3 | 1.89 | 0.40 |
| 1:A:112:ASN:HA | 1:A:113:PRO:HD3 | 1.86 | 0.40 |
| 1:A:266:THR:HG21 | 1:A:273:VAL:O | 2.22 | 0.40 |
| 1:A:307:MET:C | 1:A:308:GLU:HG3 | 2.42 | 0.40 |
| 1:A:42:LYS:HE2 | 1:A:48:THR:HB | 2.04 | 0.40 |
| 1:B:128:VAL:HG12 | 1:B:132:LYS:HE2 | 2.02 | 0.40 |
| 1:B:261:THR:O | 1:B:265:ASN:ND2 | 2.55 | 0.40 |
| 1:B:339:GLU:CD | 1:B:339:GLU:N | 2.75 | 0.40 |
| 1:B:43:SER:O | 1:B:44:PHE:O | 2.40 | 0.40 |
| 1:C:146:GLN:HE21 | 1:C:494:LEU:HD11 | 1.85 | 0.40 |
| 1:D:115:ASP:HB3 | 1:D:436:GLN:HG3 | 2.02 | 0.40 |
| 1:D:117:LYS:HG2 | 1:D:121:ASP:OD2 | 2.22 | 0.40 |
| 1:D:229:ASN:C | 1:D:231:ARG:N | 2.74 | 0.40 |
| 1:D:279:PRO:HB3 | 1:D:288:MET:HE3 | 2.03 | 0.40 |
| 1:D:66:PHE:O | 1:D:67:GLU:C | 2.59 | 0.40 |
| 1:E:150:ILE:CG2 | 1:E:151:SER:N | 2.84 | 0.40 |
| 1:E:174:VAL:HG23 | 1:E:370:ALA:CB | 2.51 | 0.40 |
| 1:F:149:THR:HG23 | 1:F:156:GLU:N | 2.37 | 0.40 |
| 1:F:195:PHE:CD1 | 1:F:195:PHE:C | 2.95 | 0.40 |
| 1:F:261:THR:O | 1:F:265:ASN:ND2 | 2.55 | 0.40 |
| 1:F:270:ILE:HG23 | 2:T:25:ILE:HG22 | 2.03 | 0.40 |
| 1:F:296:THR:CG2 | 1:F:335:GLY:HA3 | 2.29 | 0.40 |
| 1:G:199:TYR:O | 1:G:199:TYR:CD1 | 2.73 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:249:ILE:HB | 1:G:275:ALA:HB1 | 2.01 | 0.40 |
| 1:G:270:ILE:O | 1:G:271:VAL:HG13 | 2.20 | 0.40 |
| 1:G:359:ASP:O | 1:G:360:TYR:CB | 2.69 | 0.40 |
| 1:G:486:GLY:HA3 | 1:G:491:MET:HE2 | 2.03 | 0.40 |
| 1:A:26:ALA:HA | 1:G:8:PHE:CE2 | 2.56 | 0.40 |
| 1:H:501:ARG:O | 1:H:505:GLN:HG3 | 2.22 | 0.40 |
| 1:H:8:PHE:O | 1:H:9:GLY:C | 2.59 | 0.40 |
| 1:I:201:SER:O | 1:I:204:PHE:HB2 | 2.21 | 0.40 |
| 1:I:347:ALA:O | 1:I:350:ARG:HB2 | 2.22 | 0.40 |
| 1:I:354:GLU:CG | 1:I:355:GLU:H | 2.34 | 0.40 |
| 1:I:166:MET:HE1 | 1:I:407:VAL:HG21 | 2.04 | 0.40 |
| 1:J:115:ASP:O | 1:J:116:LEU:C | 2.60 | 0.40 |
| 1:J:401:HIS:O | 1:J:402:ALA:C | 2.58 | 0.40 |
| 1:J:37:ASN:HB3 | 1:J:51:LYS:CG | 2.50 | 0.40 |
| 1:J:56:VAL:O | 1:J:57:ALA:C | 2.59 | 0.40 |
| 1:M:142:LYS:O | 1:M:146:GLN:HB2 | 2.22 | 0.40 |
| 1:M:257:GLU:O | 1:M:261:THR:HG23 | 2.21 | 0.40 |
| 1:M:401:HIS:O | 1:M:402:ALA:C | 2.59 | 0.40 |
| 1:M:501:ARG:O | 1:M:505:GLN:HG3 | 2.22 | 0.40 |
| 1:N:166:MET:HE2 | 1:N:171:LYS:HG2 | 2.04 | 0.40 |
| 1:N:231:ARG:O | 1:N:233:MET:N | 2.54 | 0.40 |
| 2:P:7:HIS:O | 2:P:8:ASP:CB | 2.64 | 0.40 |
| 2:Q:8:ASP:O | 2:Q:87:SER:HA | 2.21 | 0.40 |
| 2:R:47:ARG:HD3 | 2:R:49:LEU:HB2 | 2.03 | 0.40 |
| 2:T:3:ILE:CD1 | 2:T:3:ILE:H | 2.27 | 0.40 |
| 2:T:47:ARG:CD | 2:T:49:LEU:HB2 | 2.51 | 0.40 |
| 2:T:7:HIS:C | 2:T:9:ARG:H | 2.25 | 0.40 |
| 2:O:74:LYS:CE | 2:U:68:ASN:HD22 | 2.34 | 0.40 |
| 2:T:37:ARG:NE | 2:U:76:GLU:OE1 | 2.44 | 0.40 |
| 1:A:112:ASN:HD22 | 1:A:115:ASP:CG | 2.25 | 0.40 |
| 1:A:203:TYR:H | 1:A:203:TYR:HD1 | 1.68 | 0.40 |
| 1:A:284:ARG:O | 1:A:285:ARG:C | 2.59 | 0.40 |
| 1:A:320:ALA:HA | 1:A:334:ASP:O | 2.20 | 0.40 |
| 1:A:406:ALA:O | 1:A:410:GLY:N | 2.53 | 0.40 |
| 1:B:208:PRO:O | 1:B:212:ALA:HB3 | 2.22 | 0.40 |
| 1:B:261:THR:HG23 | 1:B:262:LEU:H | 1.87 | 0.40 |
| 1:B:349:ILE:HG22 | 1:B:349:ILE:O | 2.21 | 0.40 |
| 1:B:368:ARG:CD | 1:B:372:LEU:HD11 | 2.51 | 0.40 |
| 1:C:207:LYS:CB | 1:C:208:PRO:CD | 2.96 | 0.40 |
| 1:C:207:LYS:HZ2 | 1:C:207:LYS:HB2 | 1.86 | 0.40 |
| 1:C:207:LYS:CB | 1:C:207:LYS:NZ | 2.83 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:321:LYS:HG3 | 1:C:334:ASP:HB3 | 2.03 | 0.40 |
| 1:C:434:GLU:HA | 1:C:437:ASN:HD22 | 1.87 | 0.40 |
| 1:C:478:TYR:CE2 | 1:C:480:ALA:HA | 2.56 | 0.40 |
| 1:D:443:ALA:O | 1:D:444:LEU:C | 2.59 | 0.40 |
| 1:F:290:GLN:O | 1:F:294:THR:N | 2.54 | 0.40 |
| 1:G:128:VAL:HG12 | 1:G:132:LYS:HE2 | 2.02 | 0.40 |
| 1:G:14:VAL:O | 1:G:18:ARG:HG3 | 2.20 | 0.40 |
| 1:H:219:PHE:O | 1:H:247:LEU:HD22 | 2.21 | 0.40 |
| 1:I:81:ALA:HA | 1:I:506:TYR:CD2 | 2.56 | 0.40 |
| 1:J:18:ARG:O | 1:J:19:GLY:C | 2.60 | 0.40 |
| 1:J:216:GLU:O | 1:J:217:SER:C | 2.59 | 0.40 |
| 1:J:226:LYS:HD2 | 1:J:226:LYS:N | 2.36 | 0.40 |
| 1:J:231:ARG:HH11 | 1:J:231:ARG:CB | 2.35 | 0.40 |
| 1:K:128:VAL:O | 1:K:132:LYS:HG3 | 2.22 | 0.40 |
| 1:K:209:GLU:HA | 1:K:209:GLU:OE1 | 2.22 | 0.40 |
| 1:K:228:SER:HA | 1:K:255:GLU:HB2 | 2.03 | 0.40 |
| 1:K:421:ARG:O | 1:K:422:VAL:C | 2.59 | 0.40 |
| 1:K:32:GLY:HA2 | 1:K:454:ILE:HG23 | 2.02 | 0.40 |
| 1:L:222:LEU:CD1 | 1:L:293:ALA:HA | 2.51 | 0.40 |
| 1:L:236:VAL:CG2 | 1:L:237:LEU:N | 2.82 | 0.40 |
| 1:L:351:GLN:O | 1:L:354:GLU:HB3 | 2.21 | 0.40 |
| 1:M:227:ILE:CD1 | 1:M:309:LEU:HD11 | 2.51 | 0.40 |
| 1:M:323:VAL:CG2 | 1:M:332:ILE:HG22 | 2.52 | 0.40 |
| 1:M:445:ARG:HB3 | 1:M:445:ARG:HE | 1.73 | 0.40 |
| 1:M:7:LYS:HG3 | 1:M:66:PHE:CZ | 2.57 | 0.40 |
| 1:N:201:SER:HA | 1:N:202:PRO:HD3 | 1.90 | 0.40 |
| 2:S:71:TYR:O | 2:S:73:VAL:N | 2.54 | 0.40 |
| 2:T:20:LYS:HA | 2:T:28:THR:CG2 | 2.52 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:A:425:LYS:NZ | 1:J:484:GLU:OE2[4_445] | 2.13 | 0.07 |

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|----------|-------------|----|
| 1 | A | 522/547 (95%) | 396 (76%) | 92 (18%) | 34 (6%) | 1 | 8 |
| 1 | B | 522/547 (95%) | 399 (76%) | 94 (18%) | 29 (6%) | 2 | 12 |
| 1 | C | 522/547 (95%) | 397 (76%) | 88 (17%) | 37 (7%) | 1 | 6 |
| 1 | D | 522/547 (95%) | 395 (76%) | 95 (18%) | 32 (6%) | 2 | 10 |
| 1 | E | 522/547 (95%) | 390 (75%) | 98 (19%) | 34 (6%) | 1 | 8 |
| 1 | F | 522/547 (95%) | 399 (76%) | 93 (18%) | 30 (6%) | 2 | 12 |
| 1 | G | 522/547 (95%) | 390 (75%) | 98 (19%) | 34 (6%) | 1 | 8 |
| 1 | H | 522/547 (95%) | 377 (72%) | 115 (22%) | 30 (6%) | 2 | 12 |
| 1 | I | 522/547 (95%) | 384 (74%) | 113 (22%) | 25 (5%) | 2 | 16 |
| 1 | J | 522/547 (95%) | 387 (74%) | 110 (21%) | 25 (5%) | 2 | 16 |
| 1 | K | 522/547 (95%) | 376 (72%) | 121 (23%) | 25 (5%) | 2 | 16 |
| 1 | L | 522/547 (95%) | 372 (71%) | 124 (24%) | 26 (5%) | 2 | 15 |
| 1 | M | 522/547 (95%) | 383 (73%) | 110 (21%) | 29 (6%) | 2 | 12 |
| 1 | N | 522/547 (95%) | 384 (74%) | 112 (22%) | 26 (5%) | 2 | 15 |
| 2 | O | 95/97 (98%) | 69 (73%) | 20 (21%) | 6 (6%) | 1 | 9 |
| 2 | P | 95/97 (98%) | 65 (68%) | 24 (25%) | 6 (6%) | 1 | 9 |
| 2 | Q | 95/97 (98%) | 67 (70%) | 21 (22%) | 7 (7%) | 1 | 6 |
| 2 | R | 95/97 (98%) | 68 (72%) | 18 (19%) | 9 (10%) | 1 | 3 |
| 2 | S | 95/97 (98%) | 73 (77%) | 16 (17%) | 6 (6%) | 1 | 9 |
| 2 | T | 95/97 (98%) | 67 (70%) | 20 (21%) | 8 (8%) | 1 | 4 |
| 2 | U | 95/97 (98%) | 64 (67%) | 25 (26%) | 6 (6%) | 1 | 9 |
| All | All | 7973/8337 (96%) | 5902 (74%) | 1607 (20%) | 464 (6%) | 2 | 11 |

All (464) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 29 | VAL |
| 1 | A | 44 | PHE |
| 1 | A | 233 | MET |
| 1 | A | 279 | PRO |
| 1 | A | 309 | LEU |
| 1 | A | 311 | LYS |
| 1 | A | 353 | ILE |
| 1 | A | 358 | SER |
| 1 | B | 29 | VAL |
| 1 | B | 44 | PHE |
| 1 | B | 206 | ASN |
| 1 | B | 233 | MET |
| 1 | B | 279 | PRO |
| 1 | B | 309 | LEU |
| 1 | B | 311 | LYS |
| 1 | B | 353 | ILE |
| 1 | B | 354 | GLU |
| 1 | B | 358 | SER |
| 1 | B | 373 | ALA |
| 1 | C | 29 | VAL |
| 1 | C | 44 | PHE |
| 1 | C | 206 | ASN |
| 1 | C | 233 | MET |
| 1 | C | 279 | PRO |
| 1 | C | 309 | LEU |
| 1 | C | 311 | LYS |
| 1 | C | 353 | ILE |
| 1 | C | 358 | SER |
| 1 | D | 44 | PHE |
| 1 | D | 206 | ASN |
| 1 | D | 233 | MET |
| 1 | D | 309 | LEU |
| 1 | D | 311 | LYS |
| 1 | D | 342 | ILE |
| 1 | D | 353 | ILE |
| 1 | D | 354 | GLU |
| 1 | D | 358 | SER |
| 1 | E | 44 | PHE |
| 1 | E | 233 | MET |
| 1 | E | 279 | PRO |
| 1 | E | 309 | LEU |
| 1 | E | 311 | LYS |
| 1 | E | 312 | ALA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 353 | ILE |
| 1 | E | 354 | GLU |
| 1 | F | 29 | VAL |
| 1 | F | 44 | PHE |
| 1 | F | 233 | MET |
| 1 | F | 279 | PRO |
| 1 | F | 309 | LEU |
| 1 | F | 311 | LYS |
| 1 | F | 353 | ILE |
| 1 | F | 358 | SER |
| 1 | G | 44 | PHE |
| 1 | G | 233 | MET |
| 1 | G | 279 | PRO |
| 1 | G | 309 | LEU |
| 1 | G | 311 | LYS |
| 1 | G | 336 | VAL |
| 1 | G | 353 | ILE |
| 1 | H | 146 | GLN |
| 1 | H | 270 | ILE |
| 1 | H | 401 | HIS |
| 1 | H | 425 | LYS |
| 1 | I | 146 | GLN |
| 1 | I | 267 | MET |
| 1 | I | 270 | ILE |
| 1 | I | 401 | HIS |
| 1 | J | 270 | ILE |
| 1 | K | 270 | ILE |
| 1 | K | 425 | LYS |
| 1 | L | 146 | GLN |
| 1 | L | 270 | ILE |
| 1 | L | 425 | LYS |
| 1 | M | 146 | GLN |
| 1 | M | 270 | ILE |
| 1 | M | 323 | VAL |
| 1 | M | 425 | LYS |
| 1 | N | 270 | ILE |
| 2 | O | 7 | HIS |
| 2 | P | 7 | HIS |
| 2 | P | 51 | ASN |
| 2 | Q | 7 | HIS |
| 2 | Q | 49 | LEU |
| 2 | Q | 51 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | R | 7 | HIS |
| 2 | S | 7 | HIS |
| 2 | S | 51 | ASN |
| 2 | T | 7 | HIS |
| 2 | U | 7 | HIS |
| 2 | U | 49 | LEU |
| 1 | A | 206 | ASN |
| 1 | A | 253 | ASP |
| 1 | A | 293 | ALA |
| 1 | A | 336 | VAL |
| 1 | A | 342 | ILE |
| 1 | A | 354 | GLU |
| 1 | A | 373 | ALA |
| 1 | B | 284 | ARG |
| 1 | B | 312 | ALA |
| 1 | B | 334 | ASP |
| 1 | B | 342 | ILE |
| 1 | C | 228 | SER |
| 1 | C | 231 | ARG |
| 1 | C | 284 | ARG |
| 1 | C | 354 | GLU |
| 1 | C | 373 | ALA |
| 1 | D | 29 | VAL |
| 1 | D | 279 | PRO |
| 1 | D | 312 | ALA |
| 1 | D | 373 | ALA |
| 1 | E | 29 | VAL |
| 1 | E | 169 | VAL |
| 1 | E | 206 | ASN |
| 1 | E | 231 | ARG |
| 1 | E | 293 | ALA |
| 1 | E | 305 | ILE |
| 1 | E | 336 | VAL |
| 1 | E | 342 | ILE |
| 1 | E | 373 | ALA |
| 1 | F | 206 | ASN |
| 1 | F | 228 | SER |
| 1 | F | 231 | ARG |
| 1 | F | 305 | ILE |
| 1 | F | 312 | ALA |
| 1 | F | 354 | GLU |
| 1 | F | 373 | ALA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 9 | GLY |
| 1 | G | 29 | VAL |
| 1 | G | 253 | ASP |
| 1 | G | 293 | ALA |
| 1 | G | 312 | ALA |
| 1 | G | 338 | GLU |
| 1 | G | 342 | ILE |
| 1 | G | 354 | GLU |
| 1 | G | 358 | SER |
| 1 | G | 373 | ALA |
| 1 | H | 389 | MET |
| 1 | H | 429 | LEU |
| 1 | I | 85 | ALA |
| 1 | I | 256 | GLY |
| 1 | I | 352 | GLN |
| 1 | I | 389 | MET |
| 1 | I | 425 | LYS |
| 1 | I | 429 | LEU |
| 1 | J | 85 | ALA |
| 1 | J | 146 | GLN |
| 1 | J | 267 | MET |
| 1 | J | 352 | GLN |
| 1 | J | 389 | MET |
| 1 | J | 425 | LYS |
| 1 | J | 429 | LEU |
| 1 | J | 432 | GLN |
| 1 | K | 85 | ALA |
| 1 | K | 146 | GLN |
| 1 | K | 160 | LYS |
| 1 | K | 286 | LYS |
| 1 | K | 389 | MET |
| 1 | K | 401 | HIS |
| 1 | K | 429 | LEU |
| 1 | K | 432 | GLN |
| 1 | L | 85 | ALA |
| 1 | L | 267 | MET |
| 1 | L | 286 | LYS |
| 1 | L | 389 | MET |
| 1 | L | 398 | ASP |
| 1 | L | 429 | LEU |
| 1 | L | 432 | GLN |
| 1 | M | 223 | ALA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 267 | MET |
| 1 | M | 356 | ALA |
| 1 | M | 389 | MET |
| 1 | M | 401 | HIS |
| 1 | M | 429 | LEU |
| 1 | M | 432 | GLN |
| 1 | N | 85 | ALA |
| 1 | N | 146 | GLN |
| 1 | N | 155 | ASP |
| 1 | N | 232 | GLU |
| 1 | N | 267 | MET |
| 1 | N | 401 | HIS |
| 1 | N | 425 | LYS |
| 1 | N | 429 | LEU |
| 1 | N | 432 | GLN |
| 2 | O | 51 | ASN |
| 2 | P | 5 | PRO |
| 2 | P | 21 | SER |
| 2 | Q | 80 | ASN |
| 2 | R | 14 | ARG |
| 2 | R | 51 | ASN |
| 2 | S | 14 | ARG |
| 2 | T | 21 | SER |
| 2 | T | 51 | ASN |
| 2 | T | 72 | GLY |
| 2 | U | 21 | SER |
| 2 | U | 52 | GLY |
| 1 | A | 228 | SER |
| 1 | A | 268 | ARG |
| 1 | A | 282 | GLY |
| 1 | A | 284 | ARG |
| 1 | A | 289 | LEU |
| 1 | A | 312 | ALA |
| 1 | A | 334 | ASP |
| 1 | A | 363 | GLU |
| 1 | A | 390 | LYS |
| 1 | B | 231 | ARG |
| 1 | B | 237 | LEU |
| 1 | B | 263 | VAL |
| 1 | B | 293 | ALA |
| 1 | C | 9 | GLY |
| 1 | C | 153 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 293 | ALA |
| 1 | C | 312 | ALA |
| 1 | C | 336 | VAL |
| 1 | C | 338 | GLU |
| 1 | C | 342 | ILE |
| 1 | D | 231 | ARG |
| 1 | D | 268 | ARG |
| 1 | D | 334 | ASP |
| 1 | E | 153 | ASN |
| 1 | E | 228 | SER |
| 1 | E | 268 | ARG |
| 1 | E | 280 | GLY |
| 1 | E | 358 | SER |
| 1 | F | 251 | ALA |
| 1 | F | 284 | ARG |
| 1 | F | 362 | ARG |
| 1 | G | 206 | ASN |
| 1 | G | 360 | TYR |
| 1 | G | 362 | ARG |
| 1 | H | 85 | ALA |
| 1 | H | 155 | ASP |
| 1 | H | 232 | GLU |
| 1 | H | 267 | MET |
| 1 | H | 327 | LYS |
| 1 | H | 352 | GLN |
| 1 | H | 356 | ALA |
| 1 | H | 421 | ARG |
| 1 | H | 432 | GLN |
| 1 | H | 462 | PRO |
| 1 | I | 277 | LYS |
| 1 | I | 323 | VAL |
| 1 | I | 432 | GLN |
| 1 | J | 286 | LYS |
| 1 | J | 401 | HIS |
| 1 | J | 462 | PRO |
| 1 | K | 231 | ARG |
| 1 | K | 232 | GLU |
| 1 | K | 273 | VAL |
| 1 | K | 327 | LYS |
| 1 | L | 160 | LYS |
| 1 | L | 203 | TYR |
| 1 | L | 327 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 401 | HIS |
| 1 | L | 421 | ARG |
| 1 | M | 85 | ALA |
| 1 | M | 203 | TYR |
| 1 | M | 231 | ARG |
| 1 | M | 232 | GLU |
| 1 | M | 277 | LYS |
| 1 | M | 421 | ARG |
| 1 | M | 462 | PRO |
| 1 | M | 509 | SER |
| 1 | N | 66 | PHE |
| 1 | N | 203 | TYR |
| 1 | N | 252 | GLU |
| 1 | N | 286 | LYS |
| 1 | N | 389 | MET |
| 1 | N | 421 | ARG |
| 1 | N | 509 | SER |
| 2 | O | 14 | ARG |
| 2 | O | 21 | SER |
| 2 | O | 45 | ASN |
| 2 | Q | 21 | SER |
| 2 | R | 21 | SER |
| 2 | R | 30 | SER |
| 2 | S | 21 | SER |
| 2 | T | 49 | LEU |
| 2 | T | 80 | ASN |
| 2 | U | 51 | ASN |
| 1 | A | 207 | LYS |
| 1 | A | 231 | ARG |
| 1 | A | 360 | TYR |
| 1 | A | 361 | ASP |
| 1 | B | 153 | ASN |
| 1 | B | 230 | ILE |
| 1 | B | 268 | ARG |
| 1 | B | 278 | ALA |
| 1 | B | 289 | LEU |
| 1 | B | 305 | ILE |
| 1 | C | 253 | ASP |
| 1 | C | 260 | ALA |
| 1 | C | 280 | GLY |
| 1 | C | 289 | LEU |
| 1 | C | 362 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 228 | SER |
| 1 | D | 251 | ALA |
| 1 | D | 253 | ASP |
| 1 | D | 293 | ALA |
| 1 | D | 303 | GLU |
| 1 | D | 305 | ILE |
| 1 | E | 253 | ASP |
| 1 | E | 284 | ARG |
| 1 | E | 294 | THR |
| 1 | E | 390 | LYS |
| 1 | F | 207 | LYS |
| 1 | F | 293 | ALA |
| 1 | F | 303 | GLU |
| 1 | G | 207 | LYS |
| 1 | G | 228 | SER |
| 1 | G | 230 | ILE |
| 1 | H | 203 | TYR |
| 1 | I | 66 | PHE |
| 1 | I | 155 | ASP |
| 1 | I | 160 | LYS |
| 1 | I | 165 | ALA |
| 1 | I | 260 | ALA |
| 1 | I | 421 | ARG |
| 1 | J | 165 | ALA |
| 1 | J | 256 | GLY |
| 1 | J | 315 | GLU |
| 1 | J | 421 | ARG |
| 1 | K | 66 | PHE |
| 1 | K | 155 | ASP |
| 1 | K | 235 | PRO |
| 1 | K | 288 | MET |
| 1 | K | 304 | GLU |
| 1 | K | 421 | ARG |
| 1 | K | 462 | PRO |
| 1 | L | 352 | GLN |
| 1 | L | 462 | PRO |
| 1 | M | 89 | THR |
| 1 | M | 155 | ASP |
| 1 | M | 160 | LYS |
| 1 | M | 252 | GLU |
| 1 | M | 370 | ALA |
| 1 | N | 231 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 442 | VAL |
| 1 | N | 462 | PRO |
| 2 | Q | 72 | GLY |
| 2 | T | 5 | PRO |
| 2 | T | 53 | GLU |
| 1 | A | 260 | ALA |
| 1 | A | 294 | THR |
| 1 | A | 305 | ILE |
| 1 | A | 392 | LYS |
| 1 | C | 57 | ALA |
| 1 | C | 182 | GLY |
| 1 | C | 305 | ILE |
| 1 | D | 230 | ILE |
| 1 | D | 263 | VAL |
| 1 | D | 289 | LEU |
| 1 | D | 294 | THR |
| 1 | E | 158 | VAL |
| 1 | E | 207 | LYS |
| 1 | E | 260 | ALA |
| 1 | E | 289 | LEU |
| 1 | E | 334 | ASP |
| 1 | E | 363 | GLU |
| 1 | E | 392 | LYS |
| 1 | F | 230 | ILE |
| 1 | F | 342 | ILE |
| 1 | F | 392 | LYS |
| 1 | G | 169 | VAL |
| 1 | G | 294 | THR |
| 1 | G | 305 | ILE |
| 1 | G | 392 | LYS |
| 1 | H | 153 | ASN |
| 1 | H | 160 | LYS |
| 1 | H | 231 | ARG |
| 1 | H | 288 | MET |
| 1 | H | 315 | GLU |
| 1 | H | 398 | ASP |
| 1 | H | 509 | SER |
| 1 | I | 235 | PRO |
| 1 | I | 259 | LEU |
| 1 | I | 442 | VAL |
| 1 | I | 462 | PRO |
| 1 | J | 160 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 231 | ARG |
| 1 | J | 232 | GLU |
| 1 | J | 235 | PRO |
| 1 | J | 288 | MET |
| 1 | J | 398 | ASP |
| 1 | L | 158 | VAL |
| 1 | L | 407 | VAL |
| 1 | L | 442 | VAL |
| 1 | M | 66 | PHE |
| 1 | M | 442 | VAL |
| 1 | N | 160 | LYS |
| 2 | O | 52 | GLY |
| 2 | P | 69 | ASP |
| 2 | R | 5 | PRO |
| 2 | S | 80 | ASN |
| 2 | U | 69 | ASP |
| 1 | B | 169 | VAL |
| 1 | B | 207 | LYS |
| 1 | C | 207 | LYS |
| 1 | C | 251 | ALA |
| 1 | C | 278 | ALA |
| 1 | C | 310 | GLU |
| 1 | C | 361 | ASP |
| 1 | D | 207 | LYS |
| 1 | D | 336 | VAL |
| 1 | E | 237 | LEU |
| 1 | F | 158 | VAL |
| 1 | G | 231 | ARG |
| 1 | G | 466 | ALA |
| 1 | H | 165 | ALA |
| 1 | K | 315 | GLU |
| 1 | K | 442 | VAL |
| 1 | L | 153 | ASN |
| 1 | L | 155 | ASP |
| 1 | L | 159 | GLY |
| 1 | M | 286 | LYS |
| 1 | N | 342 | ILE |
| 2 | Q | 52 | GLY |
| 2 | R | 31 | ALA |
| 2 | R | 49 | LEU |
| 1 | A | 278 | ALA |
| 1 | F | 474 | GLY |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 323 | VAL |
| 1 | I | 472 | GLY |
| 1 | J | 137 | PRO |
| 1 | L | 280 | GLY |
| 1 | M | 235 | PRO |
| 1 | N | 256 | GLY |
| 1 | N | 323 | VAL |
| 2 | P | 72 | GLY |
| 2 | S | 72 | GLY |
| 1 | A | 9 | GLY |
| 1 | B | 336 | VAL |
| 1 | D | 9 | GLY |
| 1 | D | 280 | GLY |
| 1 | G | 201 | SER |
| 1 | G | 282 | GLY |
| 1 | L | 56 | VAL |
| 1 | N | 32 | GLY |
| 1 | C | 169 | VAL |
| 1 | F | 9 | GLY |
| 1 | F | 280 | GLY |
| 1 | F | 336 | VAL |
| 1 | G | 158 | VAL |
| 1 | H | 442 | VAL |
| 1 | L | 32 | GLY |
| 2 | R | 52 | GLY |
| 1 | C | 271 | VAL |
| 1 | C | 465 | VAL |
| 1 | D | 271 | VAL |
| 1 | D | 282 | GLY |
| 1 | G | 271 | VAL |
| 1 | G | 465 | VAL |
| 1 | H | 235 | PRO |
| 1 | I | 234 | LEU |
| 1 | J | 342 | ILE |
| 1 | J | 442 | VAL |
| 1 | K | 56 | VAL |
| 1 | K | 387 | VAL |
| 1 | M | 234 | LEU |
| 1 | B | 271 | VAL |
| 1 | F | 271 | VAL |
| 1 | H | 387 | VAL |
| 1 | H | 472 | GLY |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 56 | VAL |

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 | 393/414 (95%) | 369 (94%) | 24 (6%) | 22 | 59 |
| 1 | B | 393/414 (95%) | 368 (94%) | 25 (6%) | 20 | 57 |
| 1 | C | 393/414 (95%) | 369 (94%) | 24 (6%) | 22 | 59 |
| 1 | D | 393/414 (95%) | 369 (94%) | 24 (6%) | 22 | 59 |
| 1 | E | 393/414 (95%) | 368 (94%) | 25 (6%) | 20 | 57 |
| 1 | F | 393/414 (95%) | 368 (94%) | 25 (6%) | 20 | 57 |
| 1 | G | 393/414 (95%) | 367 (93%) | 26 (7%) | 19 | 55 |
| 1 | H | 403/414 (97%) | 385 (96%) | 18 (4%) | 32 | 71 |
| 1 | I | 403/414 (97%) | 383 (95%) | 20 (5%) | 28 | 67 |
| 1 | J | 403/414 (97%) | 385 (96%) | 18 (4%) | 32 | 71 |
| 1 | K | 403/414 (97%) | 387 (96%) | 16 (4%) | 36 | 74 |
| 1 | L | 403/414 (97%) | 386 (96%) | 17 (4%) | 34 | 73 |
| 1 | M | 403/414 (97%) | 386 (96%) | 17 (4%) | 34 | 73 |
| 1 | N | 403/414 (97%) | 386 (96%) | 17 (4%) | 34 | 73 |
| 2 | O | 79/80 (99%) | 73 (92%) | 6 (8%) | 15 | 48 |
| 2 | P | 79/80 (99%) | 74 (94%) | 5 (6%) | 21 | 57 |
| 2 | Q | 79/80 (99%) | 72 (91%) | 7 (9%) | 11 | 40 |
| 2 | R | 79/80 (99%) | 70 (89%) | 9 (11%) | 7 | 27 |
| 2 | S | 79/80 (99%) | 73 (92%) | 6 (8%) | 15 | 48 |
| 2 | T | 79/80 (99%) | 71 (90%) | 8 (10%) | 9 | 33 |
| 2 | U | 79/80 (99%) | 72 (91%) | 7 (9%) | 11 | 40 |
| All | All | 6125/6356 (96%) | 5781 (94%) | 344 (6%) | 25 | 62 |

All (344) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 18 | ARG |
| 1 | A | 44 | PHE |
| 1 | A | 62 | LEU |
| 1 | A | 74 | VAL |
| 1 | A | 77 | VAL |
| 1 | A | 97 | GLN |
| 1 | A | 153 | ASN |
| 1 | A | 195 | PHE |
| 1 | A | 199 | TYR |
| 1 | A | 233 | MET |
| 1 | A | 247 | LEU |
| 1 | A | 252 | GLU |
| 1 | A | 255 | GLU |
| 1 | A | 257 | GLU |
| 1 | A | 267 | MET |
| 1 | A | 290 | GLN |
| 1 | A | 291 | ASP |
| 1 | A | 303 | GLU |
| 1 | A | 315 | GLU |
| 1 | A | 348 | GLN |
| 1 | A | 360 | TYR |
| 1 | A | 422 | VAL |
| 1 | A | 453 | GLN |
| 1 | A | 494 | LEU |
| 1 | B | 18 | ARG |
| 1 | B | 44 | PHE |
| 1 | B | 62 | LEU |
| 1 | B | 74 | VAL |
| 1 | B | 77 | VAL |
| 1 | B | 97 | GLN |
| 1 | B | 153 | ASN |
| 1 | B | 195 | PHE |
| 1 | B | 199 | TYR |
| 1 | B | 203 | TYR |
| 1 | B | 222 | LEU |
| 1 | B | 233 | MET |
| 1 | B | 247 | LEU |
| 1 | B | 255 | GLU |
| 1 | B | 257 | GLU |
| 1 | B | 267 | MET |
| 1 | B | 290 | GLN |
| 1 | B | 291 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 303 | GLU |
| 1 | B | 315 | GLU |
| 1 | B | 348 | GLN |
| 1 | B | 360 | TYR |
| 1 | B | 422 | VAL |
| 1 | B | 453 | GLN |
| 1 | B | 494 | LEU |
| 1 | C | 18 | ARG |
| 1 | C | 23 | LEU |
| 1 | C | 44 | PHE |
| 1 | C | 62 | LEU |
| 1 | C | 74 | VAL |
| 1 | C | 77 | VAL |
| 1 | C | 97 | GLN |
| 1 | C | 153 | ASN |
| 1 | C | 195 | PHE |
| 1 | C | 199 | TYR |
| 1 | C | 233 | MET |
| 1 | C | 247 | LEU |
| 1 | C | 255 | GLU |
| 1 | C | 257 | GLU |
| 1 | C | 267 | MET |
| 1 | C | 290 | GLN |
| 1 | C | 291 | ASP |
| 1 | C | 303 | GLU |
| 1 | C | 305 | ILE |
| 1 | C | 315 | GLU |
| 1 | C | 348 | GLN |
| 1 | C | 360 | TYR |
| 1 | C | 453 | GLN |
| 1 | C | 494 | LEU |
| 1 | D | 18 | ARG |
| 1 | D | 44 | PHE |
| 1 | D | 62 | LEU |
| 1 | D | 74 | VAL |
| 1 | D | 77 | VAL |
| 1 | D | 97 | GLN |
| 1 | D | 153 | ASN |
| 1 | D | 195 | PHE |
| 1 | D | 199 | TYR |
| 1 | D | 233 | MET |
| 1 | D | 247 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 255 | GLU |
| 1 | D | 257 | GLU |
| 1 | D | 267 | MET |
| 1 | D | 290 | GLN |
| 1 | D | 291 | ASP |
| 1 | D | 303 | GLU |
| 1 | D | 315 | GLU |
| 1 | D | 348 | GLN |
| 1 | D | 360 | TYR |
| 1 | D | 421 | ARG |
| 1 | D | 422 | VAL |
| 1 | D | 453 | GLN |
| 1 | D | 494 | LEU |
| 1 | E | 18 | ARG |
| 1 | E | 23 | LEU |
| 1 | E | 44 | PHE |
| 1 | E | 62 | LEU |
| 1 | E | 74 | VAL |
| 1 | E | 77 | VAL |
| 1 | E | 97 | GLN |
| 1 | E | 153 | ASN |
| 1 | E | 195 | PHE |
| 1 | E | 199 | TYR |
| 1 | E | 247 | LEU |
| 1 | E | 255 | GLU |
| 1 | E | 257 | GLU |
| 1 | E | 267 | MET |
| 1 | E | 279 | PRO |
| 1 | E | 290 | GLN |
| 1 | E | 291 | ASP |
| 1 | E | 303 | GLU |
| 1 | E | 315 | GLU |
| 1 | E | 348 | GLN |
| 1 | E | 360 | TYR |
| 1 | E | 422 | VAL |
| 1 | E | 453 | GLN |
| 1 | E | 461 | GLU |
| 1 | E | 494 | LEU |
| 1 | F | 18 | ARG |
| 1 | F | 23 | LEU |
| 1 | F | 44 | PHE |
| 1 | F | 62 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 74 | VAL |
| 1 | F | 97 | GLN |
| 1 | F | 153 | ASN |
| 1 | F | 195 | PHE |
| 1 | F | 199 | TYR |
| 1 | F | 233 | MET |
| 1 | F | 247 | LEU |
| 1 | F | 252 | GLU |
| 1 | F | 255 | GLU |
| 1 | F | 257 | GLU |
| 1 | F | 267 | MET |
| 1 | F | 290 | GLN |
| 1 | F | 291 | ASP |
| 1 | F | 303 | GLU |
| 1 | F | 315 | GLU |
| 1 | F | 348 | GLN |
| 1 | F | 360 | TYR |
| 1 | F | 421 | ARG |
| 1 | F | 422 | VAL |
| 1 | F | 453 | GLN |
| 1 | F | 494 | LEU |
| 1 | G | 18 | ARG |
| 1 | G | 23 | LEU |
| 1 | G | 44 | PHE |
| 1 | G | 62 | LEU |
| 1 | G | 74 | VAL |
| 1 | G | 77 | VAL |
| 1 | G | 97 | GLN |
| 1 | G | 153 | ASN |
| 1 | G | 195 | PHE |
| 1 | G | 199 | TYR |
| 1 | G | 203 | TYR |
| 1 | G | 233 | MET |
| 1 | G | 247 | LEU |
| 1 | G | 255 | GLU |
| 1 | G | 257 | GLU |
| 1 | G | 267 | MET |
| 1 | G | 290 | GLN |
| 1 | G | 291 | ASP |
| 1 | G | 303 | GLU |
| 1 | G | 315 | GLU |
| 1 | G | 348 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 360 | TYR |
| 1 | G | 422 | VAL |
| 1 | G | 453 | GLN |
| 1 | G | 475 | ASN |
| 1 | G | 494 | LEU |
| 1 | H | 20 | VAL |
| 1 | H | 37 | ASN |
| 1 | H | 59 | GLU |
| 1 | H | 129 | GLU |
| 1 | H | 153 | ASN |
| 1 | H | 172 | GLU |
| 1 | H | 197 | ARG |
| 1 | H | 230 | ILE |
| 1 | H | 233 | MET |
| 1 | H | 284 | ARG |
| 1 | H | 288 | MET |
| 1 | H | 291 | ASP |
| 1 | H | 331 | THR |
| 1 | H | 364 | LYS |
| 1 | H | 389 | MET |
| 1 | H | 426 | LEU |
| 1 | H | 432 | GLN |
| 1 | H | 433 | ASN |
| 1 | I | 11 | ASP |
| 1 | I | 20 | VAL |
| 1 | I | 37 | ASN |
| 1 | I | 59 | GLU |
| 1 | I | 129 | GLU |
| 1 | I | 147 | VAL |
| 1 | I | 153 | ASN |
| 1 | I | 172 | GLU |
| 1 | I | 230 | ILE |
| 1 | I | 233 | MET |
| 1 | I | 284 | ARG |
| 1 | I | 288 | MET |
| 1 | I | 291 | ASP |
| 1 | I | 331 | THR |
| 1 | I | 361 | ASP |
| 1 | I | 389 | MET |
| 1 | I | 426 | LEU |
| 1 | I | 432 | GLN |
| 1 | I | 433 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 504 | LEU |
| 1 | J | 11 | ASP |
| 1 | J | 20 | VAL |
| 1 | J | 37 | ASN |
| 1 | J | 59 | GLU |
| 1 | J | 129 | GLU |
| 1 | J | 147 | VAL |
| 1 | J | 153 | ASN |
| 1 | J | 172 | GLU |
| 1 | J | 230 | ILE |
| 1 | J | 233 | MET |
| 1 | J | 284 | ARG |
| 1 | J | 288 | MET |
| 1 | J | 291 | ASP |
| 1 | J | 361 | ASP |
| 1 | J | 389 | MET |
| 1 | J | 426 | LEU |
| 1 | J | 432 | GLN |
| 1 | J | 433 | ASN |
| 1 | K | 37 | ASN |
| 1 | K | 59 | GLU |
| 1 | K | 129 | GLU |
| 1 | K | 147 | VAL |
| 1 | K | 153 | ASN |
| 1 | K | 172 | GLU |
| 1 | K | 179 | ASP |
| 1 | K | 230 | ILE |
| 1 | K | 233 | MET |
| 1 | K | 284 | ARG |
| 1 | K | 288 | MET |
| 1 | K | 361 | ASP |
| 1 | K | 389 | MET |
| 1 | K | 426 | LEU |
| 1 | K | 432 | GLN |
| 1 | K | 433 | ASN |
| 1 | L | 11 | ASP |
| 1 | L | 20 | VAL |
| 1 | L | 37 | ASN |
| 1 | L | 59 | GLU |
| 1 | L | 129 | GLU |
| 1 | L | 153 | ASN |
| 1 | L | 172 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 230 | ILE |
| 1 | L | 233 | MET |
| 1 | L | 284 | ARG |
| 1 | L | 288 | MET |
| 1 | L | 291 | ASP |
| 1 | L | 364 | LYS |
| 1 | L | 389 | MET |
| 1 | L | 426 | LEU |
| 1 | L | 432 | GLN |
| 1 | L | 433 | ASN |
| 1 | M | 11 | ASP |
| 1 | M | 20 | VAL |
| 1 | M | 37 | ASN |
| 1 | M | 59 | GLU |
| 1 | M | 129 | GLU |
| 1 | M | 147 | VAL |
| 1 | M | 153 | ASN |
| 1 | M | 172 | GLU |
| 1 | M | 230 | ILE |
| 1 | M | 233 | MET |
| 1 | M | 284 | ARG |
| 1 | M | 288 | MET |
| 1 | M | 307 | MET |
| 1 | M | 389 | MET |
| 1 | M | 426 | LEU |
| 1 | M | 432 | GLN |
| 1 | M | 433 | ASN |
| 1 | N | 11 | ASP |
| 1 | N | 20 | VAL |
| 1 | N | 37 | ASN |
| 1 | N | 59 | GLU |
| 1 | N | 129 | GLU |
| 1 | N | 153 | ASN |
| 1 | N | 172 | GLU |
| 1 | N | 230 | ILE |
| 1 | N | 233 | MET |
| 1 | N | 284 | ARG |
| 1 | N | 288 | MET |
| 1 | N | 291 | ASP |
| 1 | N | 361 | ASP |
| 1 | N | 389 | MET |
| 1 | N | 426 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 432 | GLN |
| 1 | N | 433 | ASN |
| 2 | O | 3 | ILE |
| 2 | O | 6 | LEU |
| 2 | O | 20 | LYS |
| 2 | O | 37 | ARG |
| 2 | O | 53 | GLU |
| 2 | O | 55 | LYS |
| 2 | P | 3 | ILE |
| 2 | P | 6 | LEU |
| 2 | P | 20 | LYS |
| 2 | P | 37 | ARG |
| 2 | P | 55 | LYS |
| 2 | Q | 3 | ILE |
| 2 | Q | 6 | LEU |
| 2 | Q | 20 | LYS |
| 2 | Q | 37 | ARG |
| 2 | Q | 53 | GLU |
| 2 | Q | 55 | LYS |
| 2 | Q | 58 | ASP |
| 2 | R | 3 | ILE |
| 2 | R | 6 | LEU |
| 2 | R | 20 | LYS |
| 2 | R | 37 | ARG |
| 2 | R | 53 | GLU |
| 2 | R | 55 | LYS |
| 2 | R | 58 | ASP |
| 2 | R | 84 | LEU |
| 2 | R | 86 | MET |
| 2 | S | 3 | ILE |
| 2 | S | 6 | LEU |
| 2 | S | 20 | LYS |
| 2 | S | 37 | ARG |
| 2 | S | 53 | GLU |
| 2 | S | 55 | LYS |
| 2 | T | 3 | ILE |
| 2 | T | 6 | LEU |
| 2 | T | 20 | LYS |
| 2 | T | 28 | THR |
| 2 | T | 37 | ARG |
| 2 | T | 53 | GLU |
| 2 | T | 55 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | T | 58 | ASP |
| 2 | U | 3 | ILE |
| 2 | U | 6 | LEU |
| 2 | U | 20 | LYS |
| 2 | U | 37 | ARG |
| 2 | U | 53 | GLU |
| 2 | U | 55 | LYS |
| 2 | U | 58 | ASP |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (187) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 21 | ASN |
| 1 | A | 82 | ASN |
| 1 | A | 112 | ASN |
| 1 | A | 146 | GLN |
| 1 | A | 153 | ASN |
| 1 | A | 194 | GLN |
| 1 | A | 319 | GLN |
| 1 | A | 348 | GLN |
| 1 | A | 352 | GLN |
| 1 | A | 366 | GLN |
| 1 | A | 432 | GLN |
| 1 | A | 457 | ASN |
| 1 | A | 475 | ASN |
| 1 | B | 21 | ASN |
| 1 | B | 82 | ASN |
| 1 | B | 112 | ASN |
| 1 | B | 146 | GLN |
| 1 | B | 153 | ASN |
| 1 | B | 194 | GLN |
| 1 | B | 319 | GLN |
| 1 | B | 348 | GLN |
| 1 | B | 351 | GLN |
| 1 | B | 352 | GLN |
| 1 | B | 366 | GLN |
| 1 | B | 432 | GLN |
| 1 | B | 457 | ASN |
| 1 | B | 475 | ASN |
| 1 | C | 21 | ASN |
| 1 | C | 82 | ASN |
| 1 | C | 112 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 146 | GLN |
| 1 | C | 153 | ASN |
| 1 | C | 194 | GLN |
| 1 | C | 319 | GLN |
| 1 | C | 348 | GLN |
| 1 | C | 351 | GLN |
| 1 | C | 352 | GLN |
| 1 | C | 366 | GLN |
| 1 | C | 432 | GLN |
| 1 | C | 457 | ASN |
| 1 | C | 475 | ASN |
| 1 | D | 21 | ASN |
| 1 | D | 82 | ASN |
| 1 | D | 112 | ASN |
| 1 | D | 146 | GLN |
| 1 | D | 153 | ASN |
| 1 | D | 194 | GLN |
| 1 | D | 319 | GLN |
| 1 | D | 348 | GLN |
| 1 | D | 351 | GLN |
| 1 | D | 352 | GLN |
| 1 | D | 366 | GLN |
| 1 | D | 432 | GLN |
| 1 | D | 457 | ASN |
| 1 | D | 475 | ASN |
| 1 | E | 21 | ASN |
| 1 | E | 82 | ASN |
| 1 | E | 112 | ASN |
| 1 | E | 146 | GLN |
| 1 | E | 153 | ASN |
| 1 | E | 194 | GLN |
| 1 | E | 319 | GLN |
| 1 | E | 348 | GLN |
| 1 | E | 351 | GLN |
| 1 | E | 352 | GLN |
| 1 | E | 366 | GLN |
| 1 | E | 432 | GLN |
| 1 | E | 457 | ASN |
| 1 | F | 21 | ASN |
| 1 | F | 82 | ASN |
| 1 | F | 112 | ASN |
| 1 | F | 146 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 153 | ASN |
| 1 | F | 194 | GLN |
| 1 | F | 265 | ASN |
| 1 | F | 319 | GLN |
| 1 | F | 348 | GLN |
| 1 | F | 351 | GLN |
| 1 | F | 352 | GLN |
| 1 | F | 366 | GLN |
| 1 | F | 432 | GLN |
| 1 | F | 457 | ASN |
| 1 | G | 21 | ASN |
| 1 | G | 72 | GLN |
| 1 | G | 82 | ASN |
| 1 | G | 112 | ASN |
| 1 | G | 146 | GLN |
| 1 | G | 153 | ASN |
| 1 | G | 194 | GLN |
| 1 | G | 319 | GLN |
| 1 | G | 348 | GLN |
| 1 | G | 351 | GLN |
| 1 | G | 352 | GLN |
| 1 | G | 366 | GLN |
| 1 | G | 432 | GLN |
| 1 | G | 457 | ASN |
| 1 | H | 21 | ASN |
| 1 | H | 37 | ASN |
| 1 | H | 72 | GLN |
| 1 | H | 97 | GLN |
| 1 | H | 153 | ASN |
| 1 | H | 319 | GLN |
| 1 | H | 348 | GLN |
| 1 | H | 352 | GLN |
| 1 | H | 433 | ASN |
| 1 | H | 436 | GLN |
| 1 | I | 21 | ASN |
| 1 | I | 37 | ASN |
| 1 | I | 72 | GLN |
| 1 | I | 97 | GLN |
| 1 | I | 146 | GLN |
| 1 | I | 153 | ASN |
| 1 | I | 319 | GLN |
| 1 | I | 348 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 352 | GLN |
| 1 | I | 433 | ASN |
| 1 | I | 436 | GLN |
| 1 | J | 21 | ASN |
| 1 | J | 37 | ASN |
| 1 | J | 72 | GLN |
| 1 | J | 97 | GLN |
| 1 | J | 153 | ASN |
| 1 | J | 319 | GLN |
| 1 | J | 348 | GLN |
| 1 | J | 433 | ASN |
| 1 | J | 436 | GLN |
| 1 | K | 21 | ASN |
| 1 | K | 37 | ASN |
| 1 | K | 72 | GLN |
| 1 | K | 97 | GLN |
| 1 | K | 146 | GLN |
| 1 | K | 153 | ASN |
| 1 | K | 319 | GLN |
| 1 | K | 348 | GLN |
| 1 | K | 352 | GLN |
| 1 | K | 433 | ASN |
| 1 | K | 436 | GLN |
| 1 | L | 21 | ASN |
| 1 | L | 37 | ASN |
| 1 | L | 72 | GLN |
| 1 | L | 97 | GLN |
| 1 | L | 153 | ASN |
| 1 | L | 319 | GLN |
| 1 | L | 348 | GLN |
| 1 | L | 352 | GLN |
| 1 | L | 433 | ASN |
| 1 | L | 436 | GLN |
| 1 | M | 21 | ASN |
| 1 | M | 72 | GLN |
| 1 | M | 97 | GLN |
| 1 | M | 146 | GLN |
| 1 | M | 153 | ASN |
| 1 | M | 319 | GLN |
| 1 | M | 348 | GLN |
| 1 | M | 433 | ASN |
| 1 | M | 436 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 21 | ASN |
| 1 | N | 37 | ASN |
| 1 | N | 72 | GLN |
| 1 | N | 97 | GLN |
| 1 | N | 146 | GLN |
| 1 | N | 153 | ASN |
| 1 | N | 319 | GLN |
| 1 | N | 348 | GLN |
| 1 | N | 433 | ASN |
| 1 | N | 436 | GLN |
| 2 | O | 45 | ASN |
| 2 | O | 68 | ASN |
| 2 | O | 80 | ASN |
| 2 | P | 45 | ASN |
| 2 | P | 68 | ASN |
| 2 | P | 80 | ASN |
| 2 | Q | 45 | ASN |
| 2 | Q | 68 | ASN |
| 2 | Q | 80 | ASN |
| 2 | R | 45 | ASN |
| 2 | R | 68 | ASN |
| 2 | R | 80 | ASN |
| 2 | S | 45 | ASN |
| 2 | S | 68 | ASN |
| 2 | S | 80 | ASN |
| 2 | T | 45 | ASN |
| 2 | T | 68 | ASN |
| 2 | T | 80 | ASN |
| 2 | U | 45 | ASN |
| 2 | U | 68 | ASN |
| 2 | U | 80 | 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](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 4 | ADP | A | 1 | 3 | 25,29,29 | 0.69 | 0 | 24,45,45 | 1.03 | 1 (4%) |
| 4 | ADP | B | 1 | 3 | 25,29,29 | 0.71 | 0 | 24,45,45 | 1.05 | 1 (4%) |
| 4 | ADP | C | 1 | 3 | 25,29,29 | 0.69 | 0 | 24,45,45 | 1.01 | 1 (4%) |
| 4 | ADP | D | 1 | 3 | 25,29,29 | 0.73 | 0 | 24,45,45 | 0.96 | 1 (4%) |
| 4 | ADP | E | 1 | 3 | 25,29,29 | 0.70 | 0 | 24,45,45 | 1.23 | 1 (4%) |
| 4 | ADP | F | 1 | 3 | 25,29,29 | 0.69 | 0 | 24,45,45 | 1.01 | 1 (4%) |
| 4 | ADP | G | 1 | 3 | 25,29,29 | 0.70 | 0 | 24,45,45 | 1.02 | 1 (4%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | ADP | A | 1 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 4 | ADP | B | 1 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 4 | ADP | C | 1 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 4 | ADP | D | 1 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 4 | ADP | E | 1 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 4 | ADP | F | 1 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 4 | ADP | G | 1 | 3 | - | 0/12/32/32 | 0/3/3/3 |

There are no bond length outliers.

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | F | 1 | ADP | O3B-PB-O2B | 2.04 | 115.82 | 107.61 |
| 4 | C | 1 | ADP | O3B-PB-O2B | 2.06 | 115.93 | 107.61 |
| 4 | B | 1 | ADP | O3B-PB-O2B | 2.09 | 116.03 | 107.61 |
| 4 | A | 1 | ADP | O3B-PB-O2B | 2.12 | 116.16 | 107.61 |
| 4 | G | 1 | ADP | O3B-PB-O2B | 2.15 | 116.29 | 107.61 |
| 4 | D | 1 | ADP | O3B-PB-O2B | 2.31 | 116.92 | 107.61 |
| 4 | E | 1 | ADP | C5'-C4'-C3' | 2.37 | 124.30 | 115.29 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 22 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4 | A | 1 | ADP | 2 | 0 |
| 4 | B | 1 | ADP | 5 | 0 |
| 4 | C | 1 | ADP | 5 | 0 |
| 4 | D | 1 | ADP | 1 | 0 |
| 4 | E | 1 | ADP | 1 | 0 |
| 4 | F | 1 | ADP | 6 | 0 |
| 4 | G | 1 | ADP | 2 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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 | 524/547 (95%) | 0.11 | 18 (3%) | 46 | 20 | 4, 43, 100, 100 | 0 |
| 1 | B | 524/547 (95%) | 0.08 | 16 (3%) | 49 | 22 | 6, 44, 100, 100 | 0 |
| 1 | C | 524/547 (95%) | 0.03 | 16 (3%) | 49 | 22 | 3, 44, 100, 100 | 0 |
| 1 | D | 524/547 (95%) | 0.09 | 19 (3%) | 43 | 18 | 5, 43, 100, 100 | 0 |
| 1 | E | 524/547 (95%) | 0.18 | 31 (5%) | 23 | 9 | 6, 46, 100, 100 | 0 |
| 1 | F | 524/547 (95%) | 0.19 | 30 (5%) | 24 | 9 | 6, 47, 100, 100 | 0 |
| 1 | G | 524/547 (95%) | 0.11 | 26 (4%) | 30 | 12 | 6, 44, 100, 100 | 0 |
| 1 | H | 524/547 (95%) | -0.07 | 2 (0%) | 92 | 77 | 6, 61, 99, 100 | 0 |
| 1 | I | 524/547 (95%) | -0.07 | 1 (0%) | 94 | 85 | 6, 61, 99, 100 | 0 |
| 1 | J | 524/547 (95%) | -0.03 | 5 (0%) | 82 | 58 | 7, 61, 99, 100 | 0 |
| 1 | K | 524/547 (95%) | -0.01 | 7 (1%) | 77 | 51 | 7, 63, 99, 100 | 0 |
| 1 | L | 524/547 (95%) | 0.02 | 6 (1%) | 80 | 55 | 9, 64, 99, 100 | 0 |
| 1 | M | 524/547 (95%) | 0.03 | 11 (2%) | 64 | 34 | 7, 63, 99, 100 | 0 |
| 1 | N | 524/547 (95%) | 0.07 | 9 (1%) | 70 | 42 | 6, 62, 99, 100 | 0 |
| 2 | O | 97/97 (100%) | 0.92 | 16 (16%) | 2 | 1 | 74, 96, 100, 100 | 0 |
| 2 | P | 97/97 (100%) | 0.80 | 12 (12%) | 4 | 2 | 71, 96, 100, 100 | 0 |
| 2 | Q | 97/97 (100%) | 0.67 | 10 (10%) | 7 | 3 | 71, 96, 100, 100 | 0 |
| 2 | R | 97/97 (100%) | 0.84 | 14 (14%) | 3 | 1 | 73, 96, 100, 100 | 0 |
| 2 | S | 97/97 (100%) | 0.79 | 12 (12%) | 4 | 2 | 72, 96, 100, 100 | 0 |
| 2 | T | 97/97 (100%) | 0.89 | 18 (18%) | 1 | 1 | 74, 96, 100, 100 | 0 |
| 2 | U | 97/97 (100%) | 0.68 | 14 (14%) | 3 | 1 | 73, 96, 100, 100 | 0 |
| All | All | 8015/8337 (96%) | 0.12 | 293 (3%) | 42 | 18 | 3, 64, 100, 100 | 0 |

All (293) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 212 | ALA | 5.6 |
| 1 | F | 211 | GLY | 5.1 |
| 1 | A | 361 | ASP | 5.0 |
| 2 | T | 27 | LEU | 4.9 |
| 2 | O | 33 | ALA | 4.8 |
| 2 | O | 80 | ASN | 4.8 |
| 2 | R | 33 | ALA | 4.8 |
| 1 | C | 199 | TYR | 4.6 |
| 1 | G | 372 | LEU | 4.6 |
| 2 | O | 25 | ILE | 4.6 |
| 2 | R | 25 | ILE | 4.6 |
| 1 | G | 199 | TYR | 4.6 |
| 2 | T | 18 | GLU | 4.4 |
| 2 | U | 33 | ALA | 4.4 |
| 1 | E | 270 | ILE | 4.3 |
| 1 | E | 361 | ASP | 4.3 |
| 1 | F | 212 | ALA | 4.2 |
| 2 | T | 72 | GLY | 4.2 |
| 2 | Q | 25 | ILE | 4.2 |
| 2 | P | 23 | GLY | 4.2 |
| 1 | G | 210 | THR | 4.1 |
| 1 | G | 198 | GLY | 4.1 |
| 1 | B | 361 | ASP | 4.0 |
| 1 | C | 208 | PRO | 4.0 |
| 1 | B | 192 | GLY | 4.0 |
| 2 | T | 25 | ILE | 4.0 |
| 2 | O | 23 | GLY | 3.9 |
| 2 | S | 33 | ALA | 3.9 |
| 1 | G | 214 | GLU | 3.9 |
| 2 | R | 17 | VAL | 3.8 |
| 1 | F | 214 | GLU | 3.8 |
| 2 | R | 80 | ASN | 3.8 |
| 1 | C | 214 | GLU | 3.8 |
| 1 | C | 361 | ASP | 3.7 |
| 2 | U | 32 | ALA | 3.7 |
| 1 | D | 356 | ALA | 3.7 |
| 2 | U | 26 | VAL | 3.6 |
| 1 | E | 306 | GLY | 3.6 |
| 1 | D | 208 | PRO | 3.6 |
| 2 | R | 97 | ALA | 3.6 |
| 1 | C | 211 | GLY | 3.6 |
| 2 | Q | 72 | GLY | 3.5 |
| 1 | N | 361 | ASP | 3.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | G | 195 | PHE | 3.5 |
| 1 | A | 271 | VAL | 3.5 |
| 1 | F | 352 | GLN | 3.5 |
| 1 | G | 251 | ALA | 3.5 |
| 2 | P | 32 | ALA | 3.4 |
| 2 | U | 27 | LEU | 3.4 |
| 1 | D | 361 | ASP | 3.4 |
| 1 | G | 208 | PRO | 3.4 |
| 2 | R | 30 | SER | 3.4 |
| 1 | F | 208 | PRO | 3.4 |
| 1 | C | 192 | GLY | 3.4 |
| 2 | Q | 26 | VAL | 3.3 |
| 1 | E | 375 | GLY | 3.3 |
| 1 | M | 357 | THR | 3.3 |
| 1 | N | 181 | THR | 3.3 |
| 2 | O | 26 | VAL | 3.3 |
| 2 | S | 32 | ALA | 3.3 |
| 2 | O | 32 | ALA | 3.3 |
| 1 | L | 264 | VAL | 3.3 |
| 1 | G | 348 | GLN | 3.3 |
| 2 | T | 28 | THR | 3.3 |
| 1 | A | 208 | PRO | 3.3 |
| 2 | S | 80 | ASN | 3.2 |
| 1 | E | 372 | LEU | 3.2 |
| 1 | G | 212 | ALA | 3.2 |
| 2 | Q | 23 | GLY | 3.2 |
| 2 | O | 18 | GLU | 3.2 |
| 2 | R | 20 | LYS | 3.2 |
| 1 | A | 314 | LEU | 3.2 |
| 1 | G | 353 | ILE | 3.1 |
| 2 | T | 20 | LYS | 3.1 |
| 1 | K | 186 | GLU | 3.1 |
| 1 | F | 353 | ILE | 3.1 |
| 1 | J | 357 | THR | 3.1 |
| 1 | B | 211 | GLY | 3.1 |
| 1 | F | 172 | GLU | 3.1 |
| 1 | F | 323 | VAL | 3.1 |
| 2 | R | 18 | GLU | 3.0 |
| 1 | E | 353 | ILE | 3.0 |
| 1 | M | 358 | SER | 3.0 |
| 1 | N | 186 | GLU | 3.0 |
| 1 | F | 229 | ASN | 3.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | T | 97 | ALA | 3.0 |
| 1 | B | 353 | ILE | 3.0 |
| 1 | G | 203 | TYR | 3.0 |
| 1 | L | 381 | VAL | 3.0 |
| 1 | E | 340 | ALA | 3.0 |
| 1 | F | 210 | THR | 3.0 |
| 1 | E | 303 | GLU | 3.0 |
| 2 | O | 72 | GLY | 3.0 |
| 1 | G | 270 | ILE | 3.0 |
| 2 | Q | 71 | TYR | 2.9 |
| 1 | C | 348 | GLN | 2.9 |
| 1 | A | 358 | SER | 2.9 |
| 1 | A | 212 | ALA | 2.9 |
| 2 | T | 32 | ALA | 2.9 |
| 1 | G | 271 | VAL | 2.9 |
| 2 | R | 26 | VAL | 2.9 |
| 1 | L | 356 | ALA | 2.9 |
| 1 | F | 191 | GLU | 2.9 |
| 2 | P | 25 | ILE | 2.8 |
| 1 | E | 272 | LYS | 2.8 |
| 1 | B | 372 | LEU | 2.8 |
| 1 | F | 171 | LYS | 2.8 |
| 1 | F | 193 | MET | 2.8 |
| 2 | P | 33 | ALA | 2.8 |
| 1 | M | 362 | ARG | 2.8 |
| 1 | E | 359 | ASP | 2.8 |
| 1 | B | 352 | GLN | 2.8 |
| 2 | T | 80 | ASN | 2.8 |
| 1 | K | 360 | TYR | 2.8 |
| 2 | S | 30 | SER | 2.8 |
| 2 | T | 71 | TYR | 2.8 |
| 1 | G | 211 | GLY | 2.8 |
| 1 | G | 361 | ASP | 2.8 |
| 2 | O | 97 | ALA | 2.7 |
| 1 | E | 351 | GLN | 2.7 |
| 1 | M | 264 | VAL | 2.7 |
| 1 | B | 199 | TYR | 2.7 |
| 1 | I | 264 | VAL | 2.7 |
| 1 | L | 362 | ARG | 2.7 |
| 2 | Q | 80 | ASN | 2.7 |
| 1 | B | 357 | THR | 2.7 |
| 1 | C | 203 | TYR | 2.7 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | P | 20 | LYS | 2.7 |
| 1 | D | 366 | GLN | 2.7 |
| 1 | C | 191 | GLU | 2.7 |
| 1 | A | 229 | ASN | 2.7 |
| 1 | E | 354 | GLU | 2.6 |
| 1 | F | 361 | ASP | 2.6 |
| 1 | D | 244 | GLY | 2.6 |
| 1 | A | 362 | ARG | 2.6 |
| 1 | F | 348 | GLN | 2.6 |
| 1 | F | 387 | VAL | 2.6 |
| 1 | F | 270 | ILE | 2.6 |
| 1 | E | 307 | MET | 2.6 |
| 1 | G | 172 | GLU | 2.6 |
| 2 | P | 35 | SER | 2.6 |
| 2 | P | 51 | ASN | 2.6 |
| 1 | A | 356 | ALA | 2.6 |
| 2 | S | 51 | ASN | 2.6 |
| 2 | P | 18 | GLU | 2.6 |
| 1 | D | 340 | ALA | 2.6 |
| 2 | O | 22 | ALA | 2.6 |
| 2 | T | 51 | ASN | 2.6 |
| 2 | U | 23 | GLY | 2.6 |
| 1 | K | 295 | LEU | 2.6 |
| 2 | T | 26 | VAL | 2.5 |
| 2 | O | 83 | VAL | 2.5 |
| 1 | C | 212 | ALA | 2.5 |
| 1 | B | 351 | GLN | 2.5 |
| 1 | D | 319 | GLN | 2.5 |
| 1 | K | 384 | ALA | 2.5 |
| 1 | C | 270 | ILE | 2.5 |
| 1 | N | 357 | THR | 2.5 |
| 2 | S | 17 | VAL | 2.5 |
| 2 | P | 82 | GLU | 2.5 |
| 1 | J | 356 | ALA | 2.5 |
| 2 | R | 32 | ALA | 2.5 |
| 2 | O | 30 | SER | 2.5 |
| 1 | E | 271 | VAL | 2.5 |
| 1 | F | 357 | THR | 2.5 |
| 1 | G | 371 | LYS | 2.5 |
| 1 | G | 362 | ARG | 2.5 |
| 2 | R | 51 | ASN | 2.5 |
| 2 | U | 51 | ASN | 2.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | N | 333 | ILE | 2.5 |
| 1 | E | 177 | VAL | 2.5 |
| 1 | F | 215 | LEU | 2.5 |
| 2 | U | 28 | THR | 2.5 |
| 2 | U | 97 | ALA | 2.5 |
| 2 | U | 31 | ALA | 2.4 |
| 1 | E | 333 | ILE | 2.4 |
| 1 | B | 306 | GLY | 2.4 |
| 1 | D | 280 | GLY | 2.4 |
| 2 | O | 27 | LEU | 2.4 |
| 2 | Q | 27 | LEU | 2.4 |
| 1 | H | 288 | MET | 2.4 |
| 2 | S | 21 | SER | 2.4 |
| 2 | O | 82 | GLU | 2.4 |
| 2 | T | 17 | VAL | 2.4 |
| 1 | E | 199 | TYR | 2.4 |
| 1 | M | 365 | LEU | 2.4 |
| 2 | U | 30 | SER | 2.4 |
| 1 | F | 351 | GLN | 2.4 |
| 1 | L | 357 | THR | 2.4 |
| 1 | N | 267 | MET | 2.4 |
| 1 | G | 215 | LEU | 2.4 |
| 1 | E | 341 | ALA | 2.4 |
| 2 | P | 31 | ALA | 2.4 |
| 1 | M | 361 | ASP | 2.4 |
| 1 | A | 353 | ILE | 2.4 |
| 1 | E | 210 | THR | 2.4 |
| 2 | R | 28 | THR | 2.4 |
| 1 | E | 211 | GLY | 2.3 |
| 1 | L | 353 | ILE | 2.3 |
| 1 | D | 209 | GLU | 2.3 |
| 2 | T | 19 | THR | 2.3 |
| 1 | A | 270 | ILE | 2.3 |
| 1 | F | 356 | ALA | 2.3 |
| 1 | F | 182 | GLY | 2.3 |
| 2 | T | 52 | GLY | 2.3 |
| 1 | D | 362 | ARG | 2.3 |
| 1 | B | 210 | THR | 2.3 |
| 1 | D | 210 | THR | 2.3 |
| 2 | Q | 32 | ALA | 2.3 |
| 1 | E | 208 | PRO | 2.3 |
| 2 | S | 84 | LEU | 2.3 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | J | 181 | THR | 2.3 |
| 1 | A | 211 | GLY | 2.3 |
| 2 | S | 1 | MET | 2.3 |
| 1 | F | 174 | VAL | 2.3 |
| 1 | A | 223 | ALA | 2.3 |
| 1 | G | 207 | LYS | 2.3 |
| 2 | T | 33 | ALA | 2.3 |
| 2 | R | 72 | GLY | 2.2 |
| 2 | P | 85 | ILE | 2.2 |
| 1 | F | 190 | VAL | 2.2 |
| 1 | G | 320 | ALA | 2.2 |
| 1 | N | 360 | TYR | 2.2 |
| 1 | D | 357 | THR | 2.2 |
| 1 | D | 352 | GLN | 2.2 |
| 2 | R | 21 | SER | 2.2 |
| 1 | C | 229 | ASN | 2.2 |
| 1 | E | 195 | PHE | 2.2 |
| 1 | E | 212 | ALA | 2.2 |
| 1 | N | 266 | THR | 2.2 |
| 2 | S | 38 | GLY | 2.2 |
| 1 | D | 358 | SER | 2.2 |
| 1 | A | 357 | THR | 2.2 |
| 1 | K | 352 | GLN | 2.2 |
| 2 | Q | 18 | GLU | 2.2 |
| 1 | A | 280 | GLY | 2.2 |
| 2 | S | 35 | SER | 2.2 |
| 2 | T | 23 | GLY | 2.2 |
| 1 | C | 356 | ALA | 2.2 |
| 2 | O | 21 | SER | 2.2 |
| 2 | O | 17 | VAL | 2.2 |
| 2 | P | 80 | ASN | 2.2 |
| 1 | B | 362 | ARG | 2.2 |
| 1 | E | 327 | LYS | 2.2 |
| 1 | C | 359 | ASP | 2.2 |
| 1 | J | 365 | LEU | 2.1 |
| 1 | K | 44 | PHE | 2.1 |
| 1 | B | 271 | VAL | 2.1 |
| 1 | J | 223 | ALA | 2.1 |
| 1 | E | 174 | VAL | 2.1 |
| 1 | B | 193 | MET | 2.1 |
| 1 | M | 360 | TYR | 2.1 |
| 1 | D | 281 | PHE | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 284 | ARG | 2.1 |
| 2 | T | 83 | VAL | 2.1 |
| 1 | M | 382 | GLY | 2.1 |
| 1 | N | 180 | GLY | 2.1 |
| 1 | C | 340 | ALA | 2.1 |
| 1 | D | 199 | TYR | 2.1 |
| 1 | G | 229 | ASN | 2.1 |
| 1 | D | 271 | VAL | 2.1 |
| 1 | F | 333 | ILE | 2.1 |
| 1 | F | 390 | LYS | 2.1 |
| 1 | M | 285 | ARG | 2.1 |
| 1 | E | 196 | ASP | 2.1 |
| 1 | A | 351 | GLN | 2.1 |
| 1 | D | 335 | GLY | 2.1 |
| 1 | E | 477 | GLY | 2.1 |
| 1 | F | 170 | GLY | 2.1 |
| 1 | M | 263 | VAL | 2.1 |
| 1 | B | 229 | ASN | 2.1 |
| 1 | F | 354 | GLU | 2.1 |
| 1 | G | 373 | ALA | 2.1 |
| 2 | U | 25 | ILE | 2.1 |
| 2 | Q | 20 | LYS | 2.1 |
| 2 | U | 20 | LYS | 2.1 |
| 1 | F | 385 | THR | 2.1 |
| 1 | A | 227 | ILE | 2.1 |
| 1 | G | 244 | GLY | 2.1 |
| 2 | U | 79 | ASP | 2.1 |
| 1 | E | 363 | GLU | 2.0 |
| 1 | E | 357 | THR | 2.0 |
| 1 | M | 280 | GLY | 2.0 |
| 1 | E | 358 | SER | 2.0 |
| 2 | U | 83 | VAL | 2.0 |
| 1 | H | 44 | PHE | 2.0 |
| 1 | K | 356 | ALA | 2.0 |
| 2 | S | 18 | GLU | 2.0 |
| 1 | F | 177 | VAL | 2.0 |
| 1 | B | 280 | GLY | 2.0 |
| 1 | G | 269 | GLY | 2.0 |
| 1 | A | 348 | GLN | 2.0 |
| 1 | C | 314 | LEU | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 4 | ADP | B | 1 | 27/27 | 0.89 | 0.29 | 3.27 | 13,34,39,49 | 0 |
| 4 | ADP | A | 1 | 27/27 | 0.92 | 0.29 | 2.19 | 14,31,39,48 | 0 |
| 4 | ADP | C | 1 | 27/27 | 0.93 | 0.26 | 2.00 | 16,31,38,47 | 0 |
| 4 | ADP | G | 1 | 27/27 | 0.94 | 0.26 | 1.73 | 15,31,39,49 | 0 |
| 4 | ADP | D | 1 | 27/27 | 0.92 | 0.26 | 1.72 | 11,31,36,48 | 0 |
| 4 | ADP | F | 1 | 27/27 | 0.90 | 0.26 | 1.05 | 20,35,41,47 | 0 |
| 4 | ADP | E | 1 | 27/27 | 0.90 | 0.26 | 1.02 | 8,32,39,50 | 0 |
| 3 | MG | G | 550 | 1/1 | 0.90 | 0.27 | - | 12,12,12,12 | 0 |
| 3 | MG | A | 550 | 1/1 | 0.92 | 0.33 | - | 2,2,2,2 | 0 |
| 3 | MG | C | 550 | 1/1 | 0.90 | 0.32 | - | 13,13,13,13 | 0 |
| 3 | MG | B | 550 | 1/1 | 0.93 | 0.28 | - | 14,14,14,14 | 0 |
| 3 | MG | E | 550 | 1/1 | 0.92 | 0.30 | - | 9,9,9,9 | 0 |
| 3 | MG | F | 550 | 1/1 | 0.82 | 0.35 | - | 13,13,13,13 | 0 |
| 3 | MG | D | 550 | 1/1 | 0.76 | 0.32 | - | 5,5,5,5 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.