



wwPDB EM Map/Model Validation Report ⓘ

Aug 31, 2016 – 01:24 PM EDT

PDB ID : 5LCW
EMDB ID: : EMD-4037
Title : Cryo-EM structure of the Anaphase-promoting complex/Cyclosome, in complex with the Mitotic checkpoint complex (APC/C-MCC) at 4.2 angstrom resolution
Authors : Alfieri, C.; Chang, L.; Zhang, Z.; Yang, J.; Maslen, S.; Skehel, M.; Barford, D.
Deposited on : 2016-06-22
Resolution : 4.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

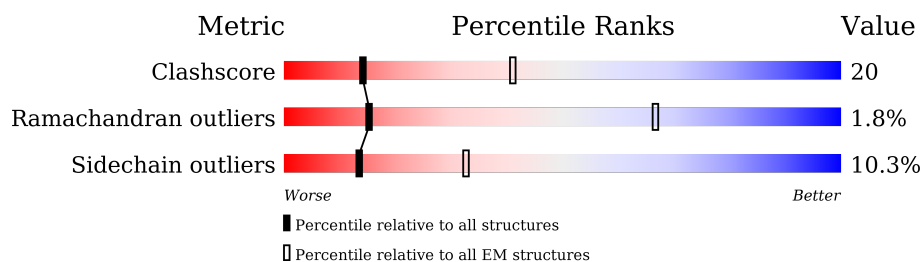
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 1944 | |
| 2 | B | 84 | |
| 3 | C | 597 | |
| 3 | P | 597 | |
| 4 | D | 121 | |
| 5 | E | 110 | |
| 6 | F | 824 | |
| 6 | H | 824 | |
| 7 | G | 85 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 7 | W | 85 |  |
| 8 | I | 808 |  |
| 9 | J | 620 |  |
| 9 | K | 620 |  |
| 10 | L | 185 |  |
| 11 | M | 74 |  |
| 12 | N | 822 |  |
| 13 | O | 755 |  |
| 14 | Q | 374 |  |
| 15 | R | 499 |  |
| 16 | S | 342 |  |
| 17 | X | 599 |  |
| 17 | Y | 599 |  |
| 18 | Z | 205 |  |

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 72075 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Anaphase-promoting complex subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1 | A | 1441 | Total | C | N | O | S | 0 | 0 |
| | | | 10949 | 7039 | 1853 | 1983 | 74 | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| A | 356 | PHE | PRO | conflict | UNP Q9H1A4 |

- Molecule 2 is a protein called Anaphase-promoting complex subunit 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2 | B | 79 | Total | C | N | O | S | 0 | 0 |
| | | | 643 | 411 | 116 | 100 | 16 | | |

- Molecule 3 is a protein called Cell division cycle protein 23 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3 | C | 524 | Total | C | N | O | S | 0 | 0 |
| | | | 4306 | 2774 | 727 | 781 | 24 | | |
| 3 | P | 491 | Total | C | N | O | S | 0 | 0 |
| | | | 4043 | 2611 | 679 | 729 | 24 | | |

- Molecule 4 is a protein called Anaphase-promoting complex subunit 15.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 4 | D | 18 | Total | C | N | O | 0 | 0 |
| | | | 153 | 104 | 23 | 26 | | |

- Molecule 5 is a protein called Anaphase-promoting complex subunit 16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5 | E | 56 | Total | C | N | O | S | 0 | 0 |
| | | | 450 | 290 | 74 | 85 | 1 | | |

- Molecule 6 is a protein called Cell division cycle protein 27 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6 | F | 483 | Total | C | N | O | S | 0 | 0 |
| | | | 3849 | 2470 | 649 | 704 | 26 | | |
| 6 | H | 483 | Total | C | N | O | S | 0 | 0 |
| | | | 3853 | 2473 | 650 | 704 | 26 | | |

- Molecule 7 is a protein called Anaphase-promoting complex subunit CDC26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7 | G | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 213 | 133 | 40 | 39 | 1 | | |
| 7 | W | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 213 | 133 | 40 | 39 | 1 | | |

- Molecule 8 is a protein called Anaphase-promoting complex subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 8 | I | 733 | Total | C | N | O | S | 0 | 0 |
| | | | 5716 | 3665 | 951 | 1067 | 33 | | |

- Molecule 9 is a protein called Cell division cycle protein 16 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9 | J | 504 | Total | C | N | O | S | 0 | 0 |
| | | | 4047 | 2601 | 684 | 737 | 25 | | |
| 9 | K | 493 | Total | C | N | O | S | 0 | 0 |
| | | | 3988 | 2563 | 672 | 729 | 24 | | |

- Molecule 10 is a protein called Anaphase-promoting complex subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10 | L | 182 | Total | C | N | O | S | 0 | 0 |
| | | | 1435 | 898 | 263 | 268 | 6 | | |

- Molecule 11 is a protein called Anaphase-promoting complex subunit 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 11 | M | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 493 | 310 | 79 | 102 | 2 | | |

- Molecule 12 is a protein called Anaphase-promoting complex subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12 | N | 703 | Total | C | N | O | S | 0 | 0 |
| | | | 5403 | 3436 | 971 | 971 | 25 | | |

- Molecule 13 is a protein called Anaphase-promoting complex subunit 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13 | O | 685 | Total | C | N | O | S | 0 | 0 |
| | | | 5402 | 3446 | 940 | 988 | 28 | | |

- Molecule 14 is a protein called Cell division cycle protein 20 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14 | Q | 354 | Total | C | N | O | S | 0 | 0 |
| | | | 2671 | 1676 | 488 | 496 | 11 | | |

- Molecule 15 is a protein called Cell division cycle protein 20 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15 | R | 383 | Total | C | N | O | S | 0 | 0 |
| | | | 2953 | 1855 | 538 | 548 | 12 | | |

- Molecule 16 is a protein called Mitotic checkpoint serine/threonine-protein kinase BUB1 beta,Mitotic checkpoint serine/threonine-protein kinase BUB1 beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16 | S | 277 | Total | C | N | O | S | 0 | 0 |
| | | | 2077 | 1292 | 380 | 400 | 5 | | |

- Molecule 17 is a protein called Anaphase-promoting complex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17 | X | 484 | Total | C | N | O | S | 0 | 0 |
| | | | 3773 | 2393 | 652 | 704 | 24 | | |
| 17 | Y | 496 | Total | C | N | O | S | 0 | 0 |
| | | | 3868 | 2449 | 669 | 724 | 26 | | |

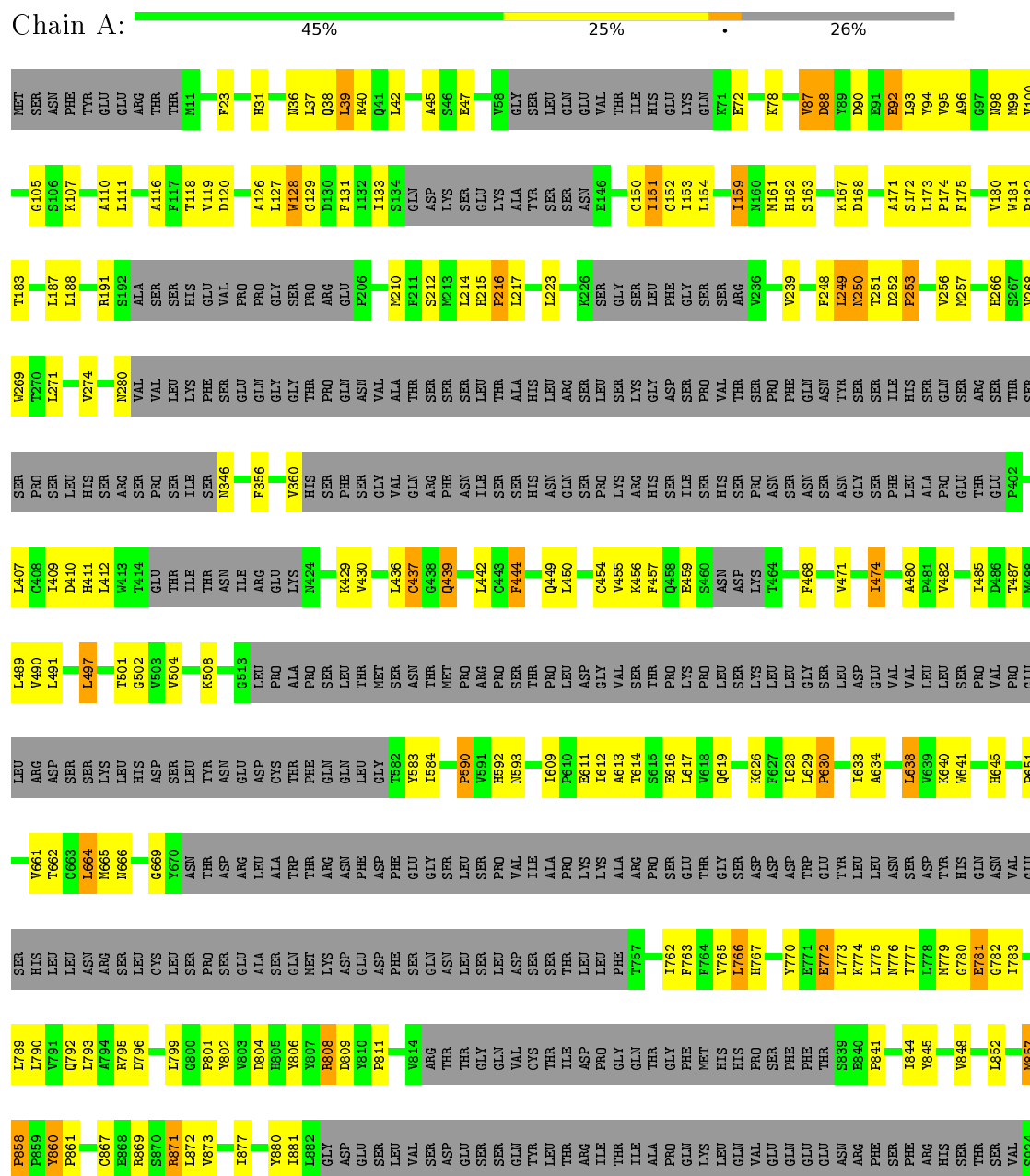
- Molecule 18 is a protein called Mitotic spindle assembly checkpoint protein MAD2A.

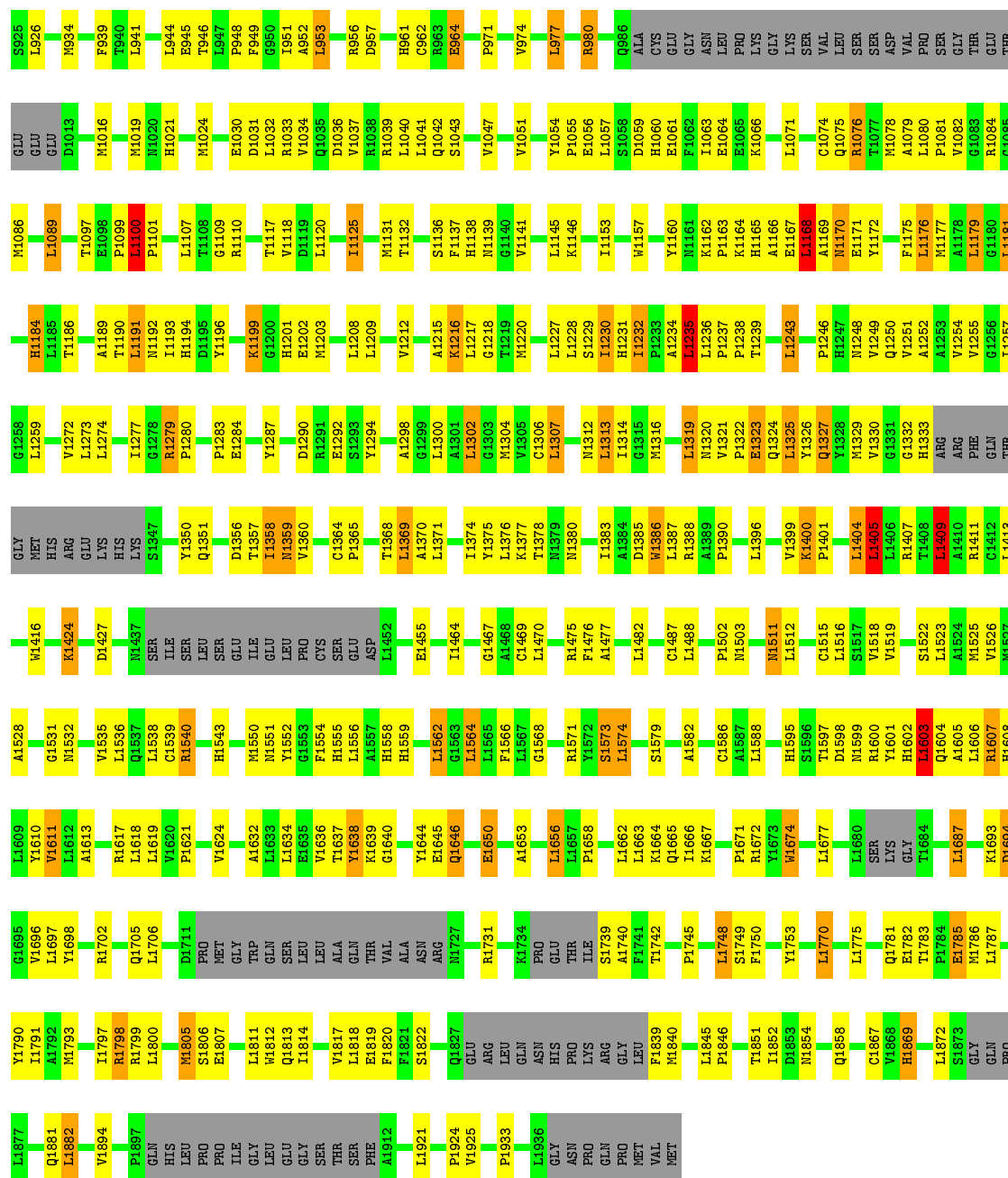
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18 | Z | 195 | Total | C | N | O | S | 0 | 0 |
| | | | 1577 | 1012 | 256 | 305 | 4 | | |

3 Residue-property plots

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

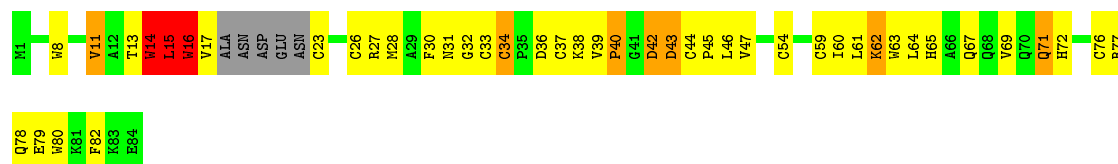
- Molecule 1: Anaphase-promoting complex subunit 1





• Molecule 2: Anaphase-promoting complex subunit 11

Chain B: 40% 42% 8% 6%




• Molecule 3: Cell division cycle protein 23 homolog

Chain C: 55% 30% 12%

| | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Tyr | ASP | ASP | GLU | GLU | GLU | ASP | ASP | GLU | ASP | ASP | GLN | GLY | GLU | VAL | ASN | ASP | ASP | GLN | TRP | MET |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Molecule 5: Anaphase-promoting complex subunit 16

Chain E:  34% 15% 0% 49%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Met | Ala | Ala | Ala | Ser | Ser | Ser | Ser | Ser | Ser | Ala | Gly | Gly | Val | Ser | Gly | Ser | Ser | Ser | Ser | Val | Thr | Gly | Gly | Gly | Ser | Gly | Phe | Ser | Val | Val | Asp | Leu | Ala | Pro | Pro | Arg | Lys | Ala | Ala | Leu | Phe | Thr | Thr | Pro | Met | Leu | Met | Glu | Asp | Gly | Gly | Ser | Glu | R52 | C85 | E66 | S57 | V88 | F59 | S60 | Y64 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Molecule 6: Cell division cycle protein 27 homolog

Chain F: 40% 17% 41%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|
| Met | Thr | Val | Leu | Q5 | P7 | A15 | Y19 | R22 | F26 | L27 | R30 | L31 | Y32 | L41 | F42 | L43 | L44 | A45 | R50 | Y88 | R89 | L60 | L61 | K62 | T67 | Q70 | C71 | K72 | Y73 | L74 | L75 | C78 | R89 | Q90 | I91 | V96 | F97 | N98 | H103 | D104 | T117 | L118 |
|-----|-----|-----|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| L121 | Y125 | D129 | K130 | K133 | G134 | S135 | E136 | G137 | S141 | L142 | S143 | L144 | K145 | P146 | F147 | F152 | E160 | K161 | P162 | D163 | P164 | D165 | G166 | T167 | F168 | K169 | F170 | THR | THR | LEU | LEU | GLN | ASN | ASP | PER | PER | PER | ASN | ASN | CYS | CYS | THR | THR | GLN | VAL | PRO | PRO | ASN | HIS | HIS | LEU | LEU | HIS | ASP |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLN | GLU | PRO | GLU | THR | VAL | LEU | THR | GLU | GLU | THR | THR | PRO | GLN | ASP | THR | THR | ILE | GLU | LEU | ASN | ARG | ARG | LEU | ASN | ASN | SER | SER | LYS | TYR | TYR | SER | LEU | ASN | ASP | ASP | SER | SER | SER | VAL | VAL | ALA | VAL | ILE | ILE | SER | PRO | PRO | ASP | THR | VAL | VAL | PRO | LEU | LEU | GLY | GLY | THR | THR | GLY | THR | SER | SER | ILE | ILE | LYS | LYS |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLN | VAL | GLN | ASN | LYS | PRO | LYS | THR | GLY | ARG | SER | LEU | LEU | GLY | GLY | PRO | ALA | ALA | LEU | SER | SER | PRO | LEU | THR | PRO | SER | ASP | PHE | GLY | ILE | ILE | LEU | PRO | LEU | GLU | GLU | THR | THR | SER | SER | PRO | PRO | GLY | PRO | ASP | GLY | GLY | GLY | SER | SER | TYR | TYR | LEU | LEU | GLN | ASN | TYR | THR | THR | ASN | THR | PRO | PRO | PRO | VAL | VAL | ILE | ILE | ASP | VAL | VAL | SER | PRO | PRO | THR | THR | GLY | GLY | ALA | PRO |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | LYS | LYS | SER | VAL | ALA | ILE | GLY | GLN | THR | GLY | THR | LYS | SER | VAL | PHE | SER | GLN | SER | GLY | ASN | SER | ARG | GLU | GLU | VAL | THR | THR | PRO | ILE | LEU | ALA | GLN | THR | THR | GLN | SER | SER | GLY | PRO | PRO | GLN | THR | THR | SER | SER | THR | THR | THR | PRO | PRO | ASN | ALA | LEU | ALA | PRO | ARG |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ARG | SER | SER | ARG | LEU | PHE | THR | SER | ASP | SER | SER | THR | THR | LYS | GLU | ASN | SER | LYS | LYS | LEU | LYS | MET | PHE | PRO | PRO | LYS | ILE | PRO | ASN | ARG | LYS | THR | LYS | LYS | LYS | ILE | ILE | THR | GLN | PRO | ASN | ASN | ILE | ASN | ASP | LEU | GLU | ILE | THR | LYS | ASP | LEU | ILE | THR | ILE |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| IIE | GLU | GLY | LYS | IIE | THR | THR | PRO | GLN | IIE | GLN | GLS | A451 | A457 | A458 | A459 | A460 | A461 | A462 | A465 | A466 | A467 | K471 | A477 | A481 | A482 | A493 | A487 | A493 | A494 | A495 | A500 | A501 | A502 | C503 | A504 | I505 | A506 | A507 | L512 | R520 | I521 | F522 | V525 | A526 | R527 | I529 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| E529 | N530 | V533 | V536 | E537 | I538 | V539 | S540 | V541 | V544 | I549 | V550 | A551 | V554 | L555 | S556 | L559 | V562 | K563 | K564 | N565 | E568 | C571 | A572 | A573 | G574 | N575 | C576 | F577 | S578 | K588 | R592 | A593 | I594 | V600 | A601 | V602 | A603 | V604 | T605 | L606 | T614 | E615 | E616 | L617 | D618 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

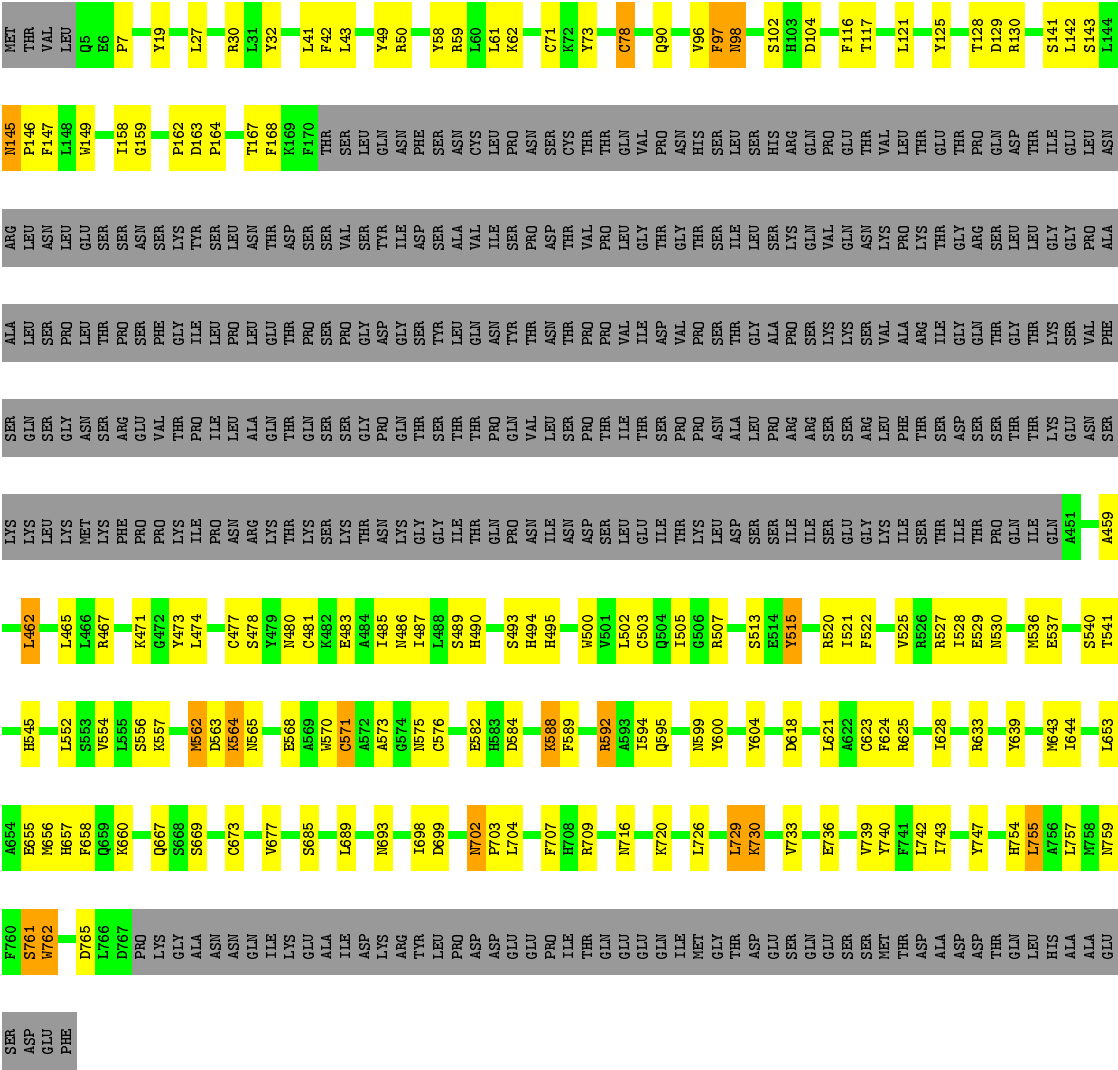
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|
| I621 | G622 | G623 | F624 | R625 | I628 | Y639 | I644 | I653 | A654 | E655 | M656 | P666 | Q667 | C673 | V677 | I689 | N693 | I696 | D699 | P700 | K701 | N702 | P703 | L704 | C705 | K706 | F707 | H708 | R709 | K720 | S721 | L726 | L729 | K730 | V733 | P734 | V739 | F740 | F741 | L742 | I743 | V744 | V745 | V746 | V747 | V748 | V749 | V750 | V751 | V752 | V753 | V754 | V755 | V756 | V757 | V758 | V759 | V760 | V761 | V762 | V763 | V764 | V765 | V766 | V767 | V768 | V769 | V770 | V771 | V772 | V773 | V774 | V775 | V776 | V777 | V778 | V779 | V780 | V781 | V782 | V783 | V784 | V785 | V786 | V787 | V788 | V789 | V790 | V791 | V792 | V793 | V794 | V795 | V796 | V797 | V798 | V799 | V800 | V801 | V802 | V803 | V804 | V805 | V806 | V807 | V808 | V809 | V810 | V811 | V812 | V813 | V814 | V815 | V816 | V817 | V818 | V819 | V820 | V821 | V822 | V823 | V824 | V825 | V826 | V827 | V828 | V829 | V830 | V831 | V832 | V833 | V834 | V835 | V836 | V837 | V838 | V839 | V840 | V841 | V842 | V843 | V844 | V845 | V846 | V847 | V848 | V849 | V850 | V851 | V852 | V853 | V854 | V855 | V856 | V857 | V858 | V859 | V860 | V861 | V862 | V863 | V864 | V865 | V866 | V867 | V868 | V869 | V870 | V871 | V872 | V873 | V874 | V875 | V876 | V877 | V878 | V879 | V880 | V881 | V882 | V883 | V884 | V885 | V886 | V887 | V888 | V889 | V890 | V891 | V892 | V893 | V894 | V895 | V896 | V897 | V898 | V899 | V900 | V901 | V902 | V903 | V904 | V905 | V906 | V907 | V908 | V909 | V910 | V911 | V912 | V913 | V914 | V915 | V916 | V917 | V918 | V919 | V920 | V921 | V922 | V923 | V924 | V925 | V926 | V927 | V928 | V929 | V930 | V931 | V932 | V933 | V934 | V935 | V936 | V937 | V938 | V939 | V940 | V941 | V942 | V943 | V944 | V945 | V946 | V947 | V948 | V949 | V950 | V951 | V952 | V953 | V954 | V955 | V956 | V957 | V958 | V959 | V960 | V961 | V962 | V963 | V964 | V965 | V966 | V967 | V968 | V969 | V970 | V971 | V972 | V973 | V974 | V975 | V976 | V977 | V978 | V979 | V980 | V981 | V982 | V983 | V984 | V985 | V986 | V987 | V988 | V989 | V990 | V991 | V992 | V993 | V994 | V995 | V996 | V997 | V998 | V999 | V1000 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-------|

■ L755
■ L756
■ L757
■ L762
■ L765
■ L766
■ L767
 PRO
 LYS
 GLY
 ALA
 ASP
 ASN
 GLN
 ILE
 LYS
 GLU
 ALA
 ILE
 ASP
 LYS
 ARG
 THR
 LEU
 PRO
 ASP
 ASP
 GLU
 PRO
 PRO
 THR
 GLN
 GLN
 GLU
 GLN
 ILE
 MET
 MET
 GLY
 THR
 ASP
 ASP
 GLU
 SER
 SER
 GLN
 GLU
 SER
 SER
 MET
 THR
 THR
 ASP
 ALA
 ASP
 ASP
 THR
 THR
 GLN
 GLU
 LEU
 LEU

ALA
ALA
GLU
SER
ASP
GLU
PHE

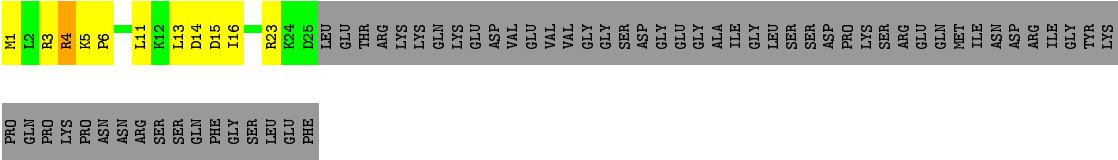
- Molecule 6: Cell division cycle protein 27 homolog

Chain H:  40% 17% 41%



• Molecule 7: Anaphase-promoting complex subunit CDC26

Chain G: 16% 12% 71%



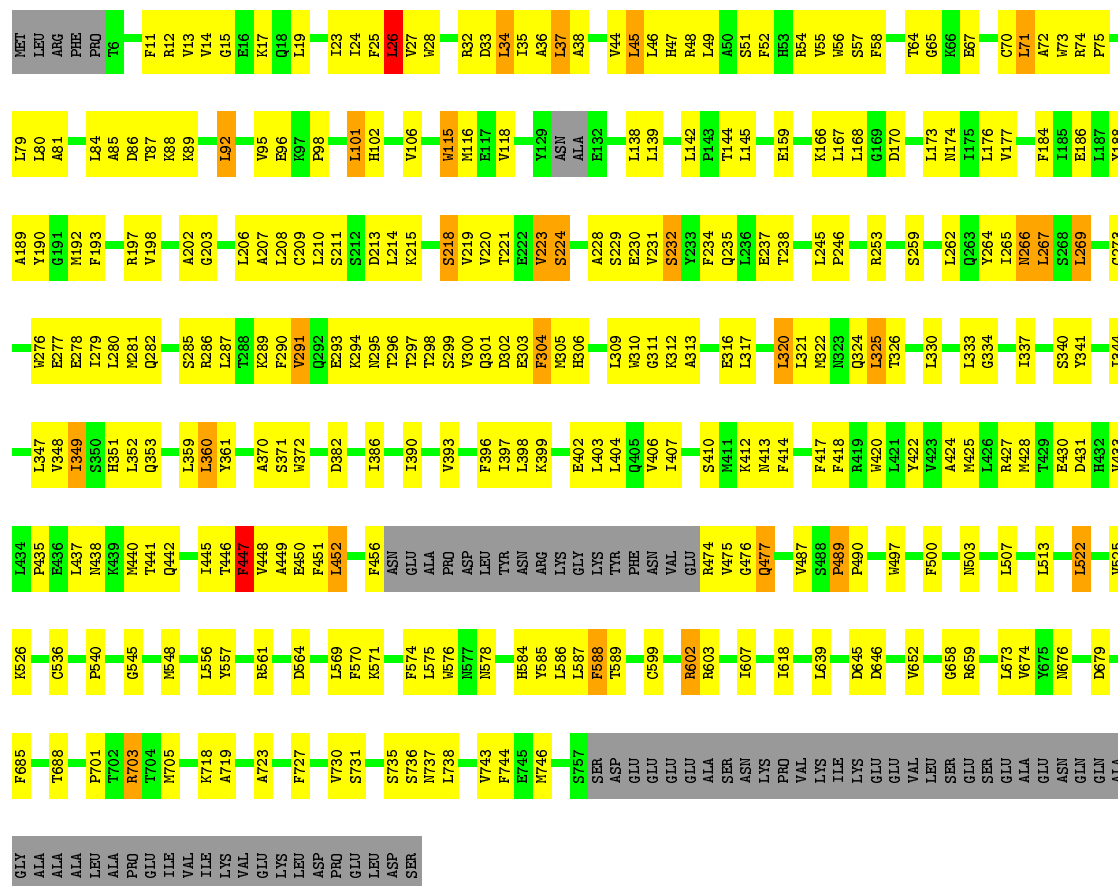
• Molecule 7: Anaphase-promoting complex subunit CDC26

Chain W: 18% 9% 71%



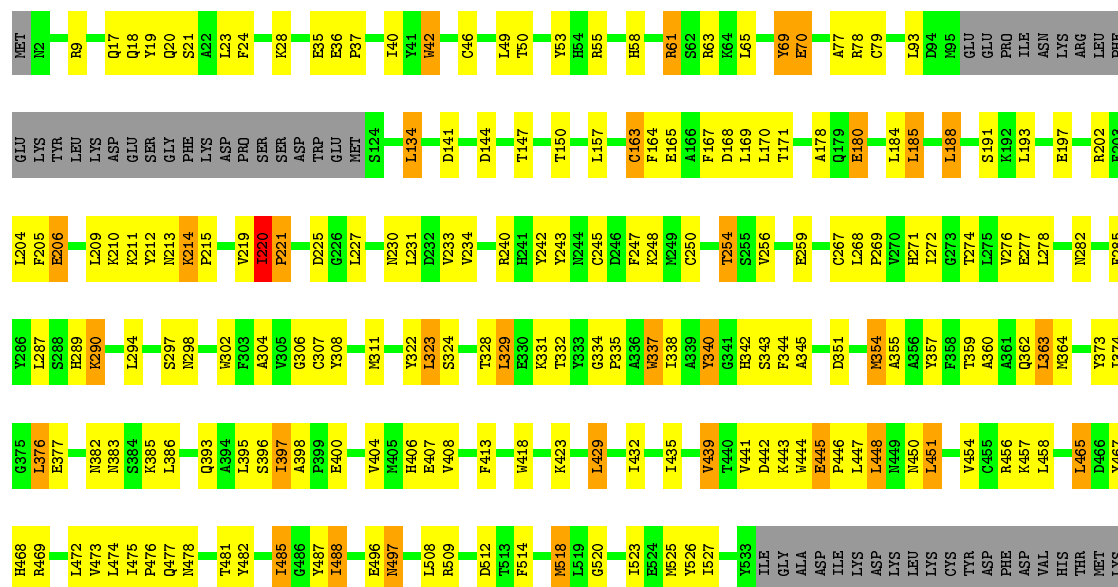
- Molecule 8: Anaphase-promoting complex subunit 4

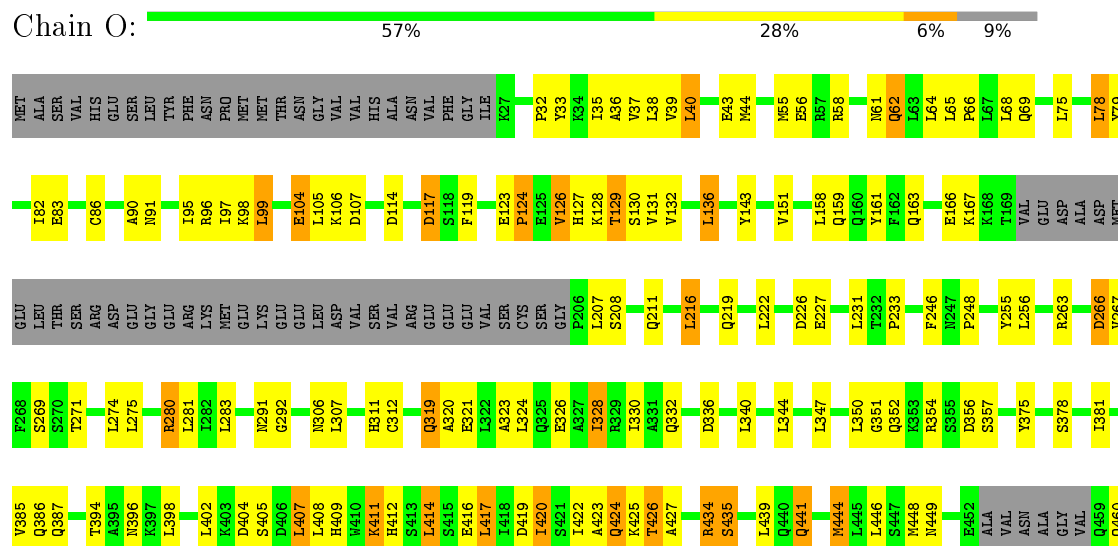
Chain I:  55% 33% 9%

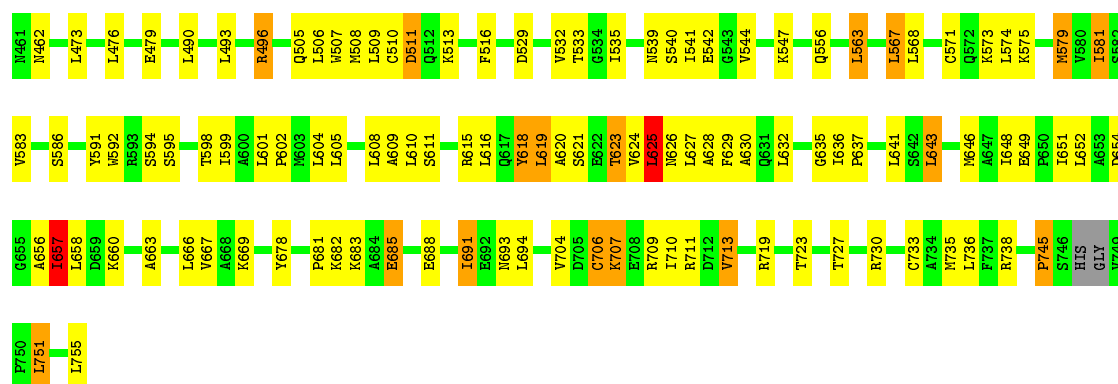


- Molecule 9: Cell division cycle protein 16 homolog

Chain J:  50% 26% 5% 19%

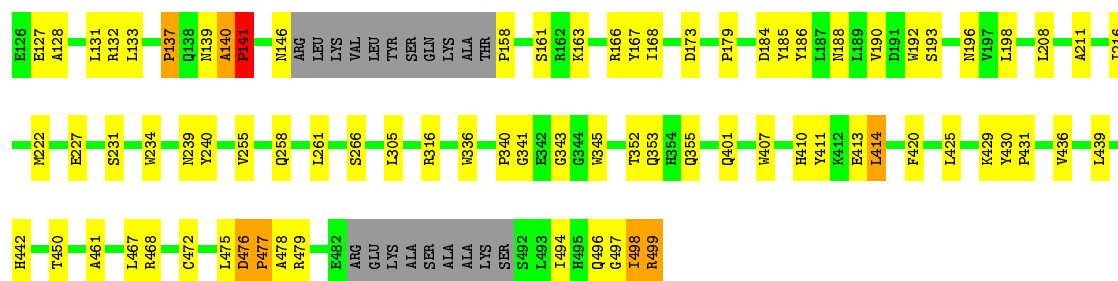






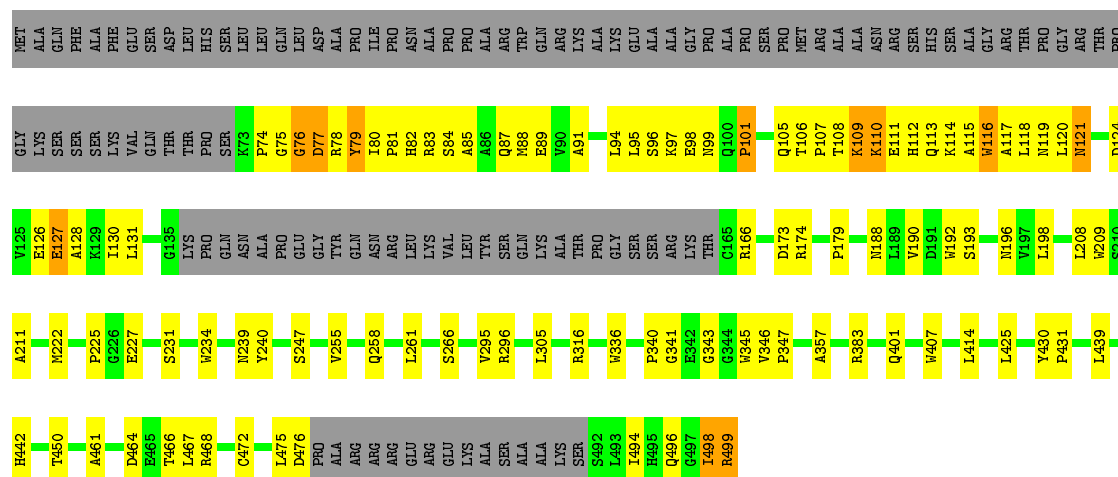
- Molecule 14: Cell division cycle protein 20 homolog

Chain Q: 74% 19% 5%



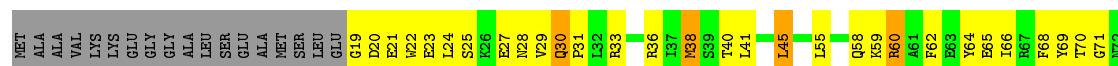
- Molecule 15: Cell division cycle protein 20 homolog

Chain R: 56% 19% 23%

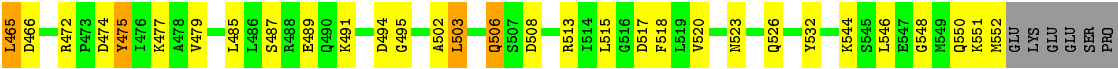


- Molecule 16: Mitotic checkpoint serine/threonine-protein kinase BUB1 beta, Mitotic checkpoint serine/threonine-protein kinase BUB1 beta

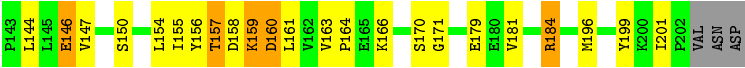
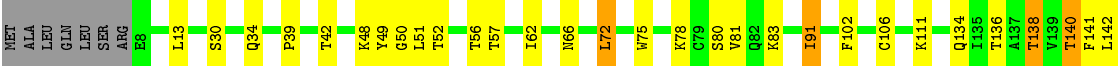
Chain S: 47% 29% 5% 19%







• Molecule 18: Mitotic spindle assembly checkpoint protein MAD2A



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | 155263 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | Not provided | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # $ Z > 2$ | RMSZ | # $ Z > 2$ |
| 1 | A | 0.67 | 6/11190 (0.1%) | 0.89 | 23/15236 (0.2%) |
| 10 | L | 0.54 | 0/1468 | 0.83 | 0/1993 |
| 11 | M | 0.66 | 0/502 | 0.95 | 0/680 |
| 12 | N | 0.63 | 3/5495 (0.1%) | 0.94 | 18/7441 (0.2%) |
| 13 | O | 0.58 | 0/5501 | 0.85 | 8/7432 (0.1%) |
| 14 | Q | 0.72 | 0/2737 | 0.86 | 4/3732 (0.1%) |
| 15 | R | 0.73 | 0/3029 | 0.86 | 2/4124 (0.0%) |
| 16 | S | 0.66 | 0/2112 | 0.88 | 12/2863 (0.4%) |
| 17 | X | 0.57 | 0/3833 | 0.82 | 3/5187 (0.1%) |
| 17 | Y | 0.58 | 0/3928 | 0.84 | 9/5311 (0.2%) |
| 18 | Z | 0.64 | 0/1605 | 0.79 | 2/2176 (0.1%) |
| 2 | B | 0.81 | 2/665 (0.3%) | 0.98 | 2/896 (0.2%) |
| 3 | C | 0.57 | 0/4404 | 0.83 | 4/5945 (0.1%) |
| 3 | P | 0.60 | 0/4138 | 0.86 | 5/5587 (0.1%) |
| 4 | D | 0.69 | 0/159 | 0.89 | 0/218 |
| 5 | E | 0.60 | 0/459 | 0.80 | 0/619 |
| 6 | F | 0.58 | 0/3939 | 0.82 | 3/5325 (0.1%) |
| 6 | H | 0.61 | 2/3943 (0.1%) | 0.82 | 2/5329 (0.0%) |
| 7 | G | 0.63 | 0/214 | 1.02 | 1/284 (0.4%) |
| 7 | W | 0.66 | 0/214 | 0.97 | 1/284 (0.4%) |
| 8 | I | 0.66 | 1/5834 (0.0%) | 0.92 | 11/7909 (0.1%) |
| 9 | J | 0.71 | 2/4146 (0.0%) | 0.95 | 5/5616 (0.1%) |
| 9 | K | 0.73 | 1/4086 (0.0%) | 0.93 | 7/5534 (0.1%) |
| All | All | 0.64 | 17/73601 (0.0%) | 0.88 | 122/99721 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 12 | N | 0 | 16 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 16 | S | 0 | 1 |
| 8 | I | 0 | 2 |
| 9 | J | 0 | 1 |
| All | All | 0 | 21 |

All (17) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | A | 1030 | GLU | CD-OE1 | 21.93 | 1.49 | 1.25 |
| 1 | A | 1030 | GLU | CD-OE2 | 15.62 | 1.42 | 1.25 |
| 1 | A | 1199 | LYS | CE-NZ | 9.92 | 1.73 | 1.49 |
| 12 | N | 209 | ARG | NE-CZ | 9.66 | 1.45 | 1.33 |
| 1 | A | 1030 | GLU | CG-CD | 8.25 | 1.64 | 1.51 |
| 9 | J | 302 | TRP | CB-CG | -7.73 | 1.36 | 1.50 |
| 9 | K | 302 | TRP | CB-CG | -6.97 | 1.37 | 1.50 |
| 1 | A | 795 | ARG | NE-CZ | 6.82 | 1.42 | 1.33 |
| 12 | N | 330 | ARG | CZ-NH2 | -6.39 | 1.24 | 1.33 |
| 9 | J | 337 | TRP | CB-CG | -6.31 | 1.38 | 1.50 |
| 6 | H | 730 | LYS | CE-NZ | 6.22 | 1.64 | 1.49 |
| 1 | A | 792 | GLN | CG-CD | 5.81 | 1.64 | 1.51 |
| 2 | B | 16 | TRP | CD2-CE2 | -5.62 | 1.34 | 1.41 |
| 8 | I | 115 | TRP | CB-CG | -5.36 | 1.40 | 1.50 |
| 6 | H | 570 | TRP | CB-CG | -5.25 | 1.40 | 1.50 |
| 12 | N | 330 | ARG | CD-NE | 5.06 | 1.55 | 1.46 |
| 2 | B | 14 | TRP | CB-CG | 5.06 | 1.59 | 1.50 |

All (122) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 12 | N | 330 | ARG | NE-CZ-NH2 | -13.57 | 113.52 | 120.30 |
| 16 | S | 60 | ARG | NE-CZ-NH1 | 9.25 | 124.92 | 120.30 |
| 9 | K | 351 | ASP | CB-CG-OD1 | 8.97 | 126.37 | 118.30 |
| 1 | A | 1235 | LEU | CB-CG-CD2 | -8.77 | 96.09 | 111.00 |
| 3 | P | 358 | LEU | CB-CG-CD1 | -8.46 | 96.62 | 111.00 |
| 14 | Q | 141 | PRO | N-CA-CB | 8.29 | 113.25 | 103.30 |
| 12 | N | 330 | ARG | NE-CZ-NH1 | 8.21 | 124.41 | 120.30 |
| 16 | S | 45 | LEU | CB-CG-CD2 | -7.99 | 97.42 | 111.00 |
| 16 | S | 38 | MET | CA-CB-CG | 7.91 | 126.75 | 113.30 |
| 13 | O | 117 | ASP | CB-CG-OD1 | -7.83 | 111.25 | 118.30 |
| 9 | J | 220 | ILE | C-N-CD | -7.47 | 104.17 | 120.60 |
| 3 | P | 358 | LEU | CA-CB-CG | 7.47 | 132.48 | 115.30 |
| 12 | N | 56 | PRO | N-CA-CB | 7.46 | 112.25 | 103.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 12 | N | 489 | PRO | N-CA-CB | 7.24 | 111.98 | 103.30 |
| 12 | N | 477 | PRO | N-CA-CB | 7.18 | 111.92 | 103.30 |
| 16 | S | 38 | MET | CB-CA-C | -7.07 | 96.26 | 110.40 |
| 17 | Y | 82 | TYR | CB-CG-CD1 | 7.04 | 125.22 | 121.00 |
| 9 | K | 134 | LEU | CA-CB-CG | 7.04 | 131.48 | 115.30 |
| 13 | O | 117 | ASP | CB-CG-OD2 | 7.00 | 124.60 | 118.30 |
| 1 | A | 1603 | LEU | CA-CB-CG | 6.99 | 131.37 | 115.30 |
| 16 | S | 60 | ARG | NE-CZ-NH2 | -6.93 | 116.83 | 120.30 |
| 9 | J | 376 | LEU | CA-CB-CG | 6.91 | 131.19 | 115.30 |
| 15 | R | 118 | LEU | CA-CB-CG | 6.87 | 131.10 | 115.30 |
| 17 | Y | 70 | LEU | CB-CG-CD1 | 6.87 | 122.67 | 111.00 |
| 14 | Q | 477 | PRO | N-CA-CB | 6.79 | 111.44 | 103.30 |
| 17 | Y | 82 | TYR | CB-CG-CD2 | -6.76 | 116.95 | 121.00 |
| 8 | I | 320 | LEU | CB-CG-CD1 | -6.69 | 99.63 | 111.00 |
| 8 | I | 435 | PRO | N-CA-CB | 6.60 | 111.22 | 103.30 |
| 3 | C | 365 | LEU | CA-CB-CG | -6.58 | 100.18 | 115.30 |
| 1 | A | 1933 | PRO | N-CA-CB | 6.57 | 111.18 | 103.30 |
| 12 | N | 395 | ASP | N-CA-C | 6.54 | 128.65 | 111.00 |
| 9 | J | 134 | LEU | CA-CB-CG | 6.44 | 130.12 | 115.30 |
| 16 | S | 222 | PRO | N-CA-CB | 6.40 | 110.98 | 103.30 |
| 16 | S | 290 | PRO | N-CA-CB | 6.40 | 110.98 | 103.30 |
| 12 | N | 63 | ALA | N-CA-C | 6.37 | 128.21 | 111.00 |
| 14 | Q | 158 | PRO | N-CA-CB | 6.37 | 110.95 | 103.30 |
| 1 | A | 1030 | GLU | CG-CD-OE2 | 6.35 | 130.99 | 118.30 |
| 1 | A | 1168 | LEU | CA-CB-CG | 6.33 | 129.86 | 115.30 |
| 1 | A | 795 | ARG | NE-CZ-NH2 | -6.24 | 117.18 | 120.30 |
| 12 | N | 496 | ARG | N-CA-C | 6.22 | 127.80 | 111.00 |
| 9 | K | 376 | LEU | CA-CB-CG | 6.16 | 129.47 | 115.30 |
| 1 | A | 1924 | PRO | N-CA-CB | 6.12 | 110.65 | 103.30 |
| 8 | I | 223 | VAL | CB-CA-C | -6.09 | 99.82 | 111.40 |
| 12 | N | 219 | PRO | N-CA-CB | 6.08 | 110.60 | 103.30 |
| 3 | C | 358 | LEU | CB-CG-CD2 | -6.06 | 100.69 | 111.00 |
| 9 | J | 188 | LEU | CA-CB-CG | 6.03 | 129.16 | 115.30 |
| 6 | H | 462 | LEU | CA-CB-CG | 6.02 | 129.15 | 115.30 |
| 12 | N | 29 | PRO | N-CA-CB | 6.02 | 110.52 | 103.30 |
| 2 | B | 14 | TRP | CA-CB-CG | 5.98 | 125.06 | 113.70 |
| 13 | O | 625 | LEU | CA-CB-CG | 5.95 | 128.98 | 115.30 |
| 1 | A | 1882 | LEU | CA-CB-CG | 5.94 | 128.95 | 115.30 |
| 12 | N | 63 | ALA | C-N-CA | 5.93 | 136.54 | 121.70 |
| 3 | C | 306 | LEU | CA-CB-CG | 5.91 | 128.90 | 115.30 |
| 18 | Z | 184 | ARG | NE-CZ-NH1 | 5.91 | 123.25 | 120.30 |
| 16 | S | 261 | PRO | N-CA-CB | 5.90 | 110.38 | 103.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3 | P | 306 | LEU | CA-CB-CG | 5.88 | 128.82 | 115.30 |
| 9 | K | 323 | LEU | CA-CB-CG | -5.87 | 101.80 | 115.30 |
| 1 | A | 1302 | LEU | CA-CB-CG | 5.80 | 128.64 | 115.30 |
| 6 | F | 462 | LEU | CA-CB-CG | 5.78 | 128.59 | 115.30 |
| 1 | A | 664 | LEU | CA-CB-CG | 5.78 | 128.58 | 115.30 |
| 16 | S | 38 | MET | CG-SD-CE | 5.76 | 109.41 | 100.20 |
| 14 | Q | 137 | PRO | N-CA-CB | 5.75 | 110.20 | 103.30 |
| 1 | A | 1243 | LEU | CA-CB-CG | 5.75 | 128.51 | 115.30 |
| 3 | C | 26 | PHE | CB-CG-CD1 | 5.72 | 124.80 | 120.80 |
| 16 | S | 557 | PRO | N-CA-CB | 5.69 | 110.13 | 103.30 |
| 13 | O | 563 | LEU | CA-CB-CG | 5.68 | 128.36 | 115.30 |
| 12 | N | 55 | PRO | N-CA-CB | 5.67 | 110.10 | 103.30 |
| 17 | X | 446 | LEU | CA-CB-CG | 5.62 | 128.23 | 115.30 |
| 17 | Y | 418 | LEU | CA-CB-CG | 5.61 | 128.20 | 115.30 |
| 6 | F | 765 | ASP | CB-CG-OD1 | 5.59 | 123.33 | 118.30 |
| 12 | N | 482 | PRO | N-CA-CB | 5.59 | 110.00 | 103.30 |
| 1 | A | 1313 | LEU | CA-CB-CG | 5.57 | 128.12 | 115.30 |
| 17 | Y | 199 | CYS | N-CA-C | 5.57 | 126.03 | 111.00 |
| 1 | A | 1409 | LEU | CA-CB-CG | 5.56 | 128.09 | 115.30 |
| 16 | S | 263 | PRO | N-CA-CB | 5.56 | 109.97 | 103.30 |
| 18 | Z | 140 | THR | CA-CB-CG2 | -5.56 | 104.62 | 112.40 |
| 1 | A | 188 | LEU | CA-CB-CG | 5.55 | 128.06 | 115.30 |
| 12 | N | 125 | TYR | C-N-CA | 5.53 | 135.53 | 121.70 |
| 17 | X | 418 | LEU | CA-CB-CG | 5.52 | 127.99 | 115.30 |
| 8 | I | 45 | LEU | CB-CG-CD2 | 5.49 | 120.33 | 111.00 |
| 1 | A | 1030 | GLU | CG-CD-OE1 | -5.48 | 107.34 | 118.30 |
| 13 | O | 751 | LEU | CA-CB-CG | 5.46 | 127.85 | 115.30 |
| 6 | H | 571 | CYS | CA-CB-SG | -5.45 | 104.20 | 114.00 |
| 8 | I | 645 | ASP | CB-CG-OD2 | 5.43 | 123.19 | 118.30 |
| 1 | A | 953 | LEU | CA-CB-CG | 5.43 | 127.78 | 115.30 |
| 13 | O | 216 | LEU | CA-CB-CG | 5.42 | 127.76 | 115.30 |
| 2 | B | 61 | LEU | CA-CB-CG | 5.40 | 127.72 | 115.30 |
| 6 | F | 130 | ARG | NE-CZ-NH2 | -5.39 | 117.60 | 120.30 |
| 13 | O | 64 | LEU | CA-CB-CG | 5.38 | 127.67 | 115.30 |
| 17 | Y | 59 | LEU | CA-CB-CG | 5.36 | 127.62 | 115.30 |
| 8 | I | 602 | ARG | NE-CZ-NH1 | 5.34 | 122.97 | 120.30 |
| 15 | R | 383 | ARG | NE-CZ-NH1 | -5.34 | 117.63 | 120.30 |
| 1 | A | 651 | PRO | N-CA-CB | 5.34 | 109.70 | 103.30 |
| 8 | I | 603 | ARG | NE-CZ-NH1 | 5.32 | 122.96 | 120.30 |
| 9 | K | 451 | LEU | CB-CG-CD2 | -5.31 | 101.97 | 111.00 |
| 17 | Y | 446 | LEU | CA-CB-CG | 5.29 | 127.46 | 115.30 |
| 8 | I | 447 | PHE | N-CA-CB | -5.29 | 101.09 | 110.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 1748 | LEU | CA-CB-CG | 5.28 | 127.45 | 115.30 |
| 12 | N | 197 | PRO | N-CA-CB | 5.25 | 109.60 | 103.30 |
| 3 | P | 49 | LEU | CA-CB-CG | 5.25 | 127.38 | 115.30 |
| 9 | K | 448 | LEU | CB-CG-CD2 | 5.25 | 119.93 | 111.00 |
| 1 | A | 1032 | LEU | CA-CB-CG | 5.24 | 127.35 | 115.30 |
| 3 | P | 365 | LEU | CA-CB-CG | 5.23 | 127.33 | 115.30 |
| 1 | A | 1405 | LEU | CA-CB-CG | 5.23 | 127.32 | 115.30 |
| 1 | A | 977 | LEU | CA-CB-CG | 5.21 | 127.29 | 115.30 |
| 7 | G | 14 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 9 | J | 225 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 8 | I | 26 | LEU | CA-CB-CG | 5.19 | 127.24 | 115.30 |
| 9 | K | 359 | THR | N-CA-CB | 5.19 | 120.15 | 110.30 |
| 12 | N | 386 | LEU | CA-CB-CG | 5.18 | 127.22 | 115.30 |
| 17 | X | 466 | ASP | CB-CG-OD2 | 5.18 | 122.96 | 118.30 |
| 7 | W | 3 | ARG | NE-CZ-NH1 | 5.17 | 122.89 | 120.30 |
| 1 | A | 1243 | LEU | CB-CG-CD2 | 5.17 | 119.79 | 111.00 |
| 1 | A | 1059 | ASP | CB-CG-OD2 | 5.17 | 122.95 | 118.30 |
| 17 | Y | 466 | ASP | CB-CG-OD2 | 5.16 | 122.94 | 118.30 |
| 17 | Y | 203 | LEU | CA-CB-CG | 5.11 | 127.06 | 115.30 |
| 12 | N | 78 | VAL | N-CA-C | -5.05 | 97.36 | 111.00 |
| 13 | O | 407 | LEU | CA-CB-CG | 5.05 | 126.91 | 115.30 |
| 8 | I | 703 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 12 | N | 547 | LEU | CA-CB-CG | 5.04 | 126.89 | 115.30 |
| 8 | I | 659 | ARG | N-CA-C | 5.02 | 124.56 | 111.00 |
| 16 | S | 301 | PRO | N-CA-CB | 5.00 | 109.30 | 103.30 |

There are no chirality outliers.

All (21) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|---------|
| 1 | A | 1191 | LEU | Peptide |
| 8 | I | 658 | GLY | Peptide |
| 8 | I | 727 | PHE | Peptide |
| 9 | J | 220 | ILE | Peptide |
| 12 | N | 162 | PHE | Peptide |
| 12 | N | 164 | SER | Peptide |
| 12 | N | 280 | GLU | Peptide |
| 12 | N | 281 | TYR | Peptide |
| 12 | N | 351 | PHE | Peptide |
| 12 | N | 352 | PRO | Peptide |
| 12 | N | 353 | ASP | Peptide |
| 12 | N | 367 | ARG | Peptide |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 12 | N | 369 | ASP | Peptide |
| 12 | N | 387 | LEU | Peptide |
| 12 | N | 390 | GLY | Peptide |
| 12 | N | 394 | CYS | Peptide |
| 12 | N | 395 | ASP | Peptide |
| 12 | N | 485 | VAL | Peptide |
| 12 | N | 62 | ARG | Peptide |
| 12 | N | 77 | GLU | Peptide |
| 16 | S | 235 | LYS | Peptide |

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 | 10949 | 0 | 10690 | 418 | 0 |
| 2 | B | 643 | 0 | 617 | 80 | 0 |
| 3 | C | 4306 | 0 | 4272 | 161 | 0 |
| 3 | P | 4043 | 0 | 4000 | 137 | 0 |
| 4 | D | 153 | 0 | 148 | 8 | 0 |
| 5 | E | 450 | 0 | 435 | 10 | 0 |
| 6 | F | 3849 | 0 | 3783 | 108 | 0 |
| 6 | H | 3853 | 0 | 3794 | 128 | 0 |
| 7 | G | 213 | 0 | 220 | 11 | 0 |
| 7 | W | 213 | 0 | 220 | 12 | 0 |
| 8 | I | 5716 | 0 | 5587 | 345 | 0 |
| 9 | J | 4047 | 0 | 3949 | 185 | 0 |
| 9 | K | 3988 | 0 | 3908 | 174 | 0 |
| 10 | L | 1435 | 0 | 1382 | 55 | 0 |
| 11 | M | 493 | 0 | 469 | 24 | 0 |
| 12 | N | 5403 | 0 | 5103 | 276 | 0 |
| 13 | O | 5402 | 0 | 5436 | 221 | 0 |
| 14 | Q | 2671 | 0 | 2516 | 103 | 0 |
| 15 | R | 2953 | 0 | 2839 | 111 | 0 |
| 16 | S | 2077 | 0 | 1827 | 327 | 0 |
| 17 | X | 3773 | 0 | 3831 | 163 | 0 |
| 17 | Y | 3868 | 0 | 3925 | 169 | 0 |
| 18 | Z | 1577 | 0 | 1592 | 89 | 0 |
| All | All | 72075 | 0 | 70543 | 2914 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (2914) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 16:S:38:MET:CE | 18:Z:181:VAL:HG23 | 1.22 | 1.65 |
| 16:S:22:TRP:CZ3 | 16:S:41:LEU:HB2 | 1.31 | 1.64 |
| 16:S:19:GLY:CA | 18:Z:134:GLN:HE21 | 1.16 | 1.54 |
| 8:I:413:ASN:HA | 8:I:447:PHE:CZ | 1.38 | 1.53 |
| 1:A:1199:LYS:CE | 1:A:1199:LYS:NZ | 1.73 | 1.45 |
| 16:S:19:GLY:CA | 18:Z:134:GLN:NE2 | 1.74 | 1.43 |
| 16:S:68:PHE:CE2 | 16:S:81:TYR:CD2 | 2.10 | 1.40 |
| 16:S:38:MET:CE | 18:Z:181:VAL:CG2 | 2.00 | 1.38 |
| 16:S:30:GLN:N | 16:S:36:ARG:HH22 | 1.20 | 1.38 |
| 16:S:19:GLY:C | 18:Z:134:GLN:HE21 | 1.23 | 1.38 |
| 16:S:29:VAL:HG13 | 16:S:36:ARG:NH1 | 1.40 | 1.36 |
| 16:S:22:TRP:CZ3 | 16:S:41:LEU:CB | 2.10 | 1.34 |
| 17:X:442:GLN:CD | 17:X:472:ARG:NE | 1.78 | 1.34 |
| 16:S:36:ARG:NH1 | 16:S:90:PRO:HB2 | 1.42 | 1.33 |
| 16:S:58:GLN:HG3 | 16:S:62:PHE:CE2 | 1.61 | 1.32 |
| 16:S:38:MET:HE2 | 18:Z:181:VAL:CG2 | 1.58 | 1.32 |
| 16:S:19:GLY:HA3 | 18:Z:134:GLN:NE2 | 1.34 | 1.29 |
| 12:N:362:LYS:HB2 | 12:N:410:LEU:CD2 | 1.62 | 1.28 |
| 2:B:16:TRP:NE1 | 2:B:44:CYS:CB | 1.96 | 1.26 |
| 8:I:413:ASN:HA | 8:I:447:PHE:CE1 | 1.68 | 1.25 |
| 1:A:1332:GLY:O | 1:A:1358:ILE:HD12 | 1.31 | 1.25 |
| 16:S:68:PHE:CZ | 16:S:81:TYR:HD2 | 1.54 | 1.25 |
| 16:S:21:GLU:O | 16:S:45:LEU:HD22 | 1.35 | 1.24 |
| 17:X:442:GLN:OE1 | 17:X:472:ARG:CZ | 1.85 | 1.22 |
| 1:A:1235:LEU:CD2 | 1:A:1257:ILE:HG13 | 1.70 | 1.21 |
| 16:S:29:VAL:HG12 | 18:Z:140:THR:CG2 | 1.72 | 1.20 |
| 16:S:38:MET:HE3 | 18:Z:181:VAL:CG2 | 1.71 | 1.20 |
| 8:I:430:GLU:HG2 | 14:Q:429:LYS:CG | 1.71 | 1.20 |
| 17:Y:42:ARG:HA | 17:Y:82:TYR:CE2 | 1.78 | 1.17 |
| 1:A:1332:GLY:O | 1:A:1358:ILE:CD1 | 1.91 | 1.17 |
| 2:B:16:TRP:CD1 | 2:B:44:CYS:HB3 | 1.79 | 1.16 |
| 12:N:362:LYS:CB | 12:N:410:LEU:HD23 | 1.76 | 1.16 |
| 16:S:68:PHE:CE2 | 16:S:81:TYR:HD2 | 1.51 | 1.15 |
| 16:S:29:VAL:HA | 16:S:36:ARG:HH12 | 1.11 | 1.15 |
| 16:S:71:GLY:C | 16:S:74:PRO:HD2 | 1.68 | 1.14 |
| 9:K:129:LYS:O | 9:K:133:CYS:SG | 2.05 | 1.14 |
| 16:S:132:CYS:HB2 | 16:S:135:PRO:HG3 | 1.13 | 1.13 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:279:ILE:HD11 | 8:I:337:ILE:HA | 1.23 | 1.13 |
| 13:O:75:LEU:HD11 | 13:O:161:TYR:CE2 | 1.82 | 1.12 |
| 17:X:201:LEU:HD11 | 17:Y:40:HIS:HB3 | 1.20 | 1.12 |
| 13:O:75:LEU:CD2 | 13:O:161:TYR:OH | 1.98 | 1.11 |
| 8:I:290:PHE:CA | 8:I:320:LEU:HD11 | 1.81 | 1.11 |
| 8:I:413:ASN:CA | 8:I:447:PHE:CZ | 2.31 | 1.11 |
| 12:N:765:LEU:HD21 | 16:S:200:VAL:HG21 | 1.30 | 1.11 |
| 16:S:29:VAL:CG1 | 16:S:36:ARG:NH1 | 2.14 | 1.11 |
| 9:K:250:CYS:SG | 9:K:274:THR:HG21 | 1.91 | 1.11 |
| 16:S:29:VAL:HG12 | 18:Z:140:THR:HG21 | 1.29 | 1.10 |
| 16:S:76:ASP:O | 16:S:77:VAL:HG23 | 1.49 | 1.10 |
| 16:S:58:GLN:O | 16:S:62:PHE:CD2 | 2.04 | 1.10 |
| 12:N:362:LYS:HB2 | 12:N:410:LEU:HD23 | 1.10 | 1.10 |
| 9:J:441:VAL:HG21 | 9:J:444:TRP:HD1 | 1.16 | 1.09 |
| 16:S:21:GLU:O | 16:S:45:LEU:CD2 | 1.99 | 1.09 |
| 2:B:16:TRP:NE1 | 2:B:44:CYS:HB3 | 1.58 | 1.09 |
| 16:S:22:TRP:CH2 | 16:S:38:MET:O | 2.05 | 1.09 |
| 8:I:313:ALA:HB3 | 8:I:317:LEU:HB2 | 1.18 | 1.08 |
| 16:S:132:CYS:HA | 16:S:133:ASN:HB2 | 1.34 | 1.08 |
| 9:J:454:VAL:O | 9:J:458:LEU:HD12 | 1.51 | 1.08 |
| 16:S:20:ASP:OD1 | 18:Z:184:ARG:HD2 | 1.53 | 1.08 |
| 8:I:209:CYS:SG | 8:I:584:HIS:CE1 | 2.46 | 1.07 |
| 16:S:36:ARG:NH1 | 16:S:90:PRO:CB | 2.17 | 1.07 |
| 16:S:30:GLN:H | 16:S:91:GLN:HB2 | 1.18 | 1.07 |
| 12:N:180:PHE:CD1 | 12:N:299:TRP:CZ3 | 2.43 | 1.07 |
| 16:S:30:GLN:N | 16:S:36:ARG:NH2 | 2.00 | 1.07 |
| 13:O:75:LEU:O | 13:O:79:TYR:CD2 | 2.08 | 1.07 |
| 9:J:332:THR:HA | 9:J:363:LEU:HD21 | 1.37 | 1.06 |
| 16:S:132:CYS:SG | 16:S:135:PRO:HA | 1.95 | 1.06 |
| 8:I:302:ASP:N | 8:I:303:GLU:N | 2.04 | 1.06 |
| 1:A:1235:LEU:HD21 | 1:A:1257:ILE:CG1 | 1.85 | 1.06 |
| 6:H:656:MET:HE2 | 6:H:660:LYS:HE2 | 1.30 | 1.05 |
| 8:I:209:CYS:SG | 8:I:584:HIS:ND1 | 2.30 | 1.05 |
| 17:X:442:GLN:OE1 | 17:X:472:ARG:NH2 | 1.87 | 1.05 |
| 12:N:393:THR:O | 12:N:395:ASP:HB3 | 1.54 | 1.04 |
| 6:F:130:ARG:HG2 | 17:Y:506:GLN:NE2 | 1.71 | 1.04 |
| 8:I:300:VAL:HA | 8:I:303:GLU:OE1 | 1.55 | 1.04 |
| 17:Y:452:LEU:HD22 | 17:Y:461:ALA:N | 1.73 | 1.04 |
| 17:X:452:LEU:CD2 | 17:X:457:THR:O | 2.06 | 1.04 |
| 16:S:68:PHE:CZ | 16:S:81:TYR:CD2 | 2.37 | 1.03 |
| 17:X:442:GLN:HG2 | 17:X:472:ARG:CD | 1.86 | 1.03 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:56:TRP:CE3 | 8:I:98:PRO:HB3 | 1.93 | 1.03 |
| 12:N:362:LYS:CB | 12:N:410:LEU:CD2 | 2.34 | 1.03 |
| 16:S:30:GLN:N | 16:S:91:GLN:HB2 | 1.74 | 1.03 |
| 17:Y:452:LEU:CD2 | 17:Y:457:THR:O | 2.06 | 1.03 |
| 15:R:98:GLU:CG | 15:R:101:PRO:HD3 | 1.88 | 1.02 |
| 16:S:38:MET:HE3 | 18:Z:181:VAL:HG21 | 1.40 | 1.02 |
| 14:Q:185:TYR:CD1 | 16:S:27:GLU:HB3 | 1.94 | 1.02 |
| 16:S:79:ASP:OD2 | 16:S:120:ARG:HG2 | 1.59 | 1.02 |
| 12:N:425:ARG:HH11 | 12:N:425:ARG:HG2 | 1.20 | 1.02 |
| 16:S:29:VAL:CA | 16:S:36:ARG:HH12 | 1.73 | 1.02 |
| 2:B:14:TRP:HA | 2:B:15:LEU:HB2 | 1.41 | 1.02 |
| 13:O:581:ILE:HD11 | 13:O:619:LEU:HB3 | 1.42 | 1.01 |
| 1:A:1232:ILE:HG13 | 1:A:1235:LEU:HB2 | 1.40 | 1.01 |
| 17:X:452:LEU:HD22 | 17:X:461:ALA:N | 1.73 | 1.01 |
| 8:I:295:ASN:O | 8:I:316:GLU:HB2 | 1.61 | 1.01 |
| 14:Q:410:HIS:HB3 | 14:Q:475:LEU:HD21 | 1.40 | 1.01 |
| 13:O:75:LEU:CG | 13:O:161:TYR:CE2 | 2.44 | 1.00 |
| 16:S:71:GLY:O | 16:S:74:PRO:HD2 | 1.59 | 1.00 |
| 8:I:289:LYS:HG3 | 8:I:324:GLN:OE1 | 1.61 | 1.00 |
| 2:B:16:TRP:HD1 | 2:B:33:CYS:HA | 1.24 | 1.00 |
| 16:S:66:ILE:HA | 16:S:69:TYR:HD2 | 1.24 | 1.00 |
| 8:I:430:GLU:HG2 | 14:Q:429:LYS:HG3 | 1.38 | 1.00 |
| 13:O:75:LEU:CD1 | 13:O:161:TYR:CE2 | 2.45 | 0.99 |
| 1:A:1162:LYS:HG3 | 1:A:1163:PRO:HD2 | 1.44 | 0.99 |
| 17:Y:42:ARG:HG3 | 17:Y:82:TYR:OH | 1.61 | 0.99 |
| 16:S:19:GLY:C | 18:Z:134:GLN:NE2 | 2.04 | 0.99 |
| 8:I:430:GLU:HG2 | 14:Q:429:LYS:HG2 | 1.45 | 0.99 |
| 16:S:22:TRP:HH2 | 16:S:38:MET:CA | 1.76 | 0.99 |
| 17:X:442:GLN:HG2 | 17:X:472:ARG:HD2 | 1.40 | 0.99 |
| 13:O:435:SER:HB3 | 13:O:654:ASP:HB2 | 1.43 | 0.98 |
| 8:I:313:ALA:HB2 | 8:I:317:LEU:HD12 | 1.43 | 0.98 |
| 3:C:344:ARG:HH21 | 11:M:25:PRO:HG2 | 1.27 | 0.98 |
| 1:A:1235:LEU:HD21 | 1:A:1257:ILE:HG13 | 1.00 | 0.98 |
| 16:S:29:VAL:HG13 | 16:S:36:ARG:HH11 | 1.26 | 0.98 |
| 14:Q:128:ALA:HB3 | 18:Z:156:TYR:CZ | 1.99 | 0.98 |
| 15:R:225:PRO:HD2 | 16:S:166:GLU:O | 1.64 | 0.98 |
| 9:K:250:CYS:SG | 9:K:274:THR:CG2 | 2.52 | 0.97 |
| 17:X:201:LEU:HD11 | 17:Y:40:HIS:CB | 1.94 | 0.97 |
| 9:J:55:ARG:HH11 | 9:K:264:HIS:HA | 1.24 | 0.97 |
| 16:S:33:ARG:HB2 | 16:S:130:ARG:HH11 | 1.30 | 0.97 |
| 8:I:186:GLU:OE1 | 8:I:197:ARG:NH1 | 1.97 | 0.97 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:144:THR:HG21 | 8:I:159:GLU:HA | 1.46 | 0.97 |
| 16:S:132:CYS:HB2 | 16:S:135:PRO:CG | 1.93 | 0.97 |
| 8:I:313:ALA:CB | 8:I:317:LEU:HD12 | 1.95 | 0.96 |
| 3:C:134:THR:HG23 | 3:C:143:LYS:HG3 | 1.47 | 0.96 |
| 13:O:75:LEU:HD21 | 13:O:161:TYR:OH | 1.62 | 0.96 |
| 16:S:40:THR:HB | 16:S:87:GLN:O | 1.65 | 0.96 |
| 8:I:313:ALA:HB3 | 8:I:317:LEU:CB | 1.95 | 0.96 |
| 2:B:17:VAL:HG13 | 2:B:31:ASN:ND2 | 1.80 | 0.96 |
| 16:S:79:ASP:OD2 | 16:S:120:ARG:CG | 2.13 | 0.96 |
| 8:I:209:CYS:HG | 8:I:584:HIS:HD1 | 1.11 | 0.95 |
| 16:S:79:ASP:OD2 | 16:S:120:ARG:CB | 2.15 | 0.95 |
| 12:N:574:ILE:HD12 | 12:N:625:LYS:HG2 | 1.49 | 0.95 |
| 3:P:233:PHE:CZ | 3:P:237:ILE:HD11 | 2.02 | 0.95 |
| 16:S:22:TRP:CH2 | 16:S:38:MET:HA | 2.02 | 0.95 |
| 17:X:442:GLN:CD | 17:X:472:ARG:HE | 1.61 | 0.95 |
| 13:O:75:LEU:CD2 | 13:O:161:TYR:CZ | 2.50 | 0.94 |
| 16:S:22:TRP:HA | 16:S:45:LEU:HD11 | 1.47 | 0.94 |
| 17:X:442:GLN:NE2 | 17:X:472:ARG:HE | 1.66 | 0.94 |
| 17:Y:305:ILE:HG23 | 17:Y:340:GLU:OE1 | 1.68 | 0.94 |
| 1:A:1322:PRO:HG3 | 1:A:1375:TYR:OH | 1.67 | 0.94 |
| 8:I:413:ASN:HA | 8:I:447:PHE:HZ | 1.24 | 0.94 |
| 9:J:254:THR:HG23 | 9:J:271:HIS:HD2 | 1.32 | 0.94 |
| 16:S:86:GLU:HG3 | 16:S:98:MET:CE | 1.98 | 0.94 |
| 16:S:22:TRP:CH2 | 16:S:41:LEU:HB2 | 2.02 | 0.94 |
| 13:O:75:LEU:HD21 | 13:O:161:TYR:CE2 | 2.03 | 0.94 |
| 13:O:75:LEU:O | 13:O:79:TYR:HD2 | 1.47 | 0.93 |
| 9:K:214:LYS:O | 9:K:216:SER:N | 2.01 | 0.93 |
| 12:N:538:GLU:HG2 | 12:N:561:LEU:HG | 1.47 | 0.93 |
| 6:H:762:TRP:HA | 6:H:765:ASP:HB3 | 1.48 | 0.93 |
| 8:I:290:PHE:HA | 8:I:320:LEU:HD11 | 1.46 | 0.93 |
| 16:S:38:MET:HE1 | 18:Z:199:TYR:HE2 | 1.30 | 0.93 |
| 6:H:656:MET:CE | 6:H:660:LYS:HE2 | 1.98 | 0.93 |
| 2:B:16:TRP:CZ3 | 12:N:630:LYS:HE2 | 2.04 | 0.93 |
| 12:N:78:VAL:O | 12:N:81:ASN:N | 2.01 | 0.93 |
| 2:B:14:TRP:CA | 2:B:15:LEU:HB2 | 1.99 | 0.92 |
| 2:B:16:TRP:HZ2 | 2:B:45:PRO:N | 1.65 | 0.92 |
| 9:J:441:VAL:HG21 | 9:J:444:TRP:CD1 | 2.03 | 0.92 |
| 12:N:273:MET:HG3 | 12:N:277:CYS:SG | 2.09 | 0.92 |
| 16:S:22:TRP:HZ3 | 16:S:41:LEU:CB | 1.63 | 0.92 |
| 16:S:163:GLU:CD | 16:S:196:PHE:CE1 | 2.43 | 0.92 |
| 17:X:40:HIS:HB3 | 17:Y:201:LEU:HD11 | 1.51 | 0.92 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:S:163:GLU:OE1 | 16:S:196:PHE:CE1 | 2.22 | 0.92 |
| 12:N:180:PHE:CD1 | 12:N:299:TRP:CH2 | 2.57 | 0.92 |
| 14:Q:352:THR:HG21 | 18:Z:50:GLY:O | 1.70 | 0.91 |
| 1:A:1332:GLY:O | 1:A:1358:ILE:CG1 | 2.18 | 0.91 |
| 13:O:75:LEU:HD21 | 13:O:161:TYR:CZ | 2.04 | 0.91 |
| 16:S:76:ASP:O | 16:S:77:VAL:CG2 | 2.17 | 0.91 |
| 16:S:71:GLY:O | 16:S:74:PRO:O | 1.86 | 0.91 |
| 16:S:30:GLN:NE2 | 16:S:91:GLN:HG3 | 1.86 | 0.91 |
| 16:S:36:ARG:HH12 | 16:S:90:PRO:HB2 | 1.18 | 0.90 |
| 16:S:86:GLU:HG3 | 16:S:98:MET:HE1 | 1.50 | 0.90 |
| 2:B:46:LEU:HB2 | 12:N:632:MET:SD | 2.09 | 0.90 |
| 8:I:300:VAL:O | 8:I:303:GLU:HB2 | 1.70 | 0.90 |
| 2:B:16:TRP:CD1 | 2:B:33:CYS:HA | 2.05 | 0.90 |
| 13:O:75:LEU:HD23 | 13:O:161:TYR:OH | 1.71 | 0.90 |
| 16:S:163:GLU:OE1 | 16:S:196:PHE:CD1 | 2.24 | 0.90 |
| 8:I:26:LEU:HB3 | 8:I:37:LEU:HB3 | 1.54 | 0.90 |
| 17:X:267:LEU:HD11 | 17:Y:59:LEU:CD1 | 2.01 | 0.90 |
| 16:S:22:TRP:HZ3 | 16:S:41:LEU:HB2 | 1.07 | 0.90 |
| 16:S:58:GLN:O | 16:S:62:PHE:HD2 | 1.55 | 0.90 |
| 13:O:75:LEU:HG | 13:O:161:TYR:CZ | 2.05 | 0.90 |
| 16:S:58:GLN:HG3 | 16:S:62:PHE:HE2 | 1.00 | 0.90 |
| 3:C:414:MET:HG2 | 13:O:330:ILE:CD1 | 2.02 | 0.90 |
| 14:Q:132:ARG:HG3 | 18:Z:154:LEU:CD2 | 2.02 | 0.90 |
| 9:J:211:LYS:O | 9:J:212:TYR:CD2 | 2.24 | 0.89 |
| 17:X:442:GLN:OE1 | 17:X:472:ARG:NE | 1.97 | 0.89 |
| 2:B:14:TRP:HA | 2:B:15:LEU:CB | 1.99 | 0.89 |
| 8:I:302:ASP:C | 8:I:303:GLU:N | 2.26 | 0.89 |
| 17:Y:452:LEU:HD23 | 17:Y:457:THR:O | 1.72 | 0.89 |
| 16:S:193:HIS:CE1 | 16:S:197:GLN:OE1 | 2.25 | 0.89 |
| 16:S:197:GLN:O | 16:S:200:VAL:HG22 | 1.73 | 0.89 |
| 16:S:68:PHE:HE2 | 16:S:81:TYR:CD2 | 1.82 | 0.89 |
| 17:X:452:LEU:HD23 | 17:X:457:THR:O | 1.72 | 0.89 |
| 16:S:132:CYS:CB | 16:S:135:PRO:HG3 | 2.03 | 0.89 |
| 6:F:130:ARG:HG2 | 17:Y:506:GLN:HE21 | 1.35 | 0.89 |
| 16:S:66:ILE:HA | 16:S:69:TYR:CD2 | 2.07 | 0.89 |
| 11:M:4:GLU:HG2 | 3:P:50:HIS:CE1 | 2.08 | 0.89 |
| 8:I:300:VAL:HG21 | 8:I:456:PHE:CB | 2.03 | 0.89 |
| 17:X:442:GLN:CG | 17:X:472:ARG:CD | 2.51 | 0.88 |
| 14:Q:185:TYR:CE1 | 16:S:27:GLU:HG3 | 2.09 | 0.88 |
| 13:O:55:MET:SD | 13:O:58:ARG:NH1 | 2.47 | 0.88 |
| 17:X:201:LEU:CD1 | 17:Y:40:HIS:HB3 | 2.02 | 0.88 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Y:462:LYS:HG2 | 17:Y:485:LEU:HD13 | 1.56 | 0.88 |
| 9:J:55:ARG:NH1 | 9:K:264:HIS:HA | 1.89 | 0.87 |
| 13:O:55:MET:SD | 13:O:58:ARG:CZ | 2.62 | 0.87 |
| 8:I:290:PHE:C | 8:I:320:LEU:HD11 | 1.93 | 0.87 |
| 10:L:83:TYR:CD2 | 10:L:115:GLU:HA | 2.09 | 0.87 |
| 16:S:134:GLU:O | 16:S:136:LEU:N | 2.08 | 0.87 |
| 12:N:91:PHE:O | 12:N:93:ASN:N | 2.07 | 0.87 |
| 16:S:41:LEU:CD1 | 18:Z:141:PHE:HB3 | 2.05 | 0.87 |
| 1:A:1175:PHE:CZ | 1:A:1179:LEU:HD21 | 2.10 | 0.87 |
| 14:Q:132:ARG:HB2 | 18:Z:170:SER:HB2 | 1.55 | 0.87 |
| 16:S:22:TRP:CH2 | 16:S:38:MET:CA | 2.58 | 0.87 |
| 9:J:445:GLU:OE1 | 9:J:475:ILE:HG21 | 1.75 | 0.87 |
| 9:J:167:PHE:O | 9:J:170:LEU:HD23 | 1.75 | 0.86 |
| 12:N:362:LYS:HB2 | 12:N:410:LEU:HD21 | 1.55 | 0.86 |
| 16:S:199:ARG:O | 16:S:202:ARG:HG2 | 1.73 | 0.86 |
| 14:Q:185:TYR:CD1 | 16:S:27:GLU:CB | 2.59 | 0.86 |
| 16:S:22:TRP:HH2 | 16:S:38:MET:O | 1.56 | 0.86 |
| 16:S:83:SER:O | 16:S:87:GLN:HG3 | 1.74 | 0.86 |
| 16:S:29:VAL:HA | 16:S:90:PRO:HB2 | 1.57 | 0.86 |
| 17:Y:42:ARG:HA | 17:Y:82:TYR:CZ | 2.10 | 0.86 |
| 2:B:16:TRP:CD1 | 2:B:44:CYS:CB | 2.52 | 0.86 |
| 3:P:276:ILE:HG22 | 3:P:277:ARG:H | 1.40 | 0.86 |
| 16:S:19:GLY:HA3 | 18:Z:134:GLN:CD | 1.96 | 0.86 |
| 16:S:29:VAL:CG1 | 18:Z:140:THR:HG21 | 2.05 | 0.86 |
| 6:H:653:LEU:HD22 | 9:K:523:ILE:HG21 | 1.58 | 0.86 |
| 12:N:570:ILE:HD13 | 12:N:633:ARG:HH12 | 1.41 | 0.86 |
| 12:N:570:ILE:HD13 | 12:N:633:ARG:NH1 | 1.91 | 0.86 |
| 16:S:82:ILE:CD1 | 16:S:124:LEU:CD2 | 2.54 | 0.85 |
| 16:S:71:GLY:CA | 16:S:74:PRO:HD2 | 2.05 | 0.85 |
| 16:S:29:VAL:CG1 | 18:Z:140:THR:CG2 | 2.54 | 0.85 |
| 1:A:1307:LEU:HD11 | 1:A:1582:ALA:HB2 | 1.58 | 0.85 |
| 9:K:472:LEU:HG | 9:K:481:THR:HG21 | 1.58 | 0.85 |
| 13:O:75:LEU:HD11 | 13:O:161:TYR:HE2 | 1.40 | 0.85 |
| 16:S:83:SER:HB2 | 16:S:87:GLN:NE2 | 1.91 | 0.85 |
| 8:I:286:ARG:HE | 8:I:333:LEU:HD13 | 1.40 | 0.85 |
| 8:I:413:ASN:CA | 8:I:447:PHE:CE1 | 2.56 | 0.85 |
| 12:N:180:PHE:CD1 | 12:N:299:TRP:HZ3 | 1.90 | 0.85 |
| 1:A:1619:LEU:HD21 | 1:A:1697:LEU:HD22 | 1.58 | 0.85 |
| 3:C:259:PHE:HB3 | 3:C:265:ILE:CD1 | 2.06 | 0.85 |
| 8:I:73:TRP:CZ2 | 8:I:80:LEU:HD22 | 2.11 | 0.85 |
| 17:X:442:GLN:HG2 | 17:X:472:ARG:CG | 2.06 | 0.85 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:16:TRP:HE1 | 2:B:44:CYS:CB | 1.47 | 0.85 |
| 8:I:312:LYS:HG3 | 8:I:428:MET:SD | 2.16 | 0.85 |
| 8:I:301:GLN:C | 8:I:303:GLU:N | 2.29 | 0.85 |
| 16:S:19:GLY:N | 18:Z:134:GLN:NE2 | 2.25 | 0.85 |
| 8:I:300:VAL:HG21 | 8:I:456:PHE:HB3 | 1.59 | 0.85 |
| 10:L:86:ASP:HB3 | 10:L:89:TYR:HB2 | 1.58 | 0.85 |
| 17:X:462:LYS:HG2 | 17:X:485:LEU:HD13 | 1.57 | 0.85 |
| 13:O:75:LEU:HG | 13:O:161:TYR:CE2 | 2.12 | 0.84 |
| 6:F:571:CYS:SG | 6:F:606:LEU:HD12 | 2.17 | 0.84 |
| 8:I:337:ILE:CG2 | 8:I:341:TYR:HE2 | 1.89 | 0.84 |
| 16:S:29:VAL:HG12 | 18:Z:140:THR:HG22 | 1.58 | 0.84 |
| 16:S:22:TRP:HH2 | 16:S:38:MET:C | 1.79 | 0.84 |
| 16:S:20:ASP:N | 18:Z:134:GLN:NE2 | 2.25 | 0.84 |
| 17:Y:452:LEU:HD21 | 17:Y:457:THR:O | 1.75 | 0.84 |
| 13:O:114:ASP:O | 13:O:117:ASP:OD1 | 1.93 | 0.84 |
| 16:S:78:TRP:CZ3 | 16:S:105:ALA:HA | 2.13 | 0.84 |
| 17:X:452:LEU:HD21 | 17:X:457:THR:O | 1.75 | 0.84 |
| 9:J:254:THR:HG23 | 9:J:271:HIS:CD2 | 2.11 | 0.84 |
| 14:Q:185:TYR:CG | 16:S:27:GLU:HB3 | 2.12 | 0.84 |
| 8:I:262:LEU:HA | 8:I:265:ILE:HG22 | 1.59 | 0.84 |
| 12:N:395:ASP:HB2 | 12:N:397:ILE:H | 1.43 | 0.83 |
| 8:I:310:TRP:HB2 | 8:I:313:ALA:HA | 1.59 | 0.83 |
| 13:O:75:LEU:CD2 | 13:O:161:TYR:CE2 | 2.61 | 0.83 |
| 8:I:430:GLU:CG | 14:Q:429:LYS:CG | 2.55 | 0.83 |
| 8:I:430:GLU:CG | 14:Q:429:LYS:HG2 | 2.08 | 0.83 |
| 16:S:58:GLN:CG | 16:S:62:PHE:CE2 | 2.56 | 0.83 |
| 17:Y:474:ASP:OD1 | 17:Y:502:ALA:HA | 1.78 | 0.83 |
| 9:J:476:PRO:HG2 | 3:P:182:LEU:HG | 1.60 | 0.83 |
| 13:O:539:ASN:HD22 | 13:O:542:GLU:HB2 | 1.44 | 0.83 |
| 13:O:75:LEU:HB3 | 13:O:79:TYR:CE2 | 2.14 | 0.83 |
| 14:Q:168:ILE:HG23 | 14:Q:472:CYS:HA | 1.61 | 0.83 |
| 13:O:216:LEU:HD22 | 13:O:256:LEU:HD12 | 1.59 | 0.83 |
| 17:X:474:ASP:OD1 | 17:X:502:ALA:HA | 1.78 | 0.83 |
| 8:I:295:ASN:O | 8:I:316:GLU:CB | 2.27 | 0.82 |
| 16:S:38:MET:CE | 18:Z:199:TYR:HE2 | 1.82 | 0.82 |
| 8:I:290:PHE:HE1 | 8:I:324:GLN:HB3 | 1.42 | 0.82 |
| 8:I:276:TRP:CH2 | 8:I:476:GLY:HA3 | 2.14 | 0.82 |
| 15:R:98:GLU:HG3 | 15:R:101:PRO:HD3 | 1.58 | 0.82 |
| 3:C:53:LYS:HD3 | 3:P:96:VAL:HG21 | 1.61 | 0.82 |
| 8:I:34:LEU:HD12 | 8:I:46:LEU:HD21 | 1.61 | 0.82 |
| 9:K:222:GLU:OE1 | 9:K:228:GLN:CD | 2.17 | 0.82 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:309:LEU:O | 13:O:127:HIS:HB2 | 1.80 | 0.82 |
| 8:I:349:ILE:HD12 | 13:O:407:LEU:HA | 1.62 | 0.82 |
| 16:S:29:VAL:HA | 16:S:36:ARG:NH1 | 1.93 | 0.82 |
| 6:F:537:GLU:OE1 | 6:F:602:TYR:HB3 | 1.79 | 0.82 |
| 16:S:30:GLN:H | 16:S:36:ARG:HH22 | 1.23 | 0.82 |
| 3:C:316:LEU:HD21 | 3:C:340:TYR:HA | 1.62 | 0.81 |
| 17:Y:442:GLN:HG2 | 17:Y:472:ARG:CG | 2.07 | 0.81 |
| 3:C:148:ASN:HB3 | 3:C:151:LEU:HG | 1.62 | 0.81 |
| 9:K:192:LYS:HG2 | 9:K:198:GLN:HG3 | 1.62 | 0.81 |
| 16:S:132:CYS:HA | 16:S:133:ASN:CB | 2.10 | 0.81 |
| 17:Y:42:ARG:HA | 17:Y:82:TYR:HE2 | 1.37 | 0.81 |
| 16:S:163:GLU:HB2 | 16:S:196:PHE:HE1 | 1.45 | 0.81 |
| 13:O:75:LEU:CG | 13:O:161:TYR:CZ | 2.63 | 0.81 |
| 16:S:132:CYS:HB3 | 16:S:135:PRO:CD | 2.10 | 0.81 |
| 1:A:1799:ARG:HD3 | 1:A:1805:MET:HB3 | 1.63 | 0.81 |
| 17:X:267:LEU:HD11 | 17:Y:59:LEU:HD11 | 1.60 | 0.81 |
| 17:X:442:GLN:CD | 17:X:472:ARG:CZ | 2.42 | 0.81 |
| 14:Q:128:ALA:CB | 18:Z:156:TYR:CZ | 2.63 | 0.81 |
| 12:N:180:PHE:CE1 | 12:N:299:TRP:CZ3 | 2.69 | 0.80 |
| 14:Q:163:LYS:HB2 | 14:Q:167:TYR:CD2 | 2.16 | 0.80 |
| 17:Y:305:ILE:CG2 | 17:Y:340:GLU:OE1 | 2.29 | 0.80 |
| 17:Y:366:ILE:HD11 | 17:Y:379:LYS:HD2 | 1.61 | 0.80 |
| 16:S:86:GLU:CG | 16:S:98:MET:HE3 | 2.11 | 0.80 |
| 8:I:337:ILE:HG23 | 8:I:341:TYR:HE2 | 1.45 | 0.80 |
| 17:X:230:VAL:CG2 | 17:Y:36:ASN:HB3 | 2.11 | 0.80 |
| 6:H:656:MET:HE2 | 6:H:660:LYS:CE | 2.09 | 0.80 |
| 8:I:32:ARG:HD3 | 12:N:388:HIS:CE1 | 2.16 | 0.80 |
| 17:X:230:VAL:HG21 | 17:Y:36:ASN:HB3 | 1.62 | 0.80 |
| 14:Q:163:LYS:HB2 | 14:Q:167:TYR:HD2 | 1.46 | 0.80 |
| 2:B:16:TRP:O | 2:B:32:GLY:HA2 | 1.82 | 0.80 |
| 9:J:37:PRO:HB3 | 9:J:69:TYR:CE2 | 2.16 | 0.80 |
| 2:B:17:VAL:HG13 | 2:B:31:ASN:HD22 | 1.47 | 0.80 |
| 2:B:17:VAL:HG11 | 12:N:632:MET:HB3 | 1.64 | 0.80 |
| 16:S:65:GLU:O | 16:S:69:TYR:CD2 | 2.34 | 0.80 |
| 2:B:17:VAL:HG21 | 12:N:634:THR:H | 1.46 | 0.79 |
| 1:A:1232:ILE:HD11 | 1:A:1235:LEU:HD22 | 1.63 | 0.79 |
| 17:X:442:GLN:CG | 17:X:472:ARG:HD2 | 2.10 | 0.79 |
| 8:I:56:TRP:HZ3 | 8:I:58:PHE:HB2 | 1.46 | 0.79 |
| 8:I:312:LYS:N | 8:I:428:MET:SD | 2.55 | 0.79 |
| 8:I:293:GLU:CB | 8:I:324:GLN:NE2 | 2.46 | 0.79 |
| 16:S:145:GLN:HE22 | 16:S:296:ILE:CB | 1.94 | 0.79 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:S:41:LEU:HD11 | 18:Z:141:PHE:HB3 | 1.63 | 0.79 |
| 1:A:1209:LEU:HD22 | 1:A:1228:LEU:HD23 | 1.64 | 0.79 |
| 13:O:32:PRO:O | 13:O:35:ILE:HG22 | 1.82 | 0.79 |
| 16:S:71:GLY:O | 16:S:74:PRO:CD | 2.29 | 0.79 |
| 16:S:68:PHE:HZ | 16:S:81:TYR:CB | 1.95 | 0.79 |
| 17:Y:84:ALA:HB1 | 17:Y:100:TYR:CE2 | 2.17 | 0.79 |
| 2:B:43:ASP:HA | 12:N:630:LYS:HE3 | 1.65 | 0.79 |
| 8:I:290:PHE:HD1 | 8:I:324:GLN:OE1 | 1.66 | 0.79 |
| 12:N:368:THR:OG1 | 12:N:369:ASP:HA | 1.82 | 0.78 |
| 16:S:30:GLN:O | 16:S:36:ARG:NH2 | 2.16 | 0.78 |
| 6:F:507:ARG:HD3 | 6:F:538:ILE:HD13 | 1.65 | 0.78 |
| 8:I:306:HIS:ND1 | 8:I:317:LEU:HG | 1.98 | 0.78 |
| 12:N:577:GLU:HB3 | 12:N:625:LYS:HE3 | 1.64 | 0.78 |
| 9:J:185:LEU:HD12 | 9:J:209:LEU:HD21 | 1.64 | 0.78 |
| 8:I:276:TRP:CH2 | 8:I:280:LEU:HD22 | 2.19 | 0.78 |
| 14:Q:128:ALA:CB | 18:Z:156:TYR:CE2 | 2.67 | 0.78 |
| 8:I:413:ASN:O | 8:I:447:PHE:HE1 | 1.65 | 0.78 |
| 1:A:873:VAL:HG21 | 1:A:951:ILE:HG21 | 1.66 | 0.78 |
| 3:C:493:TYR:CE2 | 3:C:497:ILE:HD11 | 2.19 | 0.78 |
| 6:H:527:ARG:HB3 | 17:Y:302:PRO:HB3 | 1.66 | 0.78 |
| 13:O:581:ILE:HD13 | 13:O:611:SER:HB3 | 1.66 | 0.78 |
| 15:R:110:LYS:HE2 | 15:R:114:LYS:HB2 | 1.66 | 0.78 |
| 9:J:445:GLU:HG2 | 9:J:446:PRO:HD3 | 1.67 | 0.77 |
| 1:A:1656:LEU:HD12 | 1:A:1656:LEU:H | 1.49 | 0.77 |
| 6:H:128:THR:HG21 | 6:H:130:ARG:NH1 | 2.00 | 0.77 |
| 8:I:56:TRP:CE3 | 8:I:98:PRO:CB | 2.67 | 0.77 |
| 15:R:115:ALA:O | 15:R:119:ASN:HB2 | 1.84 | 0.77 |
| 16:S:163:GLU:CB | 16:S:196:PHE:HE1 | 1.97 | 0.77 |
| 9:K:487:TYR:OH | 7:W:15:ASP:O | 2.01 | 0.77 |
| 16:S:82:ILE:HD12 | 16:S:124:LEU:CD2 | 2.13 | 0.77 |
| 2:B:14:TRP:CZ2 | 2:B:42:ASP:OD1 | 2.38 | 0.77 |
| 2:B:16:TRP:CZ2 | 2:B:45:PRO:N | 2.41 | 0.77 |
| 9:J:383:ASN:HB3 | 9:J:386:LEU:HD13 | 1.65 | 0.77 |
| 1:A:1097:THR:HG23 | 13:O:340:LEU:HB3 | 1.66 | 0.77 |
| 17:X:442:GLN:CD | 17:X:472:ARG:CD | 2.52 | 0.77 |
| 8:I:290:PHE:O | 8:I:320:LEU:CD1 | 2.32 | 0.77 |
| 16:S:82:ILE:HD12 | 16:S:124:LEU:HD23 | 1.66 | 0.77 |
| 8:I:326:THR:O | 8:I:330:LEU:N | 2.18 | 0.77 |
| 12:N:281:TYR:CE2 | 12:N:356:PRO:HB2 | 2.20 | 0.77 |
| 1:A:1791:ILE:HB | 13:O:598:THR:HG21 | 1.66 | 0.77 |
| 3:C:238:TYR:HD1 | 3:C:243:LEU:HD12 | 1.49 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:S:163:GLU:HB2 | 16:S:196:PHE:CE1 | 2.20 | 0.77 |
| 3:C:373:HIS:CE1 | 15:R:79:TYR:HA | 2.20 | 0.76 |
| 8:I:304:PHE:CZ | 8:I:452:LEU:HG | 2.19 | 0.76 |
| 12:N:362:LYS:CA | 12:N:410:LEU:CD2 | 2.62 | 0.76 |
| 16:S:201:SER:O | 16:S:205:LEU:HG | 1.86 | 0.76 |
| 17:X:52:ASN:HD22 | 17:Y:202:ALA:HB1 | 1.50 | 0.76 |
| 14:Q:132:ARG:HB2 | 18:Z:170:SER:CB | 2.13 | 0.76 |
| 1:A:1248:ASN:O | 1:A:1251:VAL:HG22 | 1.84 | 0.76 |
| 8:I:297:THR:N | 8:I:316:GLU:OE2 | 2.19 | 0.76 |
| 12:N:289:PHE:O | 12:N:291:LYS:N | 2.18 | 0.76 |
| 12:N:435:VAL:HA | 12:N:438:ILE:HD12 | 1.67 | 0.76 |
| 2:B:14:TRP:CE2 | 2:B:42:ASP:OD1 | 2.39 | 0.76 |
| 8:I:679:ASP:OD1 | 8:I:703:ARG:NH2 | 2.18 | 0.76 |
| 12:N:666:ILE:HG12 | 12:N:681:LEU:HD21 | 1.66 | 0.76 |
| 16:S:29:VAL:C | 16:S:36:ARG:HH22 | 1.88 | 0.76 |
| 2:B:16:TRP:CZ2 | 2:B:44:CYS:N | 2.53 | 0.76 |
| 8:I:290:PHE:CD1 | 8:I:324:GLN:OE1 | 2.38 | 0.76 |
| 10:L:40:PHE:HA | 10:L:44:GLN:OE1 | 1.86 | 0.76 |
| 12:N:670:PHE:CE1 | 12:N:715:VAL:HB | 2.20 | 0.76 |
| 16:S:132:CYS:HB3 | 16:S:135:PRO:N | 2.00 | 0.76 |
| 1:A:1229:SER:HB3 | 1:A:1236:LEU:HA | 1.67 | 0.76 |
| 12:N:425:ARG:HG2 | 12:N:425:ARG:NH1 | 1.97 | 0.76 |
| 16:S:82:ILE:CD1 | 16:S:124:LEU:HD23 | 2.16 | 0.76 |
| 13:O:411:LYS:HE2 | 13:O:412:HIS:CE1 | 2.20 | 0.76 |
| 14:Q:128:ALA:HB3 | 18:Z:156:TYR:OH | 1.85 | 0.76 |
| 15:R:225:PRO:HB2 | 16:S:166:GLU:HB2 | 1.68 | 0.76 |
| 1:A:1196:TYR:CB | 1:A:1208:LEU:HD11 | 2.16 | 0.76 |
| 7:G:6:PRO:HB3 | 9:J:406:HIS:CD2 | 2.21 | 0.76 |
| 16:S:33:ARG:HB2 | 16:S:130:ARG:NH1 | 2.01 | 0.76 |
| 8:I:290:PHE:O | 8:I:320:LEU:HD13 | 1.85 | 0.75 |
| 9:K:174:HIS:HA | 9:K:211:LYS:NZ | 2.00 | 0.75 |
| 12:N:663:GLN:HE21 | 12:N:695:ARG:HG3 | 1.51 | 0.75 |
| 15:R:225:PRO:CB | 16:S:166:GLU:HB2 | 2.16 | 0.75 |
| 1:A:1254:VAL:HG11 | 1:A:1298:ALA:HA | 1.68 | 0.75 |
| 8:I:48:ARG:HG3 | 8:I:55:VAL:HG22 | 1.68 | 0.75 |
| 13:O:356:ASP:HA | 13:O:357:SER:HB2 | 1.69 | 0.75 |
| 16:S:132:CYS:SG | 16:S:135:PRO:CA | 2.74 | 0.75 |
| 3:C:493:TYR:CZ | 3:C:497:ILE:HD11 | 2.21 | 0.75 |
| 8:I:293:GLU:CB | 8:I:324:GLN:HE21 | 1.99 | 0.75 |
| 13:O:163:GLN:O | 13:O:167:LYS:HG3 | 1.85 | 0.75 |
| 3:P:290:ARG:HH21 | 3:P:319:LEU:HD12 | 1.51 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:332:THR:CA | 9:J:363:LEU:HD21 | 2.15 | 0.75 |
| 10:L:126:ASP:OD2 | 10:L:130:LYS:O | 2.05 | 0.75 |
| 12:N:289:PHE:HA | 12:N:292:TRP:HB3 | 1.68 | 0.75 |
| 6:F:730:LYS:HE2 | 6:F:740:TYR:HE1 | 1.50 | 0.75 |
| 12:N:180:PHE:HD1 | 12:N:299:TRP:HZ3 | 1.34 | 0.75 |
| 1:A:1375:TYR:HB3 | 1:A:1378:THR:HG21 | 1.69 | 0.75 |
| 9:J:19:TYR:CD1 | 9:J:49:LEU:HD13 | 2.21 | 0.75 |
| 16:S:76:ASP:O | 16:S:77:VAL:CB | 2.33 | 0.75 |
| 9:J:406:HIS:CE1 | 9:J:450:ASN:HD22 | 2.05 | 0.75 |
| 16:S:30:GLN:H | 16:S:91:GLN:CB | 1.97 | 0.75 |
| 1:A:873:VAL:HG21 | 1:A:951:ILE:CG2 | 2.17 | 0.74 |
| 16:S:86:GLU:HG2 | 16:S:98:MET:HE3 | 1.68 | 0.74 |
| 9:K:174:HIS:CE1 | 9:K:211:LYS:HD3 | 2.22 | 0.74 |
| 3:C:327:ASP:O | 3:C:333:THR:HG21 | 1.87 | 0.74 |
| 8:I:224:SER:CB | 8:I:229:SER:HA | 2.17 | 0.74 |
| 8:I:305:MET:HB2 | 13:O:61:ASN:HD21 | 1.51 | 0.74 |
| 12:N:120:SER:O | 12:N:124:PRO:HD3 | 1.87 | 0.74 |
| 9:J:451:LEU:HD12 | 9:J:467:TYR:CE2 | 2.22 | 0.74 |
| 9:K:184:LEU:O | 9:K:188:LEU:HD23 | 1.87 | 0.74 |
| 13:O:544:VAL:HG23 | 13:O:567:LEU:HG | 1.67 | 0.74 |
| 16:S:129:GLY:O | 16:S:132:CYS:SG | 2.45 | 0.74 |
| 16:S:22:TRP:CE3 | 16:S:41:LEU:CB | 2.68 | 0.74 |
| 9:J:465:LEU:HA | 9:J:488:ILE:HD12 | 1.67 | 0.74 |
| 16:S:20:ASP:N | 18:Z:134:GLN:HE21 | 1.85 | 0.74 |
| 1:A:629:LEU:HD11 | 1:A:634:ALA:HB2 | 1.69 | 0.74 |
| 13:O:312:CYS:SG | 13:O:350:LEU:HD21 | 2.28 | 0.74 |
| 6:F:653:LEU:HA | 6:F:656:MET:SD | 2.27 | 0.74 |
| 6:F:500:TRP:HB3 | 6:H:30:ARG:NH2 | 2.02 | 0.74 |
| 8:I:26:LEU:HB3 | 8:I:37:LEU:CB | 2.17 | 0.74 |
| 8:I:430:GLU:CG | 14:Q:429:LYS:HG3 | 2.17 | 0.74 |
| 16:S:30:GLN:CA | 16:S:91:GLN:HB2 | 2.17 | 0.74 |
| 17:X:52:ASN:ND2 | 17:Y:202:ALA:HB1 | 2.01 | 0.74 |
| 8:I:279:ILE:HB | 8:I:340:SER:HB2 | 1.69 | 0.74 |
| 17:Y:452:LEU:HD22 | 17:Y:461:ALA:H | 1.49 | 0.74 |
| 12:N:630:LYS:HD3 | 12:N:633:ARG:NH1 | 2.03 | 0.73 |
| 16:S:86:GLU:CG | 16:S:98:MET:CE | 2.64 | 0.73 |
| 17:X:452:LEU:HD22 | 17:X:461:ALA:H | 1.49 | 0.73 |
| 8:I:417:PHE:HD2 | 8:I:448:VAL:HG22 | 1.53 | 0.73 |
| 13:O:75:LEU:HD11 | 13:O:161:TYR:CD2 | 2.23 | 0.73 |
| 16:S:41:LEU:O | 16:S:45:LEU:HD12 | 1.88 | 0.73 |
| 3:P:327:ASP:O | 3:P:333:THR:HG21 | 1.89 | 0.73 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:S:20:ASP:OD1 | 18:Z:184:ARG:CD | 2.35 | 0.73 |
| 13:O:405:SER:O | 13:O:409:HIS:CD2 | 2.41 | 0.73 |
| 16:S:163:GLU:CD | 16:S:196:PHE:HE1 | 1.92 | 0.73 |
| 14:Q:186:TYR:CZ | 16:S:27:GLU:HB2 | 2.23 | 0.73 |
| 12:N:626:TYR:CD2 | 12:N:633:ARG:HB3 | 2.22 | 0.73 |
| 3:P:251:TYR:OH | 3:P:268:GLN:HG3 | 1.88 | 0.73 |
| 6:F:550:VAL:HG21 | 9:K:289:HIS:HB3 | 1.70 | 0.73 |
| 10:L:44:GLN:HA | 10:L:47:ASP:OD2 | 1.88 | 0.73 |
| 10:L:74:VAL:HG21 | 10:L:137:ILE:HD11 | 1.68 | 0.73 |
| 12:N:542:VAL:HG11 | 12:N:558:GLU:HG2 | 1.71 | 0.73 |
| 13:O:539:ASN:HD22 | 13:O:542:GLU:CB | 2.01 | 0.73 |
| 1:A:776:ASN:HD22 | 1:A:779:MET:HG2 | 1.54 | 0.72 |
| 8:I:177:VAL:HG12 | 8:I:208:LEU:HD13 | 1.70 | 0.72 |
| 8:I:81:ALA:HB2 | 8:I:92:LEU:HB3 | 1.71 | 0.72 |
| 12:N:542:VAL:HG11 | 12:N:558:GLU:CG | 2.17 | 0.72 |
| 13:O:291:ASN:O | 13:O:336:ASP:HB2 | 1.89 | 0.72 |
| 16:S:193:HIS:NE2 | 16:S:197:GLN:OE1 | 2.22 | 0.72 |
| 16:S:40:THR:HG21 | 16:S:87:GLN:HB3 | 1.70 | 0.72 |
| 6:H:707:PHE:HB2 | 6:H:729:LEU:HD11 | 1.71 | 0.72 |
| 8:I:26:LEU:CB | 8:I:37:LEU:HB3 | 2.19 | 0.72 |
| 17:X:407:LEU:HD13 | 17:X:443:THR:HG21 | 1.72 | 0.72 |
| 8:I:302:ASP:CA | 8:I:303:GLU:N | 2.51 | 0.72 |
| 9:J:24:PHE:CE1 | 9:J:28:LYS:HE3 | 2.24 | 0.72 |
| 16:S:163:GLU:CG | 16:S:196:PHE:HE1 | 2.02 | 0.72 |
| 16:S:30:GLN:CA | 16:S:36:ARG:NH2 | 2.52 | 0.72 |
| 1:A:1138:HIS:HE1 | 1:A:1604:GLN:HE21 | 1.37 | 0.72 |
| 1:A:482:VAL:HG12 | 1:A:487:THR:O | 1.90 | 0.72 |
| 9:K:185:LEU:HA | 9:K:188:LEU:HD21 | 1.70 | 0.72 |
| 16:S:22:TRP:HZ3 | 16:S:41:LEU:CG | 2.02 | 0.72 |
| 17:Y:442:GLN:HG2 | 17:Y:472:ARG:HG3 | 1.71 | 0.72 |
| 3:C:358:LEU:HD21 | 3:C:368:TRP:CD2 | 2.24 | 0.72 |
| 9:J:441:VAL:O | 9:J:442:ASP:HB3 | 1.89 | 0.72 |
| 9:K:63:ARG:HB2 | 9:K:65:LEU:CD1 | 2.19 | 0.72 |
| 16:S:132:CYS:CB | 16:S:135:PRO:CG | 2.64 | 0.72 |
| 6:F:145:ASN:HB2 | 6:F:146:PRO:C | 2.10 | 0.72 |
| 6:H:754:HIS:CE1 | 6:H:755:LEU:HD13 | 2.25 | 0.72 |
| 1:A:1753:TYR:HD2 | 13:O:643:LEU:HD12 | 1.53 | 0.72 |
| 1:A:1284:GLU:HB2 | 1:A:1350:TYR:CE2 | 2.24 | 0.72 |
| 8:I:674:VAL:O | 8:I:703:ARG:NH1 | 2.23 | 0.72 |
| 12:N:520:ARG:HD2 | 12:N:556:PHE:CD1 | 2.25 | 0.72 |
| 3:C:238:TYR:CD1 | 3:C:243:LEU:HD12 | 2.24 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:72:ALA:O | 8:I:80:LEU:HD12 | 1.89 | 0.72 |
| 11:M:17:ASP:HA | 11:M:20:ARG:HG2 | 1.71 | 0.72 |
| 16:S:30:GLN:CD | 16:S:91:GLN:HG3 | 2.10 | 0.72 |
| 16:S:30:GLN:HB2 | 16:S:91:GLN:HA | 1.72 | 0.72 |
| 8:I:48:ARG:HG3 | 8:I:55:VAL:CG2 | 2.20 | 0.72 |
| 13:O:620:ALA:O | 13:O:624:VAL:HG23 | 1.90 | 0.72 |
| 8:I:65:GLY:H | 8:I:84:LEU:HG | 1.54 | 0.71 |
| 3:C:242:GLN:O | 3:C:244:ILE:HG13 | 1.91 | 0.71 |
| 16:S:163:GLU:CG | 16:S:196:PHE:CE1 | 2.73 | 0.71 |
| 2:B:16:TRP:CH2 | 12:N:630:LYS:HE2 | 2.24 | 0.71 |
| 1:A:1786:MET:CE | 1:A:1786:MET:HA | 2.21 | 0.71 |
| 3:C:36:LEU:HD21 | 3:C:58:LEU:HB2 | 1.73 | 0.71 |
| 1:A:1089:LEU:HD11 | 1:A:1611:VAL:CG2 | 2.20 | 0.71 |
| 3:C:414:MET:HG2 | 13:O:330:ILE:HD11 | 1.73 | 0.71 |
| 8:I:88:LYS:O | 8:I:106:VAL:HG22 | 1.90 | 0.71 |
| 8:I:294:LYS:CB | 8:I:320:LEU:HB2 | 2.20 | 0.71 |
| 12:N:395:ASP:OD1 | 12:N:398:THR:N | 2.24 | 0.71 |
| 9:K:406:HIS:ND1 | 7:W:6:PRO:HB3 | 2.05 | 0.71 |
| 17:Y:45:ALA:HB3 | 17:Y:82:TYR:CE2 | 2.25 | 0.71 |
| 1:A:116:ALA:O | 13:O:266:ASP:HA | 1.90 | 0.71 |
| 6:F:656:MET:HG3 | 17:Y:526:GLN:HB2 | 1.72 | 0.71 |
| 12:N:60:GLU:O | 12:N:63:ALA:HB2 | 1.91 | 0.71 |
| 3:P:355:GLN:HA | 3:P:358:LEU:HD23 | 1.70 | 0.71 |
| 16:S:30:GLN:HB2 | 16:S:91:GLN:HB2 | 1.73 | 0.71 |
| 8:I:116:MET:SD | 8:I:210:LEU:HG | 2.31 | 0.71 |
| 12:N:120:SER:O | 12:N:124:PRO:CD | 2.39 | 0.71 |
| 16:S:83:SER:HB2 | 16:S:87:GLN:HE21 | 1.56 | 0.71 |
| 1:A:1469:CYS:HB2 | 1:A:1488:LEU:CD2 | 2.19 | 0.71 |
| 9:K:45:GLN:HE21 | 9:K:45:GLN:HA | 1.54 | 0.71 |
| 12:N:343:GLU:O | 12:N:347:ILE:N | 2.23 | 0.71 |
| 16:S:38:MET:HE1 | 18:Z:199:TYR:CE2 | 2.21 | 0.71 |
| 1:A:1624:VAL:HG22 | 1:A:1698:TYR:HD2 | 1.56 | 0.71 |
| 7:G:6:PRO:HB3 | 9:J:406:HIS:HD2 | 1.55 | 0.71 |
| 8:I:300:VAL:HG21 | 8:I:456:PHE:HB2 | 1.73 | 0.71 |
| 8:I:500:PHE:HE2 | 8:I:507:LEU:HD12 | 1.55 | 0.71 |
| 12:N:362:LYS:CG | 12:N:410:LEU:HD23 | 2.20 | 0.71 |
| 17:Y:42:ARG:CG | 17:Y:82:TYR:OH | 2.39 | 0.71 |
| 2:B:14:TRP:CB | 2:B:15:LEU:HB2 | 2.21 | 0.71 |
| 17:X:442:GLN:HE21 | 17:X:472:ARG:HG3 | 1.55 | 0.71 |
| 9:K:222:GLU:HB3 | 9:K:228:GLN:OE1 | 1.90 | 0.70 |
| 12:N:563:ASP:OD2 | 12:N:597:SER:HB3 | 1.90 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:N:425:ARG:CZ | 12:N:507:SER:HB2 | 2.21 | 0.70 |
| 14:Q:410:HIS:CD2 | 14:Q:475:LEU:HD11 | 2.26 | 0.70 |
| 15:R:247:SER:HB2 | 16:S:170:LYS:NZ | 2.05 | 0.70 |
| 16:S:64:TYR:O | 16:S:68:PHE:CD2 | 2.44 | 0.70 |
| 16:S:66:ILE:CA | 16:S:69:TYR:HD2 | 2.02 | 0.70 |
| 16:S:68:PHE:CZ | 16:S:81:TYR:CB | 2.75 | 0.70 |
| 1:A:1645:GLU:HG3 | 1:A:1646:GLN:H | 1.56 | 0.70 |
| 13:O:706:CYS:HB3 | 13:O:709:ARG:HB3 | 1.73 | 0.70 |
| 1:A:801:PRO:HB2 | 1:A:841:PRO:HG3 | 1.74 | 0.70 |
| 3:C:39:ILE:HD13 | 3:C:201:LEU:HB2 | 1.73 | 0.70 |
| 8:I:269:LEU:CB | 8:I:526:LYS:HZ2 | 2.05 | 0.70 |
| 9:J:254:THR:CG2 | 9:J:271:HIS:CD2 | 2.75 | 0.70 |
| 13:O:127:HIS:O | 13:O:128:LYS:HB3 | 1.91 | 0.70 |
| 17:X:442:GLN:NE2 | 17:X:472:ARG:NE | 2.29 | 0.70 |
| 12:N:519:TYR:OH | 12:N:541:ASN:HB3 | 1.90 | 0.70 |
| 16:S:132:CYS:CB | 16:S:135:PRO:CD | 2.69 | 0.70 |
| 17:X:192:TYR:HA | 17:X:195:VAL:HG22 | 1.73 | 0.70 |
| 8:I:279:ILE:HB | 8:I:340:SER:CB | 2.22 | 0.70 |
| 9:J:465:LEU:HA | 9:J:488:ILE:CD1 | 2.20 | 0.70 |
| 13:O:479:GLU:O | 13:O:656:ALA:O | 2.09 | 0.70 |
| 1:A:1390:PRO:HG2 | 1:A:1396:LEU:HG | 1.74 | 0.70 |
| 9:K:417:GLU:HB2 | 9:K:420:THR:OG1 | 1.92 | 0.70 |
| 3:P:39:ILE:HD13 | 3:P:201:LEU:HB2 | 1.72 | 0.70 |
| 17:X:442:GLN:NE2 | 17:X:472:ARG:HG3 | 2.07 | 0.70 |
| 1:A:482:VAL:HG11 | 1:A:485:ILE:HD12 | 1.74 | 0.70 |
| 15:R:74:PRO:HB2 | 15:R:75:GLY:HA2 | 1.72 | 0.70 |
| 8:I:306:HIS:CE1 | 8:I:313:ALA:O | 2.44 | 0.70 |
| 8:I:231:VAL:HG21 | 8:I:557:TYR:CZ | 2.27 | 0.70 |
| 8:I:73:TRP:CG | 8:I:80:LEU:HD13 | 2.26 | 0.70 |
| 16:S:78:TRP:CE3 | 16:S:105:ALA:HB2 | 2.26 | 0.70 |
| 16:S:22:TRP:HH2 | 16:S:38:MET:HA | 1.38 | 0.70 |
| 16:S:25:SER:H | 16:S:45:LEU:HD21 | 1.57 | 0.70 |
| 6:H:761:SER:O | 6:H:765:ASP:HB2 | 1.92 | 0.70 |
| 9:J:475:ILE:HD11 | 9:J:478:ASN:HD22 | 1.57 | 0.70 |
| 8:I:312:LYS:HE2 | 8:I:428:MET:HA | 1.72 | 0.69 |
| 3:P:276:ILE:HG22 | 3:P:277:ARG:N | 2.06 | 0.69 |
| 16:S:79:ASP:OD2 | 16:S:120:ARG:HB3 | 1.91 | 0.69 |
| 17:Y:186:ARG:HA | 17:Y:189:VAL:HG12 | 1.75 | 0.69 |
| 2:B:16:TRP:HB3 | 2:B:33:CYS:N | 2.08 | 0.69 |
| 3:C:416:PHE:HB2 | 3:C:446:LEU:HD11 | 1.74 | 0.69 |
| 8:I:290:PHE:HE1 | 8:I:324:GLN:CB | 2.05 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:252:GLN:O | 3:P:255:ILE:HG22 | 1.92 | 0.69 |
| 17:Y:192:TYR:HA | 17:Y:195:VAL:HG22 | 1.74 | 0.69 |
| 1:A:980:ARG:NH1 | 1:A:1674:TRP:CD1 | 2.61 | 0.69 |
| 8:I:290:PHE:HA | 8:I:320:LEU:CD1 | 2.22 | 0.69 |
| 8:I:289:LYS:CG | 8:I:324:GLN:OE1 | 2.38 | 0.69 |
| 3:C:358:LEU:HD13 | 3:C:367:ALA:HB3 | 1.75 | 0.69 |
| 8:I:46:LEU:HD22 | 8:I:56:TRP:HE1 | 1.58 | 0.69 |
| 9:J:185:LEU:HD13 | 9:J:206:GLU:OE1 | 1.92 | 0.69 |
| 9:J:439:VAL:HG21 | 9:J:448:LEU:HD21 | 1.73 | 0.69 |
| 13:O:657:ILE:HA | 13:O:660:LYS:CB | 2.22 | 0.69 |
| 16:S:22:TRP:CH2 | 16:S:38:MET:C | 2.60 | 0.69 |
| 1:A:1332:GLY:O | 1:A:1358:ILE:HG13 | 1.92 | 0.69 |
| 10:L:105:LEU:HD12 | 10:L:138:GLN:OE1 | 1.93 | 0.69 |
| 16:S:195:GLN:O | 16:S:199:ARG:HG3 | 1.91 | 0.69 |
| 17:Y:503:LEU:O | 17:Y:506:GLN:NE2 | 2.25 | 0.69 |
| 14:Q:131:LEU:HD13 | 18:Z:163:VAL:HG11 | 1.74 | 0.69 |
| 15:R:112:HIS:NE2 | 15:R:116:TRP:HZ3 | 1.91 | 0.69 |
| 6:F:554:VAL:HG21 | 9:K:286:TYR:HD1 | 1.56 | 0.69 |
| 8:I:574:PHE:HE2 | 8:I:576:TRP:HB2 | 1.57 | 0.69 |
| 12:N:350:ASP:CB | 12:N:351:PHE:HA | 2.23 | 0.69 |
| 4:D:8:LEU:HD23 | 13:O:420:ILE:HD11 | 1.73 | 0.69 |
| 6:H:168:PHE:CB | 6:H:467:ARG:HD3 | 2.23 | 0.69 |
| 6:H:653:LEU:CD2 | 9:K:523:ILE:HG21 | 2.22 | 0.69 |
| 13:O:539:ASN:ND2 | 13:O:542:GLU:HB2 | 2.08 | 0.69 |
| 16:S:22:TRP:HZ3 | 16:S:41:LEU:CD1 | 2.04 | 0.69 |
| 6:H:730:LYS:HD3 | 6:H:740:TYR:HE1 | 1.56 | 0.69 |
| 8:I:214:LEU:O | 8:I:238:THR:OG1 | 2.11 | 0.69 |
| 14:Q:166:ARG:NH2 | 14:Q:413:GLU:OE1 | 2.24 | 0.69 |
| 16:S:22:TRP:CZ3 | 16:S:41:LEU:HB3 | 2.25 | 0.69 |
| 1:A:763:PHE:CD1 | 1:A:793:LEU:HD22 | 2.29 | 0.68 |
| 2:B:17:VAL:O | 2:B:30:PHE:O | 2.10 | 0.68 |
| 6:H:685:SER:O | 6:H:689:LEU:HD12 | 1.92 | 0.68 |
| 12:N:597:SER:OG | 12:N:600:PHE:HB2 | 1.93 | 0.68 |
| 3:C:434:ARG:HD2 | 15:R:80:ILE:HD13 | 1.74 | 0.68 |
| 16:S:71:GLY:HA2 | 16:S:74:PRO:HD2 | 1.75 | 0.68 |
| 4:D:16:LEU:H | 4:D:16:LEU:HD23 | 1.57 | 0.68 |
| 12:N:139:GLY:C | 12:N:141:LEU:H | 1.97 | 0.68 |
| 17:X:445:THR:O | 17:X:449:THR:HG23 | 1.93 | 0.68 |
| 6:F:133:LYS:HA | 6:F:136:GLU:OE1 | 1.94 | 0.68 |
| 12:N:769:SER:OG | 12:N:772:ARG:HD3 | 1.93 | 0.68 |
| 13:O:274:LEU:HD11 | 13:O:306:ASN:HB3 | 1.76 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:283:LEU:HD21 | 3:P:312:MET:CE | 2.24 | 0.68 |
| 16:S:29:VAL:CB | 16:S:36:ARG:HH12 | 2.05 | 0.68 |
| 17:Y:270:ASN:HB2 | 17:Y:273:LEU:HB3 | 1.74 | 0.68 |
| 1:A:1469:CYS:HB2 | 1:A:1488:LEU:HD21 | 1.76 | 0.68 |
| 9:J:35:GLU:CD | 9:J:63:ARG:HE | 1.96 | 0.68 |
| 9:K:285:PHE:HB2 | 9:K:308:TYR:CE1 | 2.28 | 0.68 |
| 9:K:384:SER:HB2 | 9:K:415:ASN:HD21 | 1.59 | 0.68 |
| 15:R:107:PRO:O | 15:R:109:LYS:HE2 | 1.93 | 0.68 |
| 17:Y:407:LEU:HD13 | 17:Y:443:THR:HG21 | 1.74 | 0.68 |
| 1:A:1089:LEU:HD11 | 1:A:1611:VAL:HG23 | 1.74 | 0.68 |
| 1:A:857:MET:CB | 1:A:858:PRO:HD3 | 2.24 | 0.68 |
| 12:N:516:ILE:HG13 | 12:N:554:MET:HE2 | 1.75 | 0.68 |
| 17:X:503:LEU:O | 17:X:506:GLN:NE2 | 2.27 | 0.68 |
| 17:Y:371:ASN:HD22 | 17:Y:371:ASN:H | 1.40 | 0.68 |
| 8:I:414:PHE:CE1 | 8:I:451:PHE:CE1 | 2.82 | 0.68 |
| 8:I:67:GLU:O | 8:I:85:ALA:N | 2.19 | 0.68 |
| 9:K:185:LEU:HD13 | 9:K:209:LEU:HD11 | 1.75 | 0.68 |
| 9:K:495:PHE:CZ | 9:K:525:MET:HG2 | 2.28 | 0.68 |
| 12:N:285:PHE:O | 12:N:289:PHE:HD1 | 1.76 | 0.68 |
| 12:N:350:ASP:HB3 | 12:N:351:PHE:HA | 1.76 | 0.68 |
| 2:B:16:TRP:HH2 | 12:N:630:LYS:HG2 | 1.59 | 0.68 |
| 7:G:4:ARG:HH21 | 9:J:345:ALA:HB1 | 1.57 | 0.68 |
| 1:A:980:ARG:NH2 | 1:A:1674:TRP:O | 2.27 | 0.68 |
| 3:C:388:TYR:HB2 | 3:C:405:LEU:HD13 | 1.76 | 0.68 |
| 6:F:554:VAL:HG21 | 9:K:286:TYR:CD1 | 2.29 | 0.68 |
| 8:I:360:LEU:HD21 | 8:I:390:ILE:HG23 | 1.76 | 0.68 |
| 8:I:417:PHE:CD2 | 8:I:448:VAL:HG22 | 2.28 | 0.68 |
| 9:J:285:PHE:HB2 | 9:J:308:TYR:CE1 | 2.28 | 0.68 |
| 1:A:1470:LEU:HA | 1:A:1522:SER:OG | 1.93 | 0.68 |
| 2:B:27:ARG:CB | 12:N:810:TYR:HE2 | 2.06 | 0.68 |
| 14:Q:166:ARG:CZ | 14:Q:436:VAL:HG11 | 2.23 | 0.68 |
| 17:Y:407:LEU:CD2 | 17:Y:437:LEU:HD21 | 2.24 | 0.68 |
| 1:A:1076:ARG:HE | 1:A:1543:HIS:CD2 | 2.11 | 0.68 |
| 8:I:287:LEU:HG | 8:I:456:PHE:CZ | 2.29 | 0.68 |
| 3:C:434:ARG:CD | 15:R:80:ILE:HG21 | 2.24 | 0.67 |
| 9:J:332:THR:HA | 9:J:363:LEU:CD2 | 2.21 | 0.67 |
| 9:J:397:ILE:HG22 | 9:J:398:ALA:H | 1.59 | 0.67 |
| 4:D:13:THR:HG22 | 13:O:255:TYR:HE2 | 1.59 | 0.67 |
| 8:I:330:LEU:HD23 | 8:I:425:MET:HE3 | 1.76 | 0.67 |
| 13:O:75:LEU:HB3 | 13:O:79:TYR:HE2 | 1.54 | 0.67 |
| 3:P:358:LEU:HD11 | 3:P:368:TRP:CE2 | 2.29 | 0.67 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:16:TRP:CD1 | 2:B:44:CYS:SG | 2.88 | 0.67 |
| 2:B:76:CYS:SG | 2:B:78:GLN:HG2 | 2.34 | 0.67 |
| 8:I:317:LEU:HD22 | 8:I:320:LEU:HD23 | 1.76 | 0.67 |
| 8:I:574:PHE:CE2 | 8:I:576:TRP:HB2 | 2.28 | 0.67 |
| 16:S:78:TRP:CE3 | 16:S:105:ALA:CB | 2.77 | 0.67 |
| 16:S:163:GLU:OE1 | 16:S:196:PHE:HE1 | 1.75 | 0.67 |
| 1:A:1329:MET:HE2 | 1:A:1368:THR:HA | 1.77 | 0.67 |
| 8:I:306:HIS:ND1 | 8:I:313:ALA:HB1 | 2.10 | 0.67 |
| 8:I:290:PHE:CB | 8:I:320:LEU:HD11 | 2.24 | 0.67 |
| 17:X:442:GLN:HG2 | 17:X:472:ARG:HG3 | 1.76 | 0.67 |
| 17:Y:442:GLN:CG | 17:Y:472:ARG:HG3 | 2.24 | 0.67 |
| 17:Y:445:THR:O | 17:Y:449:THR:HG23 | 1.93 | 0.67 |
| 1:A:1153:ILE:HD11 | 1:A:1184:HIS:HB3 | 1.76 | 0.67 |
| 3:P:233:PHE:CE1 | 3:P:237:ILE:HD11 | 2.28 | 0.67 |
| 1:A:1186:THR:HG23 | 1:A:1215:ALA:HB1 | 1.76 | 0.67 |
| 1:A:1470:LEU:HD12 | 1:A:1518:VAL:HG13 | 1.75 | 0.67 |
| 10:L:89:TYR:O | 10:L:151:THR:HG22 | 1.95 | 0.67 |
| 15:R:109:LYS:O | 15:R:113:GLN:HG3 | 1.95 | 0.67 |
| 16:S:197:GLN:O | 16:S:200:VAL:CG2 | 2.41 | 0.67 |
| 17:X:442:GLN:CG | 17:X:472:ARG:NE | 2.58 | 0.67 |
| 18:Z:158:ASP:O | 18:Z:160:ASP:N | 2.28 | 0.67 |
| 1:A:939:PHE:HZ | 1:A:944:LEU:HD13 | 1.59 | 0.67 |
| 8:I:15:GLY:O | 8:I:743:VAL:N | 2.26 | 0.67 |
| 9:K:222:GLU:CD | 9:K:228:GLN:HG3 | 2.14 | 0.67 |
| 13:O:657:ILE:HA | 13:O:660:LYS:HB3 | 1.77 | 0.67 |
| 16:S:83:SER:O | 16:S:87:GLN:N | 2.21 | 0.67 |
| 16:S:30:GLN:CB | 16:S:91:GLN:HB2 | 2.24 | 0.67 |
| 3:C:414:MET:CG | 13:O:330:ILE:HD11 | 2.25 | 0.67 |
| 2:B:14:TRP:HB2 | 2:B:15:LEU:HB2 | 1.76 | 0.66 |
| 8:I:28:TRP:NE1 | 8:I:723:ALA:O | 2.28 | 0.66 |
| 8:I:312:LYS:HG2 | 8:I:428:MET:HB3 | 1.76 | 0.66 |
| 1:A:1287:TYR:CD1 | 1:A:1287:TYR:O | 2.48 | 0.66 |
| 6:F:168:PHE:CB | 6:F:467:ARG:HD3 | 2.24 | 0.66 |
| 6:H:762:TRP:CA | 6:H:765:ASP:HB3 | 2.25 | 0.66 |
| 16:S:22:TRP:CE3 | 16:S:41:LEU:HB3 | 2.30 | 0.66 |
| 17:X:66:ASN:ND2 | 17:Y:268:ARG:HB3 | 2.10 | 0.66 |
| 6:F:562:MET:HB2 | 6:H:59:ARG:HH12 | 1.58 | 0.66 |
| 13:O:544:VAL:CG2 | 13:O:567:LEU:HG | 2.25 | 0.66 |
| 12:N:165:THR:N | 12:N:166:PRO:HA | 2.10 | 0.66 |
| 2:B:16:TRP:NE1 | 2:B:44:CYS:SG | 2.67 | 0.66 |
| 8:I:13:VAL:HG22 | 8:I:744:PHE:CE2 | 2.31 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:Q:475:LEU:O | 14:Q:476:ASP:HB3 | 1.94 | 0.66 |
| 17:Y:104:LEU:HD11 | 17:Y:142:MET:SD | 2.36 | 0.66 |
| 1:A:1399:VAL:HG11 | 1:A:1404:LEU:HG | 1.76 | 0.66 |
| 3:C:411:ILE:HG22 | 15:R:95:LEU:HD23 | 1.78 | 0.66 |
| 8:I:290:PHE:CE1 | 8:I:324:GLN:HB3 | 2.27 | 0.66 |
| 8:I:269:LEU:HB2 | 8:I:526:LYS:NZ | 2.10 | 0.66 |
| 8:I:73:TRP:CD1 | 8:I:80:LEU:HD13 | 2.31 | 0.66 |
| 14:Q:131:LEU:CD1 | 18:Z:163:VAL:HG11 | 2.26 | 0.66 |
| 16:S:30:GLN:HB2 | 16:S:91:GLN:CB | 2.25 | 0.66 |
| 16:S:23:GLU:OE2 | 18:Z:134:GLN:HA | 1.96 | 0.66 |
| 1:A:1051:VAL:HG21 | 1:A:1066:LYS:HB3 | 1.78 | 0.66 |
| 1:A:1138:HIS:HD2 | 1:A:1608:HIS:NE2 | 1.94 | 0.66 |
| 8:I:349:ILE:CD1 | 13:O:407:LEU:HA | 2.26 | 0.66 |
| 8:I:536:CYS:O | 8:I:540:PRO:HD3 | 1.96 | 0.66 |
| 1:A:1750:PHE:HD1 | 13:O:605:LEU:HD11 | 1.60 | 0.66 |
| 16:S:58:GLN:HG3 | 16:S:62:PHE:CZ | 2.29 | 0.66 |
| 8:I:313:ALA:HB3 | 8:I:317:LEU:CG | 2.26 | 0.66 |
| 3:C:416:PHE:CE2 | 13:O:323:ALA:HB2 | 2.31 | 0.66 |
| 13:O:417:LEU:HA | 13:O:420:ILE:HG22 | 1.78 | 0.66 |
| 3:C:251:TYR:HB3 | 3:C:269:ILE:HD11 | 1.78 | 0.66 |
| 12:N:74:TRP:CZ2 | 12:N:77:GLU:HB2 | 2.31 | 0.66 |
| 1:A:949:PHE:HA | 1:A:952:ALA:HB3 | 1.77 | 0.66 |
| 3:C:521:PHE:CD1 | 3:C:553:ILE:HG22 | 2.31 | 0.66 |
| 6:H:743:ILE:CG2 | 6:H:759:ASN:HD21 | 2.09 | 0.66 |
| 8:I:24:ILE:O | 8:I:569:LEU:HD22 | 1.96 | 0.66 |
| 17:X:63:MET:HE3 | 17:Y:266:LEU:HD22 | 1.78 | 0.66 |
| 6:H:765:ASP:O | 17:X:397:ARG:NH2 | 2.29 | 0.65 |
| 12:N:280:GLU:HA | 12:N:281:TYR:HD1 | 1.61 | 0.65 |
| 1:A:38:GLN:HE21 | 3:C:396:LYS:H | 1.41 | 0.65 |
| 6:F:50:ARG:HE | 6:H:19:TYR:HE1 | 1.44 | 0.65 |
| 9:K:250:CYS:HG | 9:K:274:THR:HG21 | 1.60 | 0.65 |
| 3:P:36:LEU:HD21 | 3:P:58:LEU:HB2 | 1.78 | 0.65 |
| 15:R:98:GLU:HG2 | 15:R:101:PRO:HG3 | 1.77 | 0.65 |
| 16:S:82:ILE:HD11 | 16:S:124:LEU:CD2 | 2.25 | 0.65 |
| 17:X:203:LEU:HD21 | 17:X:239:TRP:CH2 | 2.31 | 0.65 |
| 17:X:414:ILE:HD11 | 17:X:451:CYS:SG | 2.36 | 0.65 |
| 1:A:1196:TYR:HB2 | 1:A:1208:LEU:HD11 | 1.78 | 0.65 |
| 1:A:257:MET:HE3 | 1:A:266:HIS:HB3 | 1.77 | 0.65 |
| 2:B:39:VAL:N | 2:B:40:PRO:HD2 | 2.12 | 0.65 |
| 3:C:314:SER:HB2 | 9:J:289:HIS:CE1 | 2.31 | 0.65 |
| 9:J:37:PRO:HB3 | 9:J:69:TYR:CZ | 2.32 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:H:121:LEU:HG | 6:H:125:TYR:CE1 | 2.32 | 0.65 |
| 9:J:429:LEU:HA | 9:J:432:ILE:HG22 | 1.79 | 0.65 |
| 12:N:202:GLU:HB2 | 12:N:282:GLU:OE2 | 1.96 | 0.65 |
| 3:C:368:TRP:HB3 | 3:C:391:ALA:HB2 | 1.78 | 0.65 |
| 12:N:538:GLU:HG2 | 12:N:561:LEU:CG | 2.25 | 0.65 |
| 16:S:29:VAL:CA | 16:S:36:ARG:NH1 | 2.55 | 0.65 |
| 6:F:67:THR:HG21 | 17:Y:263:LYS:HD3 | 1.78 | 0.65 |
| 1:A:150:CYS:HB3 | 1:A:163:SER:HA | 1.78 | 0.65 |
| 1:A:1797:ILE:HG22 | 1:A:1852:ILE:HD11 | 1.78 | 0.65 |
| 16:S:163:GLU:OE1 | 16:S:196:PHE:HD1 | 1.79 | 0.65 |
| 17:X:40:HIS:HB3 | 17:Y:201:LEU:CD1 | 2.24 | 0.65 |
| 1:A:1321:VAL:HG22 | 1:A:1322:PRO:HD3 | 1.79 | 0.65 |
| 3:C:477:HIS:HD2 | 3:C:482:GLU:OE1 | 1.80 | 0.65 |
| 13:O:658:LEU:HD13 | 13:O:704:VAL:HG11 | 1.78 | 0.65 |
| 1:A:1306:CYS:HB2 | 1:A:1374:ILE:HG12 | 1.76 | 0.65 |
| 1:A:175:PHE:CD1 | 1:A:191:ARG:HG3 | 2.31 | 0.65 |
| 8:I:348:VAL:HB | 8:I:404:LEU:HD21 | 1.76 | 0.65 |
| 2:B:17:VAL:CG1 | 12:N:632:MET:HB3 | 2.26 | 0.65 |
| 17:X:371:ASN:H | 17:X:371:ASN:HD22 | 1.43 | 0.65 |
| 1:A:1799:ARG:HD3 | 1:A:1805:MET:CB | 2.26 | 0.65 |
| 3:C:531:THR:O | 3:C:535:LYS:HG2 | 1.97 | 0.65 |
| 8:I:295:ASN:O | 8:I:316:GLU:CG | 2.45 | 0.65 |
| 8:I:279:ILE:CG1 | 8:I:340:SER:HB2 | 2.26 | 0.65 |
| 9:K:376:LEU:HG | 9:K:407:GLU:OE1 | 1.97 | 0.65 |
| 15:R:98:GLU:CB | 15:R:101:PRO:HD3 | 2.26 | 0.65 |
| 1:A:1333:HIS:HB2 | 1:A:1357:THR:HA | 1.78 | 0.65 |
| 13:O:35:ILE:HG21 | 13:O:158:LEU:HD13 | 1.78 | 0.65 |
| 16:S:68:PHE:CZ | 16:S:81:TYR:HB2 | 2.32 | 0.65 |
| 16:S:75:LEU:HD13 | 16:S:75:LEU:C | 2.17 | 0.65 |
| 16:S:82:ILE:HD11 | 16:S:124:LEU:HD22 | 1.79 | 0.65 |
| 1:A:1405:LEU:HD13 | 1:A:1467:GLY:HA2 | 1.78 | 0.64 |
| 8:I:337:ILE:HG23 | 8:I:341:TYR:CE2 | 2.28 | 0.64 |
| 8:I:206:LEU:HD22 | 8:I:570:PHE:CG | 2.33 | 0.64 |
| 9:K:254:THR:HG23 | 9:K:271:HIS:CD2 | 2.32 | 0.64 |
| 13:O:625:LEU:HD13 | 13:O:666:LEU:HD22 | 1.79 | 0.64 |
| 16:S:132:CYS:HB3 | 16:S:135:PRO:HD3 | 1.79 | 0.64 |
| 16:S:79:ASP:HB2 | 16:S:120:ARG:HH11 | 1.62 | 0.64 |
| 3:P:531:THR:O | 3:P:535:LYS:HG2 | 1.97 | 0.64 |
| 14:Q:146:ASN:C | 14:Q:420:PHE:HE1 | 2.00 | 0.64 |
| 15:R:225:PRO:HB2 | 16:S:165:ARG:O | 1.98 | 0.64 |
| 16:S:144:ASN:HB3 | 16:S:295:TRP:O | 1.97 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:X:270:ASN:HB2 | 17:X:273:LEU:CB | 2.28 | 0.64 |
| 1:A:611:GLU:O | 1:A:645:HIS:NE2 | 2.30 | 0.64 |
| 8:I:290:PHE:CE1 | 8:I:324:GLN:CB | 2.80 | 0.64 |
| 12:N:74:TRP:CE3 | 12:N:76:VAL:HG13 | 2.32 | 0.64 |
| 13:O:460:GLN:HG2 | 13:O:496:ARG:NH2 | 2.11 | 0.64 |
| 14:Q:166:ARG:NH1 | 14:Q:436:VAL:HG11 | 2.12 | 0.64 |
| 6:F:707:PHE:HB2 | 6:F:729:LEU:HD11 | 1.80 | 0.64 |
| 9:K:210:LYS:O | 9:K:212:TYR:N | 2.28 | 0.64 |
| 17:X:407:LEU:CD2 | 17:X:437:LEU:HD21 | 2.26 | 0.64 |
| 1:A:1162:LYS:HG3 | 1:A:1163:PRO:CD | 2.24 | 0.64 |
| 1:A:1475:ARG:HG2 | 1:A:1476:PHE:CE1 | 2.32 | 0.64 |
| 8:I:115:TRP:CZ3 | 8:I:176:LEU:HD22 | 2.32 | 0.64 |
| 12:N:392:ASN:O | 12:N:395:ASP:HA | 1.98 | 0.64 |
| 3:P:233:PHE:CZ | 3:P:237:ILE:CD1 | 2.79 | 0.64 |
| 16:S:22:TRP:HA | 16:S:45:LEU:CD1 | 2.26 | 0.64 |
| 17:X:270:ASN:HB2 | 17:X:273:LEU:HB3 | 1.79 | 0.64 |
| 1:A:1619:LEU:HD11 | 1:A:1697:LEU:HB2 | 1.77 | 0.64 |
| 6:H:703:PRO:HB3 | 6:H:733:VAL:HG21 | 1.78 | 0.64 |
| 9:J:454:VAL:C | 9:J:458:LEU:HD12 | 2.17 | 0.64 |
| 9:J:40:ILE:HD13 | 9:J:63:ARG:HD3 | 1.79 | 0.64 |
| 9:J:294:LEU:HD12 | 9:K:54:HIS:NE2 | 2.13 | 0.64 |
| 12:N:622:TYR:O | 12:N:626:TYR:HB2 | 1.98 | 0.64 |
| 16:S:134:GLU:HG3 | 16:S:134:GLU:O | 1.98 | 0.64 |
| 17:X:442:GLN:CG | 17:X:472:ARG:HG3 | 2.27 | 0.64 |
| 6:H:145:ASN:HB2 | 6:H:146:PRO:O | 1.97 | 0.64 |
| 10:L:45:LEU:O | 10:L:155:GLN:OE1 | 2.16 | 0.64 |
| 8:I:265:ILE:HD11 | 8:I:396:PHE:CE2 | 2.33 | 0.64 |
| 1:A:1540:ARG:CZ | 12:N:486:ASP:O | 2.45 | 0.64 |
| 3:P:441:GLU:HG3 | 3:P:472:LYS:HZ1 | 1.63 | 0.64 |
| 17:X:159:LEU:HD22 | 17:X:171:ILE:HG23 | 1.80 | 0.64 |
| 17:Y:215:LYS:O | 17:Y:219:VAL:HG23 | 1.98 | 0.64 |
| 12:N:202:GLU:O | 12:N:204:ASP:N | 2.31 | 0.63 |
| 3:P:368:TRP:HB3 | 3:P:391:ALA:HB2 | 1.80 | 0.63 |
| 15:R:475:LEU:O | 15:R:476:ASP:HB2 | 1.98 | 0.63 |
| 17:X:215:LYS:O | 17:X:219:VAL:HG23 | 1.98 | 0.63 |
| 1:A:1100:LEU:HB3 | 1:A:1101:PRO:HA | 1.79 | 0.63 |
| 8:I:290:PHE:C | 8:I:320:LEU:CD1 | 2.67 | 0.63 |
| 8:I:73:TRP:CE2 | 8:I:80:LEU:HD22 | 2.32 | 0.63 |
| 9:J:445:GLU:HA | 9:J:474:LEU:HD23 | 1.79 | 0.63 |
| 9:K:372:LEU:HD11 | 9:K:407:GLU:HG3 | 1.80 | 0.63 |
| 14:Q:166:ARG:NH1 | 14:Q:413:GLU:OE1 | 2.31 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:S:84:TRP:O | 16:S:88:ASN:ND2 | 2.31 | 0.63 |
| 2:B:16:TRP:CH2 | 12:N:630:LYS:HG2 | 2.34 | 0.63 |
| 8:I:279:ILE:CB | 8:I:340:SER:HB2 | 2.28 | 0.63 |
| 8:I:305:MET:HB2 | 13:O:61:ASN:ND2 | 2.14 | 0.63 |
| 9:K:77:ALA:CB | 9:K:93:LEU:HD11 | 2.27 | 0.63 |
| 12:N:78:VAL:O | 12:N:80:GLN:N | 2.31 | 0.63 |
| 1:A:174:PRO:HA | 1:A:360:VAL:O | 1.99 | 0.63 |
| 2:B:16:TRP:C | 2:B:31:ASN:O | 2.28 | 0.63 |
| 6:F:696:ILE:HD11 | 6:F:709:ARG:HD3 | 1.81 | 0.63 |
| 8:I:24:ILE:HG22 | 8:I:38:ALA:O | 1.98 | 0.63 |
| 1:A:1229:SER:O | 1:A:1236:LEU:HB2 | 1.98 | 0.63 |
| 1:A:1601:TYR:HH | 10:L:102:PHE:HD1 | 1.45 | 0.63 |
| 3:C:61:SER:HB2 | 3:C:262:SER:HB2 | 1.79 | 0.63 |
| 8:I:313:ALA:CB | 8:I:317:LEU:CD1 | 2.72 | 0.63 |
| 6:H:130:ARG:HH12 | 9:K:473:VAL:HG22 | 1.64 | 0.63 |
| 3:P:283:LEU:HD21 | 3:P:312:MET:HE3 | 1.80 | 0.63 |
| 17:Y:159:LEU:HD22 | 17:Y:171:ILE:HG23 | 1.81 | 0.63 |
| 17:Y:373:VAL:HG11 | 17:Y:403:ALA:HB2 | 1.79 | 0.63 |
| 16:S:38:MET:HE2 | 18:Z:181:VAL:HG23 | 0.64 | 0.63 |
| 1:A:1327:GLN:HA | 1:A:1330:VAL:HG12 | 1.80 | 0.63 |
| 12:N:296:VAL:O | 12:N:299:TRP:HB3 | 1.99 | 0.63 |
| 12:N:765:LEU:HD21 | 16:S:200:VAL:CG2 | 2.20 | 0.63 |
| 17:Y:294:PHE:CD1 | 17:Y:294:PHE:C | 2.71 | 0.63 |
| 1:A:1230:ILE:HA | 1:A:1236:LEU:HD22 | 1.81 | 0.63 |
| 1:A:1409:LEU:HG | 1:A:1470:LEU:HD22 | 1.79 | 0.63 |
| 8:I:402:GLU:O | 8:I:406:VAL:HG23 | 1.98 | 0.63 |
| 15:R:225:PRO:HG2 | 16:S:166:GLU:CB | 2.28 | 0.63 |
| 17:X:452:LEU:HB3 | 17:X:461:ALA:HB2 | 1.81 | 0.63 |
| 17:Y:270:ASN:HB2 | 17:Y:273:LEU:CB | 2.28 | 0.63 |
| 1:A:1511:ASN:N | 1:A:1511:ASN:HD22 | 1.96 | 0.63 |
| 8:I:321:LEU:HD21 | 8:I:425:MET:HG2 | 1.81 | 0.63 |
| 8:I:330:LEU:HD11 | 8:I:422:TYR:HB2 | 1.79 | 0.63 |
| 12:N:501:ILE:HD12 | 12:N:501:ILE:H | 1.62 | 0.63 |
| 15:R:208:LEU:CD1 | 15:R:255:VAL:CG2 | 2.77 | 0.63 |
| 6:H:478:SER:HA | 6:H:633:ARG:HH22 | 1.63 | 0.62 |
| 13:O:114:ASP:C | 13:O:117:ASP:OD1 | 2.37 | 0.62 |
| 13:O:119:PHE:HE1 | 13:O:136:LEU:HD21 | 1.63 | 0.62 |
| 14:Q:208:LEU:CD1 | 14:Q:255:VAL:CG2 | 2.77 | 0.62 |
| 17:X:100:TYR:CD1 | 17:X:138:VAL:HG13 | 2.34 | 0.62 |
| 17:X:77:TYR:N | 17:X:106:GLN:HE21 | 1.97 | 0.62 |
| 17:Y:452:LEU:HB3 | 17:Y:461:ALA:HB2 | 1.81 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:X:203:LEU:HD22 | 17:Y:55:LEU:HB3 | 1.81 | 0.62 |
| 9:K:429:LEU:HA | 9:K:432:ILE:HG22 | 1.82 | 0.62 |
| 8:I:32:ARG:CD | 12:N:388:HIS:CE1 | 2.82 | 0.62 |
| 3:P:475:LYS:O | 3:P:479:GLN:NE2 | 2.32 | 0.62 |
| 16:S:21:GLU:C | 16:S:45:LEU:HD13 | 2.18 | 0.62 |
| 16:S:70:THR:O | 16:S:74:PRO:HD3 | 1.98 | 0.62 |
| 1:A:1604:GLN:O | 1:A:1607:ARG:HB2 | 1.99 | 0.62 |
| 8:I:17:LYS:CE | 8:I:51:SER:O | 2.47 | 0.62 |
| 15:R:192:TRP:CD2 | 15:R:198:LEU:HD13 | 2.35 | 0.62 |
| 15:R:95:LEU:HB2 | 15:R:130:ILE:HD11 | 1.80 | 0.62 |
| 1:A:1227:LEU:O | 1:A:1230:ILE:HG22 | 1.98 | 0.62 |
| 3:C:341:TYR:OH | 11:M:25:PRO:HD3 | 2.00 | 0.62 |
| 8:I:231:VAL:HG21 | 8:I:557:TYR:CE1 | 2.34 | 0.62 |
| 8:I:310:TRP:HB2 | 8:I:313:ALA:CA | 2.29 | 0.62 |
| 8:I:489:PRO:HB2 | 8:I:490:PRO:C | 2.19 | 0.62 |
| 9:K:292:VAL:HG21 | 11:M:57:TRP:HB3 | 1.81 | 0.62 |
| 9:K:19:TYR:CD1 | 9:K:49:LEU:HD13 | 2.35 | 0.62 |
| 12:N:180:PHE:HD1 | 12:N:299:TRP:CZ3 | 2.08 | 0.62 |
| 3:P:358:LEU:O | 3:P:362:PRO:HA | 1.98 | 0.62 |
| 10:L:148:GLY:HA2 | 16:S:270:SER:HB3 | 1.79 | 0.62 |
| 9:J:271:HIS:O | 9:J:274:THR:HG22 | 2.00 | 0.62 |
| 10:L:126:ASP:HB2 | 10:L:132:THR:HG23 | 1.78 | 0.62 |
| 1:A:1351:GLN:O | 10:L:42:VAL:HG21 | 2.00 | 0.62 |
| 12:N:619:LEU:HG | 12:N:637:TRP:CH2 | 2.34 | 0.62 |
| 9:K:514:PHE:CE2 | 7:W:11:LEU:HD13 | 2.34 | 0.62 |
| 17:X:437:LEU:HB2 | 17:X:444:LEU:HD11 | 1.82 | 0.62 |
| 1:A:126:ALA:HA | 1:A:152:CYS:O | 1.99 | 0.62 |
| 1:A:1677:LEU:HD21 | 1:A:1687:LEU:HG | 1.81 | 0.62 |
| 6:F:89:GLU:OE2 | 6:F:125:TYR:HE1 | 1.82 | 0.62 |
| 6:F:500:TRP:HB3 | 6:H:30:ARG:HH22 | 1.65 | 0.62 |
| 9:J:520:GLY:O | 9:J:523:ILE:HG22 | 1.99 | 0.62 |
| 16:S:22:TRP:HZ3 | 16:S:41:LEU:HD12 | 1.64 | 0.62 |
| 17:Y:196:LEU:O | 17:Y:200:PRO:HA | 1.99 | 0.62 |
| 17:Y:366:ILE:HD11 | 17:Y:379:LYS:CD | 2.29 | 0.62 |
| 1:A:1555:HIS:O | 1:A:1559:HIS:HD2 | 1.82 | 0.62 |
| 16:S:83:SER:O | 16:S:87:GLN:CG | 2.47 | 0.62 |
| 17:X:304:LEU:O | 17:X:308:MET:HG2 | 1.99 | 0.62 |
| 1:A:1196:TYR:HB3 | 1:A:1208:LEU:HD11 | 1.80 | 0.62 |
| 2:B:16:TRP:CB | 2:B:33:CYS:HB3 | 2.29 | 0.62 |
| 2:B:16:TRP:CE2 | 2:B:44:CYS:N | 2.67 | 0.62 |
| 8:I:306:HIS:CG | 8:I:313:ALA:HB1 | 2.34 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:476:PRO:HB3 | 3:P:182:LEU:HB3 | 1.82 | 0.62 |
| 3:C:434:ARG:HD3 | 15:R:80:ILE:HG21 | 1.81 | 0.62 |
| 1:A:183:THR:HG22 | 1:A:249:LEU:HG | 1.82 | 0.62 |
| 3:C:358:LEU:O | 3:C:362:PRO:HA | 1.99 | 0.62 |
| 6:H:146:PRO:HG3 | 6:H:167:THR:HA | 1.82 | 0.62 |
| 18:Z:157:THR:OG1 | 18:Z:158:ASP:N | 2.33 | 0.62 |
| 2:B:16:TRP:HD1 | 2:B:33:CYS:CA | 2.04 | 0.62 |
| 3:C:279:ILE:HD11 | 15:R:76:GLY:O | 2.00 | 0.62 |
| 9:J:77:ALA:HB1 | 9:J:93:LEU:HD11 | 1.81 | 0.62 |
| 9:J:77:ALA:CB | 9:J:93:LEU:HD11 | 2.29 | 0.62 |
| 1:A:95:VAL:HG22 | 1:A:100:VAL:HG22 | 1.81 | 0.61 |
| 6:F:729:LEU:HD13 | 6:F:739:VAL:HG22 | 1.81 | 0.61 |
| 8:I:413:ASN:ND2 | 8:I:450:GLU:OE1 | 2.33 | 0.61 |
| 9:K:62:SER:C | 9:K:63:ARG:HG3 | 2.19 | 0.61 |
| 16:S:19:GLY:HA2 | 16:S:22:TRP:HD1 | 1.65 | 0.61 |
| 1:A:1867:CYS:HB2 | 1:A:1881:GLN:NE2 | 2.16 | 0.61 |
| 9:J:445:GLU:HG2 | 9:J:446:PRO:CD | 2.29 | 0.61 |
| 12:N:281:TYR:CZ | 12:N:357:ALA:HA | 2.35 | 0.61 |
| 12:N:503:SER:O | 12:N:507:SER:HB3 | 1.99 | 0.61 |
| 6:F:146:PRO:HG3 | 6:F:167:THR:HA | 1.82 | 0.61 |
| 8:I:334:GLY:HA2 | 8:I:418:PHE:CD2 | 2.36 | 0.61 |
| 12:N:626:TYR:HD2 | 12:N:633:ARG:HB3 | 1.63 | 0.61 |
| 13:O:222:LEU:O | 13:O:226:ASP:O | 2.19 | 0.61 |
| 3:P:344:ARG:NH2 | 3:P:346:GLN:OE1 | 2.33 | 0.61 |
| 14:Q:410:HIS:CB | 14:Q:475:LEU:HD21 | 2.22 | 0.61 |
| 17:Y:45:ALA:CB | 17:Y:82:TYR:CE2 | 2.83 | 0.61 |
| 18:Z:39:PRO:O | 18:Z:42:THR:HB | 1.99 | 0.61 |
| 1:A:1791:ILE:HB | 13:O:598:THR:CG2 | 2.30 | 0.61 |
| 2:B:27:ARG:CD | 12:N:813:GLY:HA2 | 2.29 | 0.61 |
| 16:S:82:ILE:HD13 | 16:S:102:LEU:CD2 | 2.29 | 0.61 |
| 17:Y:462:LYS:HG2 | 17:Y:485:LEU:CD1 | 2.30 | 0.61 |
| 1:A:1380:ASN:HD22 | 1:A:1383:ILE:HD12 | 1.65 | 0.61 |
| 1:A:844:ILE:O | 1:A:848:VAL:HG23 | 2.00 | 0.61 |
| 6:H:515:TYR:HE2 | 6:H:545:HIS:CD2 | 2.19 | 0.61 |
| 14:Q:192:TRP:CD2 | 14:Q:198:LEU:HD13 | 2.35 | 0.61 |
| 15:R:98:GLU:HG2 | 15:R:101:PRO:HD3 | 1.79 | 0.61 |
| 1:A:39:LEU:H | 1:A:39:LEU:HD23 | 1.64 | 0.61 |
| 8:I:295:ASN:O | 8:I:316:GLU:CD | 2.39 | 0.61 |
| 8:I:56:TRP:CZ3 | 8:I:58:PHE:HB2 | 2.34 | 0.61 |
| 8:I:81:ALA:HA | 8:I:92:LEU:HA | 1.83 | 0.61 |
| 9:K:222:GLU:OE1 | 9:K:228:GLN:NE2 | 2.33 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:529:ASP:O | 13:O:532:VAL:HG12 | 1.99 | 0.61 |
| 1:A:1274:LEU:HG | 1:A:1302:LEU:HD11 | 1.81 | 0.61 |
| 12:N:362:LYS:HA | 12:N:410:LEU:CD2 | 2.29 | 0.61 |
| 12:N:456:GLY:HA2 | 12:N:548:ARG:HH21 | 1.65 | 0.61 |
| 12:N:73:GLU:O | 12:N:74:TRP:HB3 | 2.01 | 0.61 |
| 15:R:225:PRO:CD | 16:S:166:GLU:O | 2.46 | 0.61 |
| 16:S:36:ARG:HH11 | 16:S:90:PRO:CB | 2.11 | 0.61 |
| 9:J:185:LEU:HD11 | 9:J:205:PHE:CB | 2.31 | 0.61 |
| 12:N:331:PHE:CZ | 12:N:335:ILE:HD11 | 2.36 | 0.61 |
| 13:O:354:ARG:HD2 | 13:O:573:LYS:O | 2.01 | 0.61 |
| 16:S:25:SER:N | 16:S:45:LEU:HD21 | 2.15 | 0.61 |
| 3:C:344:ARG:HH21 | 11:M:25:PRO:CG | 2.10 | 0.61 |
| 12:N:769:SER:OG | 12:N:772:ARG:CD | 2.49 | 0.61 |
| 3:C:344:ARG:NH2 | 11:M:25:PRO:HG2 | 2.07 | 0.61 |
| 12:N:560:MET:HA | 12:N:560:MET:CE | 2.31 | 0.61 |
| 3:C:414:MET:CG | 13:O:330:ILE:CD1 | 2.77 | 0.61 |
| 3:P:94:PHE:O | 3:P:97:LYS:HB2 | 2.01 | 0.61 |
| 16:S:19:GLY:HA2 | 16:S:22:TRP:CD1 | 2.35 | 0.61 |
| 17:Y:77:TYR:HB2 | 17:Y:106:GLN:HG3 | 1.83 | 0.61 |
| 1:A:1137:PHE:O | 1:A:1141:VAL:HG23 | 2.01 | 0.60 |
| 6:F:699:ASP:HB2 | 6:F:702:ASN:HD21 | 1.66 | 0.60 |
| 9:J:37:PRO:HA | 9:J:65:LEU:HD11 | 1.82 | 0.60 |
| 12:N:351:PHE:HE1 | 12:N:405:LYS:HB2 | 1.67 | 0.60 |
| 17:X:407:LEU:HD22 | 17:X:437:LEU:HD21 | 1.83 | 0.60 |
| 1:A:662:THR:O | 1:A:666:ASN:ND2 | 2.33 | 0.60 |
| 13:O:114:ASP:HA | 13:O:117:ASP:OD1 | 2.00 | 0.60 |
| 14:Q:411:TYR:CE1 | 14:Q:475:LEU:HD23 | 2.36 | 0.60 |
| 16:S:58:GLN:CG | 16:S:62:PHE:HE2 | 1.94 | 0.60 |
| 3:P:170:PHE:O | 3:P:173:TYR:N | 2.33 | 0.60 |
| 14:Q:475:LEU:O | 14:Q:476:ASP:CB | 2.48 | 0.60 |
| 16:S:22:TRP:CZ3 | 16:S:41:LEU:HD12 | 2.36 | 0.60 |
| 13:O:75:LEU:C | 13:O:79:TYR:CD2 | 2.75 | 0.60 |
| 14:Q:127:GLU:O | 18:Z:159:LYS:HG2 | 2.01 | 0.60 |
| 14:Q:341:GLY:O | 14:Q:343:GLY:N | 2.35 | 0.60 |
| 17:Y:304:LEU:O | 17:Y:308:MET:HG2 | 2.01 | 0.60 |
| 1:A:1640:GLY:N | 1:A:1645:GLU:O | 2.29 | 0.60 |
| 3:C:94:PHE:O | 3:C:97:LYS:HB2 | 2.01 | 0.60 |
| 8:I:311:GLY:C | 8:I:428:MET:SD | 2.79 | 0.60 |
| 16:S:41:LEU:CD1 | 18:Z:141:PHE:CB | 2.80 | 0.60 |
| 9:J:167:PHE:HA | 9:J:170:LEU:CD2 | 2.31 | 0.60 |
| 12:N:362:LYS:CA | 12:N:410:LEU:HD21 | 2.31 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:R:116:TRP:O | 15:R:120:LEU:N | 2.32 | 0.60 |
| 15:R:295:VAL:HG23 | 16:S:274:VAL:HG23 | 1.84 | 0.60 |
| 6:F:528:ILE:HG22 | 6:F:529:GLU:HG3 | 1.82 | 0.60 |
| 17:X:279:ASP:OD1 | 17:X:310:VAL:HG21 | 2.00 | 0.60 |
| 17:Y:83:HIS:O | 17:Y:86:SER:OG | 2.16 | 0.60 |
| 1:A:1153:ILE:HG12 | 1:A:1184:HIS:CD2 | 2.37 | 0.60 |
| 2:B:16:TRP:CZ2 | 2:B:45:PRO:CA | 2.85 | 0.60 |
| 6:H:528:ILE:HG22 | 6:H:529:GLU:HG3 | 1.82 | 0.60 |
| 12:N:676:TRP:O | 12:N:713:PHE:HB2 | 2.01 | 0.60 |
| 14:Q:140:ALA:O | 14:Q:141:PRO:CB | 2.49 | 0.60 |
| 1:A:39:LEU:HD12 | 13:O:248:PRO:HB3 | 1.84 | 0.59 |
| 9:K:74:TYR:CZ | 9:K:78:ARG:HD2 | 2.37 | 0.59 |
| 16:S:78:TRP:CZ3 | 16:S:105:ALA:CA | 2.85 | 0.59 |
| 1:A:1218:GLY:N | 1:A:1259:LEU:O | 2.35 | 0.59 |
| 7:G:3:ARG:HB2 | 9:J:443:LYS:NZ | 2.17 | 0.59 |
| 6:H:594:ILE:HD11 | 6:H:604:TYR:HA | 1.84 | 0.59 |
| 8:I:304:PHE:CE2 | 8:I:452:LEU:HG | 2.37 | 0.59 |
| 9:J:17:GLN:CB | 9:K:78:ARG:HH12 | 2.15 | 0.59 |
| 13:O:619:LEU:O | 13:O:623:THR:HG22 | 2.02 | 0.59 |
| 16:S:19:GLY:N | 18:Z:134:GLN:HE22 | 1.97 | 0.59 |
| 8:I:302:ASP:O | 8:I:306:HIS:HB2 | 2.03 | 0.59 |
| 12:N:77:GLU:O | 12:N:78:VAL:HG23 | 2.03 | 0.59 |
| 3:P:389:ARG:O | 3:P:392:ILE:HG23 | 2.02 | 0.59 |
| 17:X:83:HIS:O | 17:X:86:SER:OG | 2.15 | 0.59 |
| 1:A:1274:LEU:O | 1:A:1277:ILE:HG22 | 2.01 | 0.59 |
| 6:H:73:TYR:CD1 | 6:H:117:THR:HG22 | 2.37 | 0.59 |
| 12:N:180:PHE:CD1 | 12:N:299:TRP:HH2 | 2.20 | 0.59 |
| 12:N:619:LEU:HG | 12:N:637:TRP:CZ2 | 2.37 | 0.59 |
| 3:C:145:GLN:HG3 | 13:O:246:PHE:CD2 | 2.38 | 0.59 |
| 13:O:417:LEU:HA | 13:O:420:ILE:CG2 | 2.32 | 0.59 |
| 16:S:71:GLY:O | 16:S:74:PRO:C | 2.40 | 0.59 |
| 1:A:1255:VAL:HG11 | 1:A:1606:LEU:HD21 | 1.84 | 0.59 |
| 8:I:290:PHE:CZ | 8:I:325:LEU:HB2 | 2.37 | 0.59 |
| 3:C:377:GLU:HA | 15:R:130:ILE:CG2 | 2.33 | 0.59 |
| 1:A:485:ILE:CD1 | 1:A:609:ILE:HB | 2.32 | 0.59 |
| 8:I:334:GLY:HA2 | 8:I:418:PHE:CE2 | 2.38 | 0.59 |
| 12:N:609:LEU:HD22 | 12:N:639:HIS:CD2 | 2.38 | 0.59 |
| 8:I:32:ARG:HB2 | 8:I:34:LEU:CD2 | 2.33 | 0.59 |
| 8:I:337:ILE:HD13 | 8:I:418:PHE:HZ | 1.68 | 0.59 |
| 8:I:337:ILE:HG22 | 8:I:341:TYR:HE2 | 1.65 | 0.59 |
| 12:N:341:ILE:O | 12:N:344:LEU:HB3 | 2.03 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:R:341:GLY:O | 15:R:343:GLY:N | 2.35 | 0.59 |
| 17:X:229:THR:HG21 | 17:X:233:LEU:HD12 | 1.84 | 0.59 |
| 1:A:23:PHE:HB2 | 1:A:111:LEU:HD22 | 1.83 | 0.59 |
| 8:I:299:SER:O | 8:I:303:GLU:HG3 | 2.02 | 0.59 |
| 8:I:17:LYS:NZ | 8:I:51:SER:O | 2.35 | 0.59 |
| 9:K:403:PHE:O | 9:K:407:GLU:HG2 | 2.02 | 0.59 |
| 10:L:125:THR:HA | 10:L:126:ASP:HB3 | 1.84 | 0.59 |
| 3:C:317:SER:CB | 11:M:27:GLU:HG3 | 2.32 | 0.59 |
| 17:Y:434:TYR:HA | 17:Y:444:LEU:HD13 | 1.84 | 0.59 |
| 6:H:656:MET:HE1 | 9:K:526:TYR:CD2 | 2.37 | 0.59 |
| 3:P:234:LEU:HD22 | 3:P:238:TYR:CE2 | 2.38 | 0.59 |
| 3:P:389:ARG:HA | 3:P:392:ILE:CG2 | 2.32 | 0.59 |
| 16:S:84:TRP:CE2 | 16:S:88:ASN:OD1 | 2.55 | 0.59 |
| 1:A:1167:GLU:O | 1:A:1168:LEU:HB3 | 2.03 | 0.59 |
| 2:B:46:LEU:HD23 | 2:B:47:VAL:N | 2.17 | 0.59 |
| 10:L:108:ILE:HB | 10:L:125:THR:O | 2.03 | 0.59 |
| 17:Y:229:THR:HG21 | 17:Y:233:LEU:HD12 | 1.84 | 0.59 |
| 8:I:65:GLY:HA3 | 8:I:84:LEU:HB3 | 1.85 | 0.58 |
| 1:A:1194:HIS:HB2 | 15:R:121:ASN:HD21 | 1.69 | 0.58 |
| 2:B:64:LEU:HD22 | 2:B:71:GLN:HA | 1.85 | 0.58 |
| 1:A:1060:HIS:O | 1:A:1063:ILE:HG22 | 2.03 | 0.58 |
| 1:A:1599:ASN:HB2 | 1:A:1603:LEU:HA | 1.85 | 0.58 |
| 9:J:193:LEU:O | 9:J:197:GLU:HB2 | 2.03 | 0.58 |
| 9:J:211:LYS:O | 9:J:212:TYR:CG | 2.55 | 0.58 |
| 3:P:358:LEU:HD11 | 3:P:368:TRP:CZ2 | 2.38 | 0.58 |
| 14:Q:222:MET:HB3 | 14:Q:227:GLU:HG3 | 1.85 | 0.58 |
| 1:A:880:TYR:O | 1:A:926:LEU:HD21 | 2.02 | 0.58 |
| 6:F:152:PHE:HE1 | 6:F:162:PRO:HG2 | 1.69 | 0.58 |
| 8:I:420:TRP:CD1 | 8:I:440:MET:HE2 | 2.38 | 0.58 |
| 3:C:389:ARG:HG3 | 13:O:280:ARG:HD3 | 1.85 | 0.58 |
| 12:N:148:GLY:HA3 | 12:N:152:GLU:OE2 | 2.03 | 0.58 |
| 12:N:520:ARG:HG3 | 12:N:557:CYS:SG | 2.43 | 0.58 |
| 13:O:591:TYR:HA | 13:O:594:SER:OG | 2.03 | 0.58 |
| 3:P:120:TYR:CZ | 3:P:124:LEU:HD11 | 2.39 | 0.58 |
| 16:S:20:ASP:OD2 | 18:Z:184:ARG:NH1 | 2.35 | 0.58 |
| 1:A:436:LEU:H | 1:A:501:THR:HG23 | 1.68 | 0.58 |
| 9:K:77:ALA:HB1 | 9:K:93:LEU:HD11 | 1.85 | 0.58 |
| 13:O:328:ILE:O | 13:O:332:GLN:HG3 | 2.03 | 0.58 |
| 3:P:290:ARG:HH21 | 3:P:319:LEU:CD1 | 2.14 | 0.58 |
| 1:A:1230:ILE:HD12 | 15:R:116:TRP:CD1 | 2.39 | 0.58 |
| 17:Y:384:ARG:HH22 | 17:Y:415:GLU:HB3 | 1.67 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Y:45:ALA:HB2 | 17:Y:82:TYR:CD2 | 2.38 | 0.58 |
| 1:A:1404:LEU:HD22 | 1:A:1464:ILE:HD11 | 1.85 | 0.58 |
| 2:B:27:ARG:HB2 | 12:N:810:TYR:HE2 | 1.67 | 0.58 |
| 8:I:413:ASN:O | 8:I:447:PHE:CE1 | 2.52 | 0.58 |
| 9:K:78:ARG:HG3 | 9:K:135:LEU:HD22 | 1.84 | 0.58 |
| 3:C:317:SER:HB3 | 11:M:27:GLU:HG3 | 1.84 | 0.58 |
| 17:X:475:TYR:O | 17:X:479:VAL:HG23 | 2.04 | 0.58 |
| 6:H:761:SER:O | 6:H:765:ASP:CB | 2.52 | 0.58 |
| 8:I:500:PHE:CE2 | 8:I:507:LEU:HD12 | 2.37 | 0.58 |
| 12:N:278:ARG:HB3 | 12:N:343:GLU:OE2 | 2.04 | 0.58 |
| 12:N:699:TRP:CZ3 | 12:N:728:VAL:HG21 | 2.39 | 0.58 |
| 3:C:389:ARG:CG | 13:O:280:ARG:HD3 | 2.34 | 0.58 |
| 17:Y:407:LEU:HD22 | 17:Y:437:LEU:HD21 | 1.86 | 0.58 |
| 1:A:1376:LEU:HD23 | 1:A:1377:LYS:HG3 | 1.86 | 0.58 |
| 1:A:1405:LEU:HD13 | 1:A:1467:GLY:CA | 2.33 | 0.58 |
| 2:B:27:ARG:HD2 | 12:N:813:GLY:HA2 | 1.83 | 0.58 |
| 9:K:386:LEU:HD12 | 9:K:386:LEU:H | 1.68 | 0.58 |
| 14:Q:208:LEU:HD11 | 14:Q:255:VAL:HG23 | 1.86 | 0.58 |
| 16:S:99:SER:HB2 | 16:S:131:LEU:HD13 | 1.85 | 0.58 |
| 17:Y:437:LEU:HB2 | 17:Y:444:LEU:HD11 | 1.86 | 0.58 |
| 9:J:185:LEU:HD11 | 9:J:205:PHE:HB3 | 1.86 | 0.58 |
| 8:I:430:GLU:CD | 14:Q:429:LYS:HG2 | 2.24 | 0.58 |
| 3:P:400:ARG:HG3 | 14:Q:498:ILE:HB | 1.85 | 0.58 |
| 3:C:414:MET:HB3 | 13:O:326:GLU:HB3 | 1.85 | 0.57 |
| 6:F:26:PHE:CD1 | 6:H:149:TRP:HB2 | 2.38 | 0.57 |
| 9:J:178:ALA:HB1 | 9:J:213:ASN:HD22 | 1.69 | 0.57 |
| 9:K:355:ALA:O | 9:K:359:THR:HG22 | 2.04 | 0.57 |
| 12:N:300:LEU:O | 12:N:304:PHE:HD1 | 1.87 | 0.57 |
| 17:Y:294:PHE:CD1 | 17:Y:294:PHE:O | 2.57 | 0.57 |
| 6:H:42:PHE:HB2 | 6:H:71:CYS:SG | 2.43 | 0.57 |
| 9:J:219:VAL:C | 9:J:221:PRO:HD3 | 2.24 | 0.57 |
| 12:N:612:PRO:HG2 | 12:N:615:ILE:HG12 | 1.85 | 0.57 |
| 12:N:704:VAL:HA | 12:N:719:GLU:CD | 2.25 | 0.57 |
| 16:S:30:GLN:HB2 | 16:S:91:GLN:CA | 2.33 | 0.57 |
| 17:Y:96:ALA:O | 17:Y:100:TYR:HD2 | 1.86 | 0.57 |
| 10:L:63:LEU:HD13 | 10:L:138:GLN:NE2 | 2.18 | 0.57 |
| 13:O:75:LEU:HD21 | 13:O:161:TYR:HE2 | 1.62 | 0.57 |
| 3:P:61:SER:HB2 | 3:P:262:SER:HB2 | 1.85 | 0.57 |
| 3:P:251:TYR:HB3 | 3:P:269:ILE:HD11 | 1.85 | 0.57 |
| 3:P:409:TYR:HA | 3:P:412:LEU:HD12 | 1.85 | 0.57 |
| 15:R:222:MET:HB3 | 15:R:227:GLU:HG3 | 1.86 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:K:406:HIS:CE1 | 7:W:6:PRO:HB3 | 2.39 | 0.57 |
| 1:A:214:LEU:HD21 | 1:A:407:LEU:HD13 | 1.87 | 0.57 |
| 1:A:961:HIS:ND1 | 1:A:964:GLU:OE2 | 2.37 | 0.57 |
| 3:C:170:PHE:O | 3:C:173:TYR:N | 2.38 | 0.57 |
| 6:F:544:TRP:CD2 | 15:R:499:ARG:HD3 | 2.40 | 0.57 |
| 8:I:27:VAL:C | 8:I:35:ILE:HD12 | 2.25 | 0.57 |
| 12:N:386:LEU:C | 12:N:388:HIS:HB3 | 2.25 | 0.57 |
| 13:O:414:LEU:CD1 | 13:O:417:LEU:HB2 | 2.35 | 0.57 |
| 6:H:621:LEU:HB3 | 6:H:625:ARG:NH2 | 2.20 | 0.57 |
| 8:I:36:ALA:CB | 8:I:80:LEU:HD21 | 2.35 | 0.57 |
| 6:F:533:VAL:HG13 | 6:F:568:GLU:OE1 | 2.03 | 0.57 |
| 8:I:730:VAL:HG22 | 8:I:731:SER:N | 2.19 | 0.57 |
| 16:S:68:PHE:CE2 | 16:S:81:TYR:CG | 2.88 | 0.57 |
| 17:X:462:LYS:HG2 | 17:X:485:LEU:CD1 | 2.31 | 0.57 |
| 17:X:55:LEU:HB3 | 17:Y:203:LEU:HD12 | 1.86 | 0.57 |
| 1:A:629:LEU:HD22 | 1:A:633:ILE:HG22 | 1.86 | 0.57 |
| 2:B:47:VAL:HG11 | 2:B:60:ILE:HG21 | 1.85 | 0.57 |
| 3:C:352:LEU:HD21 | 3:C:356:ARG:CZ | 2.35 | 0.57 |
| 3:C:358:LEU:HD21 | 3:C:368:TRP:CE2 | 2.40 | 0.57 |
| 8:I:413:ASN:CA | 8:I:447:PHE:HZ | 1.93 | 0.57 |
| 16:S:29:VAL:CG1 | 16:S:36:ARG:HH12 | 2.08 | 0.57 |
| 16:S:60:ARG:O | 16:S:64:TYR:HD2 | 1.88 | 0.57 |
| 17:X:170:LYS:HA | 17:Y:49:LEU:HD21 | 1.86 | 0.57 |
| 18:Z:146:GLU:CD | 18:Z:146:GLU:H | 2.08 | 0.57 |
| 1:A:215:HIS:CD2 | 1:A:217:LEU:H | 2.23 | 0.57 |
| 3:C:120:TYR:CZ | 3:C:124:LEU:HD11 | 2.40 | 0.57 |
| 8:I:56:TRP:CD2 | 8:I:98:PRO:HB3 | 2.38 | 0.57 |
| 12:N:765:LEU:HD11 | 16:S:200:VAL:HG23 | 1.87 | 0.57 |
| 16:S:68:PHE:HZ | 16:S:81:TYR:HB3 | 1.69 | 0.57 |
| 6:H:121:LEU:O | 6:H:125:TYR:HD1 | 1.87 | 0.57 |
| 13:O:105:LEU:HD11 | 13:O:151:VAL:CG1 | 2.35 | 0.57 |
| 17:Y:475:TYR:O | 17:Y:479:VAL:HG23 | 2.03 | 0.57 |
| 9:J:397:ILE:HG22 | 9:J:398:ALA:N | 2.19 | 0.57 |
| 9:K:296:PRO:HB2 | 11:M:55:MET:HG3 | 1.86 | 0.57 |
| 12:N:663:GLN:HB3 | 12:N:699:TRP:CZ2 | 2.40 | 0.57 |
| 3:P:244:ILE:C | 3:P:244:ILE:HD12 | 2.26 | 0.57 |
| 16:S:145:GLN:NE2 | 16:S:296:ILE:CB | 2.68 | 0.57 |
| 16:S:79:ASP:OD2 | 16:S:120:ARG:CA | 2.52 | 0.57 |
| 1:A:1033:ARG:NH1 | 1:A:1531:GLY:O | 2.37 | 0.56 |
| 1:A:1532:ASN:HB3 | 1:A:1535:VAL:HG23 | 1.86 | 0.56 |
| 1:A:1290:ASP:OD2 | 1:A:1600:ARG:HA | 2.05 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:257:MET:CE | 1:A:266:HIS:HB3 | 2.35 | 0.56 |
| 1:A:92:GLU:OE2 | 1:A:111:LEU:HD21 | 2.05 | 0.56 |
| 2:B:46:LEU:HD21 | 2:B:54:CYS:HB3 | 1.86 | 0.56 |
| 6:F:42:PHE:HB2 | 6:F:71:CYS:SG | 2.44 | 0.56 |
| 8:I:276:TRP:NE1 | 8:I:475:VAL:HB | 2.20 | 0.56 |
| 13:O:75:LEU:CB | 13:O:79:TYR:HE2 | 2.18 | 0.56 |
| 15:R:247:SER:HB2 | 16:S:170:LYS:HZ1 | 1.69 | 0.56 |
| 16:S:68:PHE:HE1 | 16:S:78:TRP:CD2 | 2.23 | 0.56 |
| 1:A:1332:GLY:C | 1:A:1358:ILE:HD12 | 2.21 | 0.56 |
| 6:H:669:SER:HA | 6:H:698:ILE:HD11 | 1.86 | 0.56 |
| 9:J:247:PHE:CD2 | 9:J:277:GLU:HB3 | 2.40 | 0.56 |
| 9:J:324:SER:O | 9:J:328:THR:HG23 | 2.05 | 0.56 |
| 12:N:596:LEU:HB3 | 12:N:601:TRP:NE1 | 2.19 | 0.56 |
| 13:O:599:ILE:O | 13:O:602:PRO:HD2 | 2.05 | 0.56 |
| 13:O:727:THR:O | 13:O:730:ARG:HB2 | 2.05 | 0.56 |
| 14:Q:208:LEU:HD11 | 14:Q:255:VAL:CG2 | 2.35 | 0.56 |
| 1:A:1086:MET:HG2 | 1:A:1610:TYR:CZ | 2.40 | 0.56 |
| 1:A:1163:PRO:HG3 | 1:A:1169:ALA:HA | 1.86 | 0.56 |
| 1:A:1235:LEU:HD22 | 1:A:1257:ILE:HG13 | 1.79 | 0.56 |
| 6:F:125:TYR:HD1 | 6:F:130:ARG:HE | 1.49 | 0.56 |
| 9:K:472:LEU:HG | 9:K:481:THR:CG2 | 2.33 | 0.56 |
| 14:Q:410:HIS:CG | 14:Q:475:LEU:HD11 | 2.40 | 0.56 |
| 15:R:208:LEU:HD11 | 15:R:255:VAL:HG23 | 1.87 | 0.56 |
| 16:S:88:ASN:N | 16:S:88:ASN:HD22 | 2.02 | 0.56 |
| 1:A:1057:LEU:HA | 1:A:1061:GLU:OE1 | 2.04 | 0.56 |
| 1:A:1254:VAL:CG1 | 1:A:1298:ALA:HA | 2.36 | 0.56 |
| 3:C:363:ARG:HG2 | 3:C:363:ARG:O | 2.05 | 0.56 |
| 8:I:277:GLU:O | 8:I:281:MET:N | 2.32 | 0.56 |
| 8:I:34:LEU:HD13 | 12:N:389:PRO:O | 2.05 | 0.56 |
| 12:N:386:LEU:HD21 | 12:N:399:LEU:HD22 | 1.86 | 0.56 |
| 12:N:501:ILE:HD12 | 12:N:501:ILE:N | 2.20 | 0.56 |
| 17:X:54:ARG:NH2 | 17:X:90:ASP:OD2 | 2.39 | 0.56 |
| 12:N:202:GLU:OE2 | 12:N:283:ARG:HB2 | 2.05 | 0.56 |
| 12:N:648:VAL:HG13 | 12:N:650:LEU:HG | 1.86 | 0.56 |
| 16:S:132:CYS:CB | 16:S:135:PRO:N | 2.68 | 0.56 |
| 15:R:225:PRO:HG2 | 16:S:166:GLU:HB2 | 1.86 | 0.56 |
| 17:X:66:ASN:HD21 | 17:Y:268:ARG:HB3 | 1.71 | 0.56 |
| 8:I:218:SER:HA | 8:I:235:GLN:HA | 1.88 | 0.56 |
| 9:J:451:LEU:HD12 | 9:J:467:TYR:CD2 | 2.40 | 0.56 |
| 12:N:344:LEU:HA | 12:N:347:ILE:HB | 1.87 | 0.56 |
| 15:R:208:LEU:HD11 | 15:R:255:VAL:CG2 | 2.35 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:R:98:GLU:HB3 | 15:R:101:PRO:HD3 | 1.85 | 0.56 |
| 16:S:271:ARG:HG2 | 16:S:272:ILE:N | 2.21 | 0.56 |
| 17:X:442:GLN:NE2 | 17:X:472:ARG:CG | 2.68 | 0.56 |
| 16:S:38:MET:HB3 | 18:Z:181:VAL:HG22 | 1.87 | 0.56 |
| 3:C:97:LYS:O | 3:C:97:LYS:HG2 | 2.06 | 0.56 |
| 8:I:269:LEU:CB | 8:I:526:LYS:NZ | 2.69 | 0.56 |
| 12:N:556:PHE:HA | 12:N:600:PHE:CE1 | 2.41 | 0.56 |
| 13:O:627:LEU:O | 13:O:630:ALA:HB3 | 2.06 | 0.56 |
| 3:C:89:LEU:HD12 | 3:P:60:PHE:CG | 2.40 | 0.56 |
| 14:Q:216:ILE:HD13 | 16:S:558:LEU:HB2 | 1.87 | 0.56 |
| 16:S:68:PHE:CE1 | 16:S:78:TRP:CD2 | 2.93 | 0.56 |
| 17:Y:70:LEU:HD12 | 17:Y:71:PHE:CE2 | 2.40 | 0.56 |
| 1:A:105:GLY:O | 1:A:111:LEU:HG | 2.06 | 0.56 |
| 3:C:148:ASN:HB3 | 3:C:151:LEU:CG | 2.34 | 0.56 |
| 12:N:592:TYR:HD1 | 12:N:593:ALA:N | 2.04 | 0.56 |
| 14:Q:146:ASN:C | 14:Q:420:PHE:CE1 | 2.79 | 0.56 |
| 17:X:350:PHE:HB2 | 17:X:351:TYR:CD1 | 2.41 | 0.56 |
| 17:Y:350:PHE:HB2 | 17:Y:351:TYR:CD1 | 2.40 | 0.56 |
| 1:A:1632:ALA:H | 1:A:1653:ALA:HB3 | 1.70 | 0.56 |
| 6:F:73:TYR:CD1 | 6:F:117:THR:HG22 | 2.41 | 0.56 |
| 8:I:231:VAL:HG11 | 8:I:556:LEU:HD12 | 1.88 | 0.56 |
| 12:N:704:VAL:HG23 | 12:N:705:LEU:HD22 | 1.86 | 0.56 |
| 13:O:104:GLU:N | 13:O:107:ASP:OD2 | 2.39 | 0.56 |
| 1:A:167:LYS:HG2 | 13:O:319:GLN:HE22 | 1.70 | 0.56 |
| 15:R:74:PRO:CB | 15:R:75:GLY:HA2 | 2.36 | 0.56 |
| 17:Y:199:CYS:HB3 | 17:Y:201:LEU:HD12 | 1.87 | 0.56 |
| 17:Y:475:TYR:CE1 | 17:Y:477:LYS:HB2 | 2.41 | 0.56 |
| 2:B:64:LEU:HD11 | 2:B:80:TRP:CD1 | 2.41 | 0.56 |
| 3:C:301:ASP:OD2 | 3:C:335:CYS:HB3 | 2.06 | 0.56 |
| 4:D:3:THR:O | 4:D:5:PHE:CE2 | 2.58 | 0.56 |
| 8:I:262:LEU:HA | 8:I:265:ILE:CG2 | 2.32 | 0.56 |
| 9:J:212:TYR:HB3 | 9:J:243:TYR:CD1 | 2.41 | 0.56 |
| 12:N:502:ILE:HA | 12:N:505:LEU:HD12 | 1.88 | 0.56 |
| 16:S:76:ASP:O | 16:S:77:VAL:HB | 2.06 | 0.56 |
| 17:X:475:TYR:CE1 | 17:X:477:LYS:HB2 | 2.41 | 0.56 |
| 17:Y:100:TYR:HB3 | 17:Y:142:MET:CG | 2.35 | 0.56 |
| 3:C:407:GLN:O | 3:C:411:ILE:HG12 | 2.06 | 0.56 |
| 2:B:45:PRO:HB2 | 12:N:631:ALA:HB3 | 1.87 | 0.56 |
| 16:S:41:LEU:CD2 | 16:S:90:PRO:HB3 | 2.36 | 0.56 |
| 8:I:167:LEU:HD12 | 8:I:168:LEU:N | 2.21 | 0.55 |
| 9:J:465:LEU:CA | 9:J:488:ILE:HD12 | 2.35 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:S:68:PHE:CZ | 16:S:81:TYR:CG | 2.93 | 0.55 |
| 17:X:100:TYR:HD1 | 17:X:138:VAL:HG13 | 1.70 | 0.55 |
| 17:X:168:THR:HB | 17:X:169:PRO:HD2 | 1.88 | 0.55 |
| 17:X:63:MET:CE | 17:Y:266:LEU:HD22 | 2.35 | 0.55 |
| 17:Y:168:THR:HB | 17:Y:169:PRO:HD2 | 1.88 | 0.55 |
| 17:Y:50:HIS:ND1 | 17:Y:86:SER:HA | 2.21 | 0.55 |
| 6:H:121:LEU:O | 6:H:125:TYR:CD1 | 2.59 | 0.55 |
| 8:I:291:VAL:HG13 | 8:I:303:GLU:OE2 | 2.07 | 0.55 |
| 13:O:490:LEU:HD13 | 13:O:511:ASP:HB2 | 1.86 | 0.55 |
| 13:O:394:THR:HG22 | 13:O:615:ARG:HH12 | 1.70 | 0.55 |
| 15:R:105:GLN:C | 15:R:107:PRO:HD3 | 2.26 | 0.55 |
| 17:Y:294:PHE:C | 17:Y:294:PHE:HD1 | 2.10 | 0.55 |
| 1:A:1047:VAL:O | 1:A:1109:GLY:HA2 | 2.06 | 0.55 |
| 1:A:1332:GLY:H | 1:A:1358:ILE:HB | 1.71 | 0.55 |
| 1:A:1399:VAL:CG1 | 1:A:1404:LEU:HG | 2.36 | 0.55 |
| 1:A:1839:PHE:CE1 | 1:A:1840:MET:HG3 | 2.41 | 0.55 |
| 6:F:104:ASP:N | 6:F:104:ASP:OD1 | 2.39 | 0.55 |
| 8:I:64:THR:HG22 | 8:I:84:LEU:HD11 | 1.87 | 0.55 |
| 12:N:281:TYR:OH | 12:N:357:ALA:HA | 2.06 | 0.55 |
| 3:P:441:GLU:HG3 | 3:P:472:LYS:NZ | 2.21 | 0.55 |
| 16:S:22:TRP:CZ3 | 16:S:41:LEU:CD1 | 2.86 | 0.55 |
| 1:A:1573:SER:HB2 | 1:A:1617:ARG:NH2 | 2.22 | 0.55 |
| 1:A:1786:MET:HE2 | 1:A:1786:MET:HA | 1.89 | 0.55 |
| 6:F:730:LYS:HE2 | 6:F:740:TYR:CE1 | 2.38 | 0.55 |
| 8:I:306:HIS:CE1 | 8:I:316:GLU:HB3 | 2.41 | 0.55 |
| 9:K:284:LEU:HD13 | 9:K:308:TYR:HB2 | 1.88 | 0.55 |
| 14:Q:352:THR:HB | 18:Z:51:LEU:HA | 1.88 | 0.55 |
| 16:S:64:TYR:O | 16:S:68:PHE:HD2 | 1.86 | 0.55 |
| 17:X:76:LYS:CB | 17:X:106:GLN:NE2 | 2.69 | 0.55 |
| 17:Y:203:LEU:HA | 17:Y:206:ILE:HD12 | 1.89 | 0.55 |
| 14:Q:128:ALA:HB1 | 18:Z:156:TYR:CE2 | 2.39 | 0.55 |
| 1:A:1351:GLN:O | 10:L:32:SER:HA | 2.07 | 0.55 |
| 3:P:407:GLN:O | 3:P:411:ILE:HG12 | 2.06 | 0.55 |
| 16:S:60:ARG:O | 16:S:64:TYR:CD2 | 2.60 | 0.55 |
| 8:I:497:TRP:CH2 | 8:I:507:LEU:HD13 | 2.42 | 0.55 |
| 12:N:676:TRP:HE3 | 12:N:680:GLU:HB3 | 1.70 | 0.55 |
| 3:P:180:ARG:HG3 | 3:P:212:LEU:HD21 | 1.89 | 0.55 |
| 3:P:441:GLU:HG3 | 3:P:472:LYS:CE | 2.37 | 0.55 |
| 8:I:430:GLU:OE2 | 14:Q:429:LYS:HB3 | 2.06 | 0.55 |
| 15:R:98:GLU:CG | 15:R:101:PRO:CD | 2.76 | 0.55 |
| 14:Q:185:TYR:CE1 | 16:S:27:GLU:CG | 2.87 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:X:52:ASN:HD22 | 17:Y:202:ALA:CB | 2.19 | 0.55 |
| 1:A:1054:TYR:O | 1:A:1056:GLU:N | 2.40 | 0.55 |
| 1:A:1624:VAL:HG22 | 1:A:1698:TYR:CD2 | 2.38 | 0.55 |
| 2:B:42:ASP:O | 2:B:43:ASP:HB2 | 2.07 | 0.55 |
| 8:I:52:PHE:CD1 | 8:I:743:VAL:HG21 | 2.42 | 0.55 |
| 13:O:163:GLN:HB3 | 13:O:167:LYS:HE3 | 1.88 | 0.55 |
| 13:O:219:GLN:HE22 | 13:O:231:LEU:HD13 | 1.70 | 0.55 |
| 8:I:305:MET:CB | 13:O:61:ASN:HD21 | 2.20 | 0.55 |
| 16:S:79:ASP:OD2 | 16:S:120:ARG:HA | 2.06 | 0.55 |
| 16:S:22:TRP:CZ2 | 16:S:38:MET:O | 2.59 | 0.55 |
| 1:A:1531:GLY:HA3 | 1:A:1566:PHE:CE1 | 2.42 | 0.55 |
| 1:A:809:ASP:O | 1:A:1807:GLU:O | 2.24 | 0.55 |
| 6:F:699:ASP:HB3 | 6:F:702:ASN:OD1 | 2.06 | 0.55 |
| 9:J:337:TRP:HB3 | 9:J:360:ALA:HB2 | 1.88 | 0.55 |
| 13:O:105:LEU:HD11 | 13:O:151:VAL:HG12 | 1.89 | 0.55 |
| 13:O:439:LEU:HG | 13:O:476:LEU:HD13 | 1.89 | 0.55 |
| 3:C:259:PHE:HB3 | 3:C:265:ILE:HD12 | 1.84 | 0.55 |
| 6:F:594:ILE:HD11 | 6:F:604:TYR:HA | 1.88 | 0.55 |
| 8:I:166:LYS:O | 8:I:170:ASP:HB2 | 2.06 | 0.55 |
| 12:N:165:THR:H | 12:N:166:PRO:HA | 1.71 | 0.55 |
| 13:O:657:ILE:HA | 13:O:660:LYS:HB2 | 1.89 | 0.55 |
| 17:Y:100:TYR:HD1 | 17:Y:138:VAL:HG13 | 1.72 | 0.55 |
| 8:I:213:ASP:OD1 | 8:I:215:LYS:N | 2.24 | 0.55 |
| 9:K:258:MET:HG3 | 9:K:271:HIS:CD2 | 2.42 | 0.55 |
| 10:L:75:LYS:HB2 | 10:L:161:PRO:HG3 | 1.89 | 0.55 |
| 12:N:520:ARG:HD2 | 12:N:556:PHE:HD1 | 1.69 | 0.55 |
| 16:S:68:PHE:CE1 | 16:S:78:TRP:HA | 2.42 | 0.55 |
| 17:X:203:LEU:HA | 17:X:206:ILE:HD12 | 1.89 | 0.55 |
| 1:A:1323:GLU:HG3 | 1:A:1324:GLN:N | 2.22 | 0.54 |
| 1:A:1603:LEU:HD22 | 1:A:1605:ALA:H | 1.72 | 0.54 |
| 3:C:417:TYR:CD2 | 13:O:307:LEU:HD22 | 2.42 | 0.54 |
| 9:K:324:SER:O | 9:K:328:THR:HG23 | 2.07 | 0.54 |
| 13:O:119:PHE:CE1 | 13:O:136:LEU:HD11 | 2.42 | 0.54 |
| 9:K:373:TYR:CE1 | 7:W:4:ARG:HG2 | 2.42 | 0.54 |
| 1:A:1610:TYR:O | 1:A:1613:ALA:HB3 | 2.08 | 0.54 |
| 3:C:429:ARG:HG2 | 3:C:432:ASP:HB2 | 1.88 | 0.54 |
| 8:I:46:LEU:HD22 | 8:I:56:TRP:NE1 | 2.23 | 0.54 |
| 8:I:497:TRP:CD1 | 13:O:446:LEU:HB3 | 2.42 | 0.54 |
| 8:I:607:ILE:H | 8:I:607:ILE:HD12 | 1.72 | 0.54 |
| 9:K:177:THR:HG22 | 9:K:365:LYS:HB3 | 1.87 | 0.54 |
| 12:N:681:LEU:HD22 | 12:N:713:PHE:CZ | 2.42 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:373:HIS:NE2 | 14:Q:497:GLY:O | 2.39 | 0.54 |
| 15:R:305:LEU:HD23 | 15:R:336:TRP:CD2 | 2.43 | 0.54 |
| 1:A:1079:ALA:HB1 | 1:A:1556:LEU:HA | 1.89 | 0.54 |
| 3:C:526:TRP:HE1 | 3:C:556:LEU:HD23 | 1.72 | 0.54 |
| 14:Q:305:LEU:HD23 | 14:Q:336:TRP:CD2 | 2.42 | 0.54 |
| 15:R:225:PRO:CG | 16:S:166:GLU:HB2 | 2.38 | 0.54 |
| 16:S:78:TRP:CH2 | 16:S:105:ALA:HA | 2.43 | 0.54 |
| 1:A:1189:ALA:HB3 | 1:A:1192:ASN:HB2 | 1.89 | 0.54 |
| 2:B:72:HIS:ND1 | 2:B:77:ARG:HG3 | 2.21 | 0.54 |
| 3:C:60:PHE:HB2 | 3:P:89:LEU:HD12 | 1.90 | 0.54 |
| 8:I:23:ILE:HD12 | 8:I:37:LEU:HD23 | 1.88 | 0.54 |
| 8:I:79:LEU:HD11 | 8:I:168:LEU:HD23 | 1.88 | 0.54 |
| 12:N:670:PHE:CD1 | 12:N:715:VAL:HB | 2.42 | 0.54 |
| 13:O:354:ARG:HD3 | 13:O:574:LEU:HA | 1.89 | 0.54 |
| 15:R:225:PRO:HG2 | 16:S:166:GLU:HB3 | 1.89 | 0.54 |
| 17:X:294:PHE:CD1 | 17:X:294:PHE:C | 2.80 | 0.54 |
| 17:X:267:LEU:CD1 | 17:Y:59:LEU:CD1 | 2.82 | 0.54 |
| 1:A:1037:VAL:HG22 | 1:A:1562:LEU:HD21 | 1.89 | 0.54 |
| 1:A:775:LEU:O | 1:A:948:PRO:HD3 | 2.07 | 0.54 |
| 3:C:96:VAL:HG21 | 3:P:53:LYS:HD3 | 1.89 | 0.54 |
| 17:X:491:LYS:O | 17:X:494:ASP:OD1 | 2.25 | 0.54 |
| 9:J:322:TYR:HE1 | 11:M:36:LEU:HD11 | 1.73 | 0.54 |
| 9:J:55:ARG:HD2 | 9:K:261:ASP:OD1 | 2.07 | 0.54 |
| 15:R:130:ILE:HG23 | 15:R:131:LEU:N | 2.22 | 0.54 |
| 17:Y:491:LYS:O | 17:Y:494:ASP:OD1 | 2.26 | 0.54 |
| 17:Y:517:ASP:O | 17:Y:520:VAL:HG22 | 2.08 | 0.54 |
| 1:A:612:ILE:O | 1:A:641:TRP:CZ3 | 2.61 | 0.54 |
| 8:I:344:ILE:O | 8:I:348:VAL:HG23 | 2.07 | 0.54 |
| 9:J:277:GLU:OE1 | 9:J:278:LEU:HD23 | 2.07 | 0.54 |
| 9:J:406:HIS:HE1 | 9:J:450:ASN:HD22 | 1.55 | 0.54 |
| 17:X:394:ILE:HG22 | 17:X:397:ARG:NH2 | 2.23 | 0.54 |
| 17:X:517:ASP:O | 17:X:520:VAL:HG22 | 2.08 | 0.54 |
| 6:F:30:ARG:NH2 | 6:H:500:TRP:HB3 | 2.22 | 0.54 |
| 8:I:413:ASN:N | 8:I:447:PHE:HZ | 2.06 | 0.54 |
| 9:K:484:ALA:O | 9:K:488:ILE:HG12 | 2.08 | 0.54 |
| 12:N:395:ASP:HB2 | 12:N:397:ILE:N | 2.18 | 0.54 |
| 13:O:75:LEU:C | 13:O:79:TYR:HD2 | 2.09 | 0.54 |
| 9:J:476:PRO:HB2 | 3:P:148:ASN:HD21 | 1.72 | 0.54 |
| 1:A:1378:THR:HG23 | 1:A:1380:ASN:H | 1.72 | 0.54 |
| 1:A:457:PHE:HB3 | 1:A:468:PHE:CD1 | 2.43 | 0.54 |
| 2:B:34:CYS:N | 2:B:44:CYS:SG | 2.79 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:39:VAL:N | 2:B:40:PRO:CD | 2.71 | 0.54 |
| 8:I:269:LEU:HB3 | 8:I:526:LYS:HZ2 | 1.73 | 0.54 |
| 8:I:278:GLU:HA | 8:I:281:MET:HG2 | 1.88 | 0.54 |
| 8:I:287:LEU:HG | 8:I:456:PHE:CE2 | 2.43 | 0.54 |
| 8:I:337:ILE:HD13 | 8:I:418:PHE:CZ | 2.43 | 0.54 |
| 9:J:204:LEU:HD22 | 9:K:28:LYS:NZ | 2.23 | 0.54 |
| 12:N:331:PHE:CE2 | 12:N:335:ILE:HD11 | 2.42 | 0.54 |
| 9:K:242:TYR:O | 7:W:3:ARG:NH2 | 2.40 | 0.54 |
| 9:J:53:TYR:O | 9:J:79:CYS:SG | 2.66 | 0.54 |
| 9:K:154:LYS:HE2 | 9:K:184:LEU:HD22 | 1.90 | 0.54 |
| 9:K:71:ALA:HA | 9:K:128:ILE:HD13 | 1.90 | 0.54 |
| 10:L:78:CYS:SG | 10:L:119:TRP:CE3 | 3.01 | 0.54 |
| 12:N:368:THR:CB | 12:N:369:ASP:HA | 2.38 | 0.54 |
| 16:S:28:ASN:O | 16:S:90:PRO:HG2 | 2.08 | 0.54 |
| 18:Z:30:SER:O | 18:Z:34:GLN:HG3 | 2.08 | 0.54 |
| 1:A:1921:LEU:HA | 12:N:78:VAL:HG21 | 1.90 | 0.53 |
| 6:F:130:ARG:CG | 17:Y:506:GLN:HB2 | 2.38 | 0.53 |
| 6:F:15:ALA:HA | 6:H:116:PHE:CE1 | 2.43 | 0.53 |
| 8:I:218:SER:OG | 8:I:584:HIS:ND1 | 2.41 | 0.53 |
| 12:N:123:ASP:O | 12:N:127:ARG:N | 2.41 | 0.53 |
| 9:J:476:PRO:CG | 3:P:182:LEU:HG | 2.35 | 0.53 |
| 1:A:1636:VAL:HG12 | 1:A:1666:ILE:HG13 | 1.91 | 0.53 |
| 6:F:145:ASN:HB2 | 6:F:146:PRO:O | 2.08 | 0.53 |
| 8:I:186:GLU:OE1 | 8:I:197:ARG:CZ | 2.53 | 0.53 |
| 8:I:262:LEU:CA | 8:I:265:ILE:HG22 | 2.34 | 0.53 |
| 13:O:68:LEU:HD23 | 13:O:131:VAL:HG12 | 1.89 | 0.53 |
| 1:A:1322:PRO:HG3 | 1:A:1375:TYR:HH | 1.73 | 0.53 |
| 1:A:45:ALA:O | 3:C:180:ARG:NH2 | 2.42 | 0.53 |
| 17:X:76:LYS:HB2 | 17:X:106:GLN:NE2 | 2.23 | 0.53 |
| 1:A:1797:ILE:HG22 | 1:A:1852:ILE:CD1 | 2.39 | 0.53 |
| 8:I:219:VAL:N | 8:I:234:PHE:O | 2.39 | 0.53 |
| 9:K:174:HIS:CE1 | 9:K:211:LYS:CD | 2.90 | 0.53 |
| 14:Q:132:ARG:HG3 | 18:Z:154:LEU:HD23 | 1.90 | 0.53 |
| 17:Y:199:CYS:CB | 17:Y:201:LEU:HD12 | 2.37 | 0.53 |
| 8:I:67:GLU:HB2 | 8:I:85:ALA:HB3 | 1.91 | 0.53 |
| 14:Q:132:ARG:HG3 | 18:Z:154:LEU:HD21 | 1.86 | 0.53 |
| 17:X:434:TYR:HA | 17:X:444:LEU:HD13 | 1.91 | 0.53 |
| 6:F:89:GLU:OE1 | 6:F:130:ARG:NH2 | 2.41 | 0.53 |
| 6:F:7:PRO:HG2 | 6:H:459:ALA:HB2 | 1.91 | 0.53 |
| 13:O:733:CYS:HA | 13:O:736:LEU:HD12 | 1.90 | 0.53 |
| 17:X:104:LEU:HD11 | 17:X:142:MET:SD | 2.49 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 17:Y:42:ARG:CA | 17:Y:82:TYR:CE2 | 2.72 | 0.53 |
| 1:A:1568:GLY:O | 1:A:1571:ARG:HB3 | 2.08 | 0.53 |
| 2:B:46:LEU:HD21 | 2:B:54:CYS:CB | 2.39 | 0.53 |
| 3:C:93:TYR:CE1 | 3:C:98:GLU:OE2 | 2.61 | 0.53 |
| 8:I:115:TRP:CE3 | 8:I:176:LEU:HD22 | 2.44 | 0.53 |
| 8:I:197:ARG:O | 8:I:545:GLY:HA3 | 2.09 | 0.53 |
| 10:L:78:CYS:SG | 10:L:119:TRP:HE3 | 2.32 | 0.53 |
| 12:N:395:ASP:OD2 | 12:N:397:ILE:HB | 2.09 | 0.53 |
| 12:N:501:ILE:O | 12:N:505:LEU:HG | 2.09 | 0.53 |
| 12:N:596:LEU:HB3 | 12:N:601:TRP:HE1 | 1.73 | 0.53 |
| 13:O:33:TYR:CE1 | 13:O:37:VAL:HG21 | 2.43 | 0.53 |
| 13:O:707:LYS:HA | 13:O:710:ILE:HG22 | 1.91 | 0.53 |
| 3:P:488:GLN:HE21 | 3:P:492:LYS:HD2 | 1.73 | 0.53 |
| 1:A:1100:LEU:HB3 | 1:A:1101:PRO:CA | 2.39 | 0.53 |
| 6:H:762:TRP:HA | 6:H:765:ASP:CB | 2.29 | 0.53 |
| 8:I:313:ALA:CB | 8:I:317:LEU:CG | 2.86 | 0.53 |
| 9:K:62:SER:O | 9:K:63:ARG:HG3 | 2.08 | 0.53 |
| 16:S:30:GLN:C | 16:S:36:ARG:NH2 | 2.62 | 0.53 |
| 3:C:415:PRO:HG3 | 3:C:445:LYS:CB | 2.39 | 0.53 |
| 6:F:540:SER:OG | 6:F:575:ASN:ND2 | 2.34 | 0.53 |
| 5:E:86:VAL:HG22 | 6:H:589:PHE:HE1 | 1.73 | 0.53 |
| 9:K:300:VAL:HG12 | 9:K:333:TYR:OH | 2.08 | 0.53 |
| 15:R:247:SER:HB2 | 16:S:170:LYS:HZ3 | 1.73 | 0.53 |
| 16:S:141:TYR:CE1 | 16:S:297:ALA:O | 2.62 | 0.53 |
| 17:Y:42:ARG:HG3 | 17:Y:82:TYR:HH | 1.72 | 0.53 |
| 1:A:1321:VAL:CG2 | 1:A:1322:PRO:HD3 | 2.38 | 0.52 |
| 1:A:214:LEU:CD2 | 1:A:407:LEU:HD13 | 2.39 | 0.52 |
| 2:B:47:VAL:HG21 | 2:B:82:PHE:HD2 | 1.74 | 0.52 |
| 8:I:286:ARG:NE | 8:I:333:LEU:HD13 | 2.18 | 0.52 |
| 9:J:19:TYR:CE1 | 9:J:49:LEU:HD13 | 2.44 | 0.52 |
| 9:J:37:PRO:HB3 | 9:J:69:TYR:OH | 2.08 | 0.52 |
| 9:K:174:HIS:HA | 9:K:211:LYS:HZ3 | 1.74 | 0.52 |
| 16:S:71:GLY:C | 16:S:74:PRO:CD | 2.59 | 0.52 |
| 14:Q:353:GLN:HA | 18:Z:52:THR:HB | 1.91 | 0.52 |
| 3:C:377:GLU:HA | 15:R:130:ILE:HG21 | 1.90 | 0.52 |
| 3:C:449:LEU:HD11 | 3:C:479:GLN:HE22 | 1.74 | 0.52 |
| 12:N:241:HIS:CE1 | 12:N:302:LYS:HE3 | 2.44 | 0.52 |
| 12:N:267:GLN:O | 12:N:271:GLU:HG3 | 2.10 | 0.52 |
| 16:S:25:SER:HB2 | 16:S:45:LEU:CD2 | 2.38 | 0.52 |
| 8:I:32:ARG:HG2 | 12:N:388:HIS:CE1 | 2.45 | 0.52 |
| 12:N:120:SER:O | 12:N:124:PRO:HD2 | 2.09 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:N:60:GLU:C | 12:N:63:ALA:HB2 | 2.30 | 0.52 |
| 14:Q:128:ALA:HA | 18:Z:157:THR:O | 2.09 | 0.52 |
| 17:Y:458:GLN:O | 17:Y:462:LYS:HG3 | 2.09 | 0.52 |
| 1:A:1307:LEU:CD1 | 1:A:1582:ALA:HB2 | 2.36 | 0.52 |
| 1:A:159:ILE:HB | 1:A:171:ALA:HB3 | 1.91 | 0.52 |
| 9:J:204:LEU:HD22 | 9:K:28:LYS:HZ2 | 1.74 | 0.52 |
| 9:K:383:ASN:HB3 | 9:K:386:LEU:HD13 | 1.90 | 0.52 |
| 16:S:29:VAL:CB | 16:S:36:ARG:NH1 | 2.64 | 0.52 |
| 1:A:1181:LEU:HB3 | 1:A:1611:VAL:HG11 | 1.90 | 0.52 |
| 1:A:1516:LEU:HA | 1:A:1519:VAL:HG12 | 1.91 | 0.52 |
| 8:I:279:ILE:HG12 | 8:I:340:SER:HB2 | 1.91 | 0.52 |
| 9:J:481:THR:O | 9:J:485:ILE:HG12 | 2.09 | 0.52 |
| 12:N:596:LEU:HD13 | 12:N:601:TRP:CE2 | 2.45 | 0.52 |
| 13:O:378:SER:OG | 13:O:417:LEU:HD12 | 2.09 | 0.52 |
| 3:P:239:THR:O | 3:P:275:ASN:ND2 | 2.43 | 0.52 |
| 15:R:193:SER:HB3 | 15:R:234:TRP:CE2 | 2.43 | 0.52 |
| 17:Y:42:ARG:HA | 17:Y:82:TYR:OH | 2.09 | 0.52 |
| 1:A:72:GLU:HG3 | 1:A:94:TYR:OH | 2.10 | 0.52 |
| 9:K:509:ARG:HG3 | 9:K:509:ARG:O | 2.09 | 0.52 |
| 12:N:190:LYS:O | 12:N:196:ASP:N | 2.43 | 0.52 |
| 17:Y:100:TYR:CB | 17:Y:142:MET:HG2 | 2.40 | 0.52 |
| 1:A:773:LEU:HD22 | 1:A:779:MET:HG3 | 1.92 | 0.52 |
| 3:C:228:TRP:O | 3:C:231:GLU:N | 2.38 | 0.52 |
| 8:I:116:MET:SD | 8:I:210:LEU:HB3 | 2.50 | 0.52 |
| 6:H:656:MET:CE | 9:K:526:TYR:CD2 | 2.92 | 0.52 |
| 12:N:362:LYS:HA | 12:N:410:LEU:HD22 | 1.91 | 0.52 |
| 13:O:479:GLU:OE1 | 13:O:618:TYR:OH | 2.26 | 0.52 |
| 17:X:397:ARG:HD2 | 17:X:417:TYR:OH | 2.10 | 0.52 |
| 17:X:506:GLN:HG3 | 17:X:508:ASP:OD1 | 2.10 | 0.52 |
| 17:Y:54:ARG:HH11 | 17:Y:54:ARG:HG2 | 1.73 | 0.52 |
| 1:A:1170:ASN:ND2 | 1:A:1203:MET:HG3 | 2.25 | 0.52 |
| 1:A:1639:LYS:HG3 | 1:A:1664:LYS:HB2 | 1.91 | 0.52 |
| 2:B:11:VAL:HG13 | 12:N:642:GLY:HA2 | 1.91 | 0.52 |
| 3:C:335:CYS:HG | 3:C:354:PHE:HE1 | 1.56 | 0.52 |
| 12:N:362:LYS:CB | 12:N:410:LEU:HD21 | 2.23 | 0.52 |
| 14:Q:184:ASP:HA | 16:S:28:ASN:OD1 | 2.09 | 0.52 |
| 17:Y:84:ALA:HB1 | 17:Y:100:TYR:CZ | 2.45 | 0.52 |
| 1:A:1236:LEU:HD12 | 1:A:1237:PRO:HD2 | 1.91 | 0.52 |
| 1:A:436:LEU:HD13 | 1:A:638:LEU:HD22 | 1.91 | 0.52 |
| 9:J:276:VAL:HA | 9:J:311:MET:SD | 2.50 | 0.52 |
| 9:J:469:ARG:O | 9:J:473:VAL:HG23 | 2.10 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:L:33:LEU:HG | 10:L:42:VAL:HG22 | 1.91 | 0.52 |
| 16:S:25:SER:HB2 | 16:S:45:LEU:HG | 1.92 | 0.52 |
| 17:X:423:ILE:HG13 | 17:X:424:ARG:N | 2.25 | 0.52 |
| 17:X:458:GLN:O | 17:X:462:LYS:HG3 | 2.09 | 0.52 |
| 17:Y:506:GLN:HG3 | 17:Y:508:ASP:OD1 | 2.09 | 0.52 |
| 1:A:1409:LEU:HD22 | 1:A:1413:LEU:HG | 1.91 | 0.52 |
| 1:A:1502:PRO:O | 1:A:1503:ASN:HB3 | 2.09 | 0.52 |
| 3:C:316:LEU:CD2 | 3:C:340:TYR:HA | 2.35 | 0.52 |
| 6:F:544:TRP:CE3 | 15:R:499:ARG:HD3 | 2.45 | 0.52 |
| 6:H:130:ARG:NH1 | 9:K:473:VAL:HG22 | 2.24 | 0.52 |
| 8:I:290:PHE:CE1 | 8:I:324:GLN:HB2 | 2.44 | 0.52 |
| 9:J:18:GLN:HE22 | 9:K:134:LEU:CD1 | 2.23 | 0.52 |
| 13:O:136:LEU:HD12 | 13:O:136:LEU:C | 2.30 | 0.52 |
| 17:X:77:TYR:CE1 | 17:X:107:LYS:HB2 | 2.45 | 0.52 |
| 17:X:440:ASN:HA | 17:X:471:GLN:HE22 | 1.75 | 0.52 |
| 9:J:355:ALA:O | 9:J:359:THR:HG23 | 2.11 | 0.51 |
| 6:H:703:PRO:HD2 | 10:L:180:TYR:CD2 | 2.45 | 0.51 |
| 13:O:657:ILE:HG13 | 13:O:704:VAL:HG23 | 1.92 | 0.51 |
| 3:P:303:PHE:HE1 | 3:P:307:LEU:HD22 | 1.75 | 0.51 |
| 16:S:71:GLY:O | 16:S:74:PRO:N | 2.43 | 0.51 |
| 17:Y:495:GLY:HA3 | 17:Y:518:PHE:HE2 | 1.75 | 0.51 |
| 1:A:1237:PRO:CB | 1:A:1238:PRO:HD2 | 2.40 | 0.51 |
| 1:A:1320:ASN:HB3 | 1:A:1323:GLU:HG2 | 1.91 | 0.51 |
| 1:A:442:LEU:HG | 1:A:444:PHE:CE1 | 2.44 | 0.51 |
| 1:A:482:VAL:CG2 | 1:A:593:ASN:HA | 2.40 | 0.51 |
| 8:I:27:VAL:O | 8:I:35:ILE:HD12 | 2.09 | 0.51 |
| 8:I:536:CYS:O | 8:I:540:PRO:CD | 2.58 | 0.51 |
| 9:J:24:PHE:O | 9:J:28:LYS:HG2 | 2.11 | 0.51 |
| 10:L:90:THR:HG21 | 10:L:116:PRO:HD2 | 1.91 | 0.51 |
| 15:R:407:TRP:CZ3 | 15:R:414:LEU:HD11 | 2.45 | 0.51 |
| 1:A:1385:ASP:O | 1:A:1388:ARG:HB2 | 2.10 | 0.51 |
| 8:I:52:PHE:HD1 | 8:I:743:VAL:HG21 | 1.76 | 0.51 |
| 12:N:74:TRP:CH2 | 12:N:77:GLU:HB2 | 2.46 | 0.51 |
| 14:Q:407:TRP:CZ3 | 14:Q:414:LEU:HD11 | 2.44 | 0.51 |
| 1:A:1230:ILE:HD12 | 15:R:116:TRP:HD1 | 1.75 | 0.51 |
| 1:A:1138:HIS:HE1 | 1:A:1604:GLN:NE2 | 2.06 | 0.51 |
| 1:A:1869:HIS:O | 1:A:1872:LEU:HG | 2.10 | 0.51 |
| 6:F:755:LEU:HD13 | 9:J:393:GLN:HE22 | 1.76 | 0.51 |
| 7:G:1:MET:HE1 | 9:J:338:ILE:HD12 | 1.93 | 0.51 |
| 8:I:207:ALA:HB1 | 8:I:575:LEU:HD12 | 1.91 | 0.51 |
| 8:I:393:VAL:O | 8:I:397:ILE:HG13 | 2.11 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:180:GLU:O | 9:J:184:LEU:N | 2.35 | 0.51 |
| 9:J:206:GLU:HA | 9:J:209:LEU:HG | 1.91 | 0.51 |
| 12:N:281:TYR:CE1 | 12:N:357:ALA:HA | 2.46 | 0.51 |
| 12:N:560:MET:SD | 12:N:601:TRP:CD1 | 3.04 | 0.51 |
| 2:B:15:LEU:HD21 | 12:N:635:LEU:HA | 1.91 | 0.51 |
| 12:N:60:GLU:O | 12:N:63:ALA:CB | 2.56 | 0.51 |
| 13:O:414:LEU:HD12 | 13:O:417:LEU:HB2 | 1.92 | 0.51 |
| 3:P:48:LEU:HD21 | 3:P:116:PHE:CE2 | 2.45 | 0.51 |
| 14:Q:193:SER:HB3 | 14:Q:234:TRP:CE2 | 2.45 | 0.51 |
| 15:R:110:LYS:O | 15:R:114:LYS:N | 2.39 | 0.51 |
| 15:R:166:ARG:NH2 | 15:R:472:CYS:O | 2.42 | 0.51 |
| 17:X:281:TYR:CE2 | 17:X:289:ASN:HB3 | 2.45 | 0.51 |
| 1:A:1325:LEU:HD21 | 1:A:1370:ALA:HB1 | 1.92 | 0.51 |
| 1:A:766:LEU:HD22 | 1:A:790:LEU:HD21 | 1.93 | 0.51 |
| 1:A:42:LEU:HD22 | 3:C:363:ARG:HB2 | 1.92 | 0.51 |
| 6:F:50:ARG:NE | 6:H:19:TYR:HE1 | 2.09 | 0.51 |
| 6:F:19:TYR:HE2 | 6:H:50:ARG:HD3 | 1.74 | 0.51 |
| 9:K:263:PHE:HZ | 9:K:290:LYS:HG2 | 1.76 | 0.51 |
| 12:N:233:CYS:O | 12:N:235:GLN:N | 2.44 | 0.51 |
| 3:C:117:LEU:HD23 | 3:C:117:LEU:O | 2.11 | 0.51 |
| 3:C:170:PHE:O | 3:C:173:TYR:HB3 | 2.10 | 0.51 |
| 3:C:318:TYR:HD1 | 9:J:282:ASN:OD1 | 1.93 | 0.51 |
| 12:N:500:ASP:HB2 | 12:N:501:ILE:HD12 | 1.92 | 0.51 |
| 2:B:15:LEU:HD12 | 12:N:633:ARG:HG2 | 1.92 | 0.51 |
| 13:O:114:ASP:CA | 13:O:117:ASP:OD1 | 2.58 | 0.51 |
| 17:X:76:LYS:HB3 | 17:X:106:GLN:HE22 | 1.76 | 0.51 |
| 17:Y:77:TYR:CE1 | 17:Y:107:LYS:HB2 | 2.45 | 0.51 |
| 1:A:661:VAL:HG22 | 1:A:789:LEU:HD12 | 1.92 | 0.51 |
| 3:C:216:LYS:HG2 | 3:C:243:LEU:HD11 | 1.93 | 0.51 |
| 8:I:290:PHE:HD1 | 8:I:324:GLN:CD | 2.15 | 0.51 |
| 12:N:362:LYS:N | 12:N:410:LEU:HD21 | 2.25 | 0.51 |
| 12:N:765:LEU:HD13 | 12:N:768:LEU:HD21 | 1.93 | 0.51 |
| 17:X:226:VAL:HG22 | 17:X:236:LEU:HD23 | 1.93 | 0.51 |
| 17:X:430:ALA:CB | 17:X:451:CYS:SG | 2.99 | 0.51 |
| 17:X:54:ARG:CZ | 17:X:90:ASP:OD2 | 2.59 | 0.51 |
| 1:A:1375:TYR:HB3 | 1:A:1378:THR:CG2 | 2.38 | 0.51 |
| 7:G:11:LEU:HD13 | 9:J:514:PHE:CE2 | 2.45 | 0.51 |
| 6:H:540:SER:OG | 6:H:575:ASN:ND2 | 2.35 | 0.51 |
| 8:I:588:PHE:CE1 | 8:I:599:CYS:HB2 | 2.46 | 0.51 |
| 9:J:245:CYS:HA | 9:J:247:PHE:CE1 | 2.46 | 0.51 |
| 9:K:181:GLU:HB3 | 9:K:209:LEU:HD13 | 1.93 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:K:222:GLU:CD | 9:K:228:GLN:CG | 2.79 | 0.51 |
| 12:N:278:ARG:HA | 12:N:343:GLU:OE2 | 2.10 | 0.51 |
| 3:P:170:PHE:O | 3:P:173:TYR:HB3 | 2.11 | 0.51 |
| 1:A:1235:LEU:CD2 | 1:A:1257:ILE:CG1 | 2.61 | 0.51 |
| 1:A:629:LEU:HB2 | 1:A:630:PRO:HD2 | 1.92 | 0.51 |
| 2:B:16:TRP:HB2 | 2:B:33:CYS:HB3 | 1.92 | 0.51 |
| 12:N:662:VAL:CG2 | 12:N:695:ARG:HG2 | 2.41 | 0.51 |
| 13:O:119:PHE:CE1 | 13:O:136:LEU:HD21 | 2.45 | 0.51 |
| 3:P:303:PHE:CD1 | 3:P:303:PHE:C | 2.83 | 0.51 |
| 14:Q:208:LEU:HD13 | 14:Q:255:VAL:HG21 | 1.93 | 0.51 |
| 16:S:79:ASP:CG | 16:S:120:ARG:HB3 | 2.30 | 0.51 |
| 17:Y:309:ASP:HB2 | 17:Y:340:GLU:HG2 | 1.93 | 0.51 |
| 1:A:1388:ARG:HA | 1:A:1411:ARG:HD2 | 1.92 | 0.51 |
| 1:A:1556:LEU:HD12 | 1:A:1556:LEU:O | 2.11 | 0.51 |
| 8:I:304:PHE:HZ | 8:I:448:VAL:HG13 | 1.76 | 0.51 |
| 9:K:222:GLU:OE1 | 9:K:228:GLN:CG | 2.59 | 0.51 |
| 6:H:703:PRO:HD3 | 10:L:180:TYR:CE2 | 2.46 | 0.51 |
| 12:N:181:LEU:HD22 | 12:N:299:TRP:CE2 | 2.46 | 0.51 |
| 11:M:1:MET:HB2 | 3:P:50:HIS:HB2 | 1.92 | 0.51 |
| 15:R:192:TRP:CG | 15:R:198:LEU:HD13 | 2.45 | 0.51 |
| 16:S:36:ARG:CZ | 16:S:90:PRO:O | 2.59 | 0.51 |
| 1:A:1674:TRP:CD1 | 1:A:1674:TRP:N | 2.79 | 0.50 |
| 1:A:1400:LYS:HA | 10:L:135:PHE:CZ | 2.46 | 0.50 |
| 12:N:570:ILE:HA | 12:N:573:ASN:ND2 | 2.26 | 0.50 |
| 13:O:460:GLN:HG2 | 13:O:496:ARG:HH22 | 1.74 | 0.50 |
| 3:P:228:TRP:O | 3:P:231:GLU:N | 2.38 | 0.50 |
| 3:P:494:ILE:HG21 | 3:P:516:LEU:HD13 | 1.92 | 0.50 |
| 17:X:235:TRP:CE3 | 17:X:236:LEU:HA | 2.47 | 0.50 |
| 17:Y:294:PHE:CE2 | 17:Y:311:TYR:HB2 | 2.46 | 0.50 |
| 3:C:225:PRO:O | 3:C:230:LYS:HD2 | 2.11 | 0.50 |
| 12:N:555:HIS:O | 12:N:559:VAL:HG12 | 2.11 | 0.50 |
| 13:O:648:ILE:CD1 | 13:O:663:ALA:HB1 | 2.41 | 0.50 |
| 15:R:111:GLU:O | 15:R:115:ALA:N | 2.42 | 0.50 |
| 17:X:495:GLY:HA3 | 17:X:518:PHE:CE2 | 2.46 | 0.50 |
| 17:Y:281:TYR:CE2 | 17:Y:289:ASN:HB3 | 2.46 | 0.50 |
| 8:I:138:LEU:HD13 | 8:I:253:ARG:HG2 | 1.92 | 0.50 |
| 8:I:413:ASN:N | 8:I:447:PHE:CZ | 2.78 | 0.50 |
| 9:J:37:PRO:HB3 | 9:J:69:TYR:HE2 | 1.75 | 0.50 |
| 9:K:42:TRP:CE3 | 9:K:42:TRP:HA | 2.46 | 0.50 |
| 12:N:102:ALA:HA | 12:N:107:CYS:C | 2.32 | 0.50 |
| 12:N:751:LEU:HA | 12:N:754:PHE:HD2 | 1.75 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:75:LEU:CD1 | 13:O:161:TYR:CD2 | 2.89 | 0.50 |
| 14:Q:340:PRO:HD3 | 14:Q:345:TRP:CZ2 | 2.47 | 0.50 |
| 15:R:98:GLU:HG2 | 15:R:101:PRO:CD | 2.41 | 0.50 |
| 3:C:277:ARG:HB3 | 15:R:75:GLY:O | 2.11 | 0.50 |
| 17:Y:196:LEU:O | 17:Y:200:PRO:CA | 2.59 | 0.50 |
| 17:Y:423:ILE:HG13 | 17:Y:424:ARG:N | 2.25 | 0.50 |
| 17:Y:452:LEU:CD2 | 17:Y:461:ALA:H | 2.23 | 0.50 |
| 17:Y:73:PRO:O | 17:Y:106:GLN:OE1 | 2.29 | 0.50 |
| 2:B:38:LYS:C | 2:B:40:PRO:HD2 | 2.31 | 0.50 |
| 6:H:537:GLU:OE2 | 6:H:568:GLU:OE1 | 2.28 | 0.50 |
| 9:J:354:MET:CE | 9:J:377:GLU:HB2 | 2.41 | 0.50 |
| 12:N:676:TRP:CE3 | 12:N:680:GLU:HB3 | 2.46 | 0.50 |
| 12:N:75:PHE:O | 12:N:78:VAL:N | 2.44 | 0.50 |
| 3:P:225:PRO:O | 3:P:230:LYS:HD2 | 2.11 | 0.50 |
| 16:S:21:GLU:O | 16:S:45:LEU:HD13 | 2.10 | 0.50 |
| 17:X:495:GLY:HA3 | 17:X:518:PHE:HE2 | 1.75 | 0.50 |
| 1:A:442:LEU:HG | 1:A:444:PHE:HE1 | 1.77 | 0.50 |
| 1:A:873:VAL:CG2 | 1:A:951:ILE:CG2 | 2.89 | 0.50 |
| 6:F:26:PHE:CD1 | 6:H:149:TRP:CB | 2.94 | 0.50 |
| 8:I:174:ASN:OD1 | 8:I:190:TYR:HA | 2.12 | 0.50 |
| 8:I:304:PHE:CZ | 8:I:448:VAL:CG1 | 2.95 | 0.50 |
| 12:N:370:GLN:HG2 | 12:N:373:GLN:HB2 | 1.93 | 0.50 |
| 3:P:234:LEU:HD22 | 3:P:238:TYR:CZ | 2.46 | 0.50 |
| 14:Q:192:TRP:CG | 14:Q:198:LEU:HD13 | 2.46 | 0.50 |
| 17:X:269:ASP:HB3 | 17:X:300:LEU:HD21 | 1.92 | 0.50 |
| 1:A:1234:ALA:HB1 | 1:A:1272:VAL:HB | 1.93 | 0.50 |
| 1:A:1300:LEU:HD13 | 1:A:1369:LEU:HD13 | 1.94 | 0.50 |
| 3:C:361:ASN:HB3 | 3:C:363:ARG:N | 2.27 | 0.50 |
| 8:I:245:LEU:HB3 | 8:I:246:PRO:HD3 | 1.93 | 0.50 |
| 1:A:1601:TYR:OH | 10:L:102:PHE:HD1 | 1.95 | 0.50 |
| 14:Q:425:LEU:N | 14:Q:425:LEU:HD12 | 2.27 | 0.50 |
| 17:Y:146:TYR:CD1 | 17:Y:154:ASP:HB2 | 2.47 | 0.50 |
| 17:Y:495:GLY:HA3 | 17:Y:518:PHE:CE2 | 2.46 | 0.50 |
| 18:Z:138:THR:HG23 | 18:Z:142:LEU:HD12 | 1.93 | 0.50 |
| 1:A:1523:LEU:O | 1:A:1526:VAL:HG22 | 2.11 | 0.50 |
| 1:A:1840:MET:HE2 | 1:A:1845:LEU:HG | 1.94 | 0.50 |
| 8:I:306:HIS:CE1 | 8:I:313:ALA:HB1 | 2.46 | 0.50 |
| 8:I:317:LEU:CD2 | 8:I:320:LEU:HD23 | 2.40 | 0.50 |
| 8:I:441:THR:O | 8:I:445:ILE:HG12 | 2.12 | 0.50 |
| 12:N:659:VAL:HG22 | 12:N:660:THR:N | 2.27 | 0.50 |
| 15:R:81:PRO:HG3 | 15:R:131:LEU:HD21 | 1.94 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:S:273:THR:O | 16:S:274:VAL:HB | 2.12 | 0.50 |
| 18:Z:72:LEU:HD11 | 18:Z:155:ILE:HD11 | 1.92 | 0.50 |
| 1:A:489:LEU:HD22 | 1:A:497:LEU:HD22 | 1.94 | 0.50 |
| 1:A:852:LEU:HD11 | 1:A:1819:GLU:HB3 | 1.93 | 0.50 |
| 1:A:39:LEU:HD21 | 3:C:393:GLU:HG2 | 1.93 | 0.50 |
| 3:C:415:PRO:HG3 | 3:C:445:LYS:HB3 | 1.92 | 0.50 |
| 6:H:164:PRO:HG3 | 6:H:471:LYS:HG3 | 1.93 | 0.50 |
| 8:I:47:HIS:CE1 | 8:I:54:ARG:NH1 | 2.79 | 0.50 |
| 9:K:185:LEU:HA | 9:K:188:LEU:CD2 | 2.40 | 0.50 |
| 6:H:704:LEU:HD22 | 10:L:181:ARG:HA | 1.93 | 0.50 |
| 11:M:59:ASP:C | 11:M:61:ALA:H | 2.14 | 0.50 |
| 12:N:180:PHE:CE2 | 12:N:240:PHE:HB3 | 2.47 | 0.50 |
| 15:R:77:ASP:OD1 | 15:R:77:ASP:N | 2.45 | 0.50 |
| 1:A:436:LEU:HB3 | 1:A:638:LEU:HD13 | 1.93 | 0.50 |
| 1:A:95:VAL:HG21 | 1:A:126:ALA:HB3 | 1.93 | 0.50 |
| 8:I:282:GLN:O | 8:I:285:SER:HB3 | 2.12 | 0.50 |
| 15:R:340:PRO:HD3 | 15:R:345:TRP:CZ2 | 2.47 | 0.50 |
| 17:X:294:PHE:CE2 | 17:X:311:TYR:HB2 | 2.46 | 0.50 |
| 17:Y:235:TRP:CE3 | 17:Y:236:LEU:HA | 2.47 | 0.50 |
| 1:A:1325:LEU:HD21 | 1:A:1370:ALA:CB | 2.42 | 0.49 |
| 1:A:1086:MET:HE1 | 1:A:1564:LEU:HD13 | 1.94 | 0.49 |
| 3:C:273:TYR:HB3 | 3:C:282:ALA:HB2 | 1.94 | 0.49 |
| 8:I:266:ASN:HA | 8:I:526:LYS:NZ | 2.26 | 0.49 |
| 9:J:17:GLN:HB3 | 9:K:78:ARG:HH12 | 1.77 | 0.49 |
| 15:R:209:TRP:HB2 | 16:S:227:LEU:HD13 | 1.94 | 0.49 |
| 1:A:1230:ILE:HA | 1:A:1236:LEU:HD13 | 1.94 | 0.49 |
| 1:A:485:ILE:HD11 | 1:A:609:ILE:HB | 1.94 | 0.49 |
| 13:O:311:HIS:HB2 | 13:O:320:ALA:HB2 | 1.92 | 0.49 |
| 13:O:657:ILE:HG22 | 13:O:660:LYS:HE2 | 1.94 | 0.49 |
| 16:S:199:ARG:O | 16:S:203:GLN:HG2 | 2.11 | 0.49 |
| 16:S:23:GLU:OE2 | 18:Z:134:GLN:CA | 2.60 | 0.49 |
| 1:A:480:ALA:HB1 | 1:A:590:PRO:HG3 | 1.94 | 0.49 |
| 3:C:251:TYR:HB3 | 3:C:269:ILE:CD1 | 2.42 | 0.49 |
| 6:H:465:LEU:HD22 | 6:H:495:HIS:CE1 | 2.47 | 0.49 |
| 9:J:213:ASN:OD1 | 9:J:214:LYS:N | 2.45 | 0.49 |
| 9:J:247:PHE:CE2 | 9:J:277:GLU:CB | 2.96 | 0.49 |
| 9:K:227:LEU:O | 9:K:230:ASN:HB3 | 2.13 | 0.49 |
| 9:K:406:HIS:CE1 | 7:W:6:PRO:CB | 2.95 | 0.49 |
| 12:N:409:VAL:O | 12:N:410:LEU:HB2 | 2.11 | 0.49 |
| 12:N:393:THR:HG23 | 12:N:434:THR:HG22 | 1.94 | 0.49 |
| 12:N:577:GLU:HB3 | 12:N:625:LYS:CE | 2.40 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:R:112:HIS:CD2 | 15:R:116:TRP:HZ3 | 2.29 | 0.49 |
| 17:Y:226:VAL:HG22 | 17:Y:236:LEU:HD23 | 1.94 | 0.49 |
| 1:A:1229:SER:HA | 1:A:1235:LEU:HB3 | 1.94 | 0.49 |
| 1:A:1401:PRO:HD3 | 10:L:135:PHE:CE2 | 2.47 | 0.49 |
| 1:A:1555:HIS:O | 1:A:1559:HIS:CD2 | 2.64 | 0.49 |
| 5:E:94:TRP:CZ2 | 6:F:592:ARG:HG2 | 2.46 | 0.49 |
| 6:F:739:VAL:O | 6:F:743:ILE:HG13 | 2.13 | 0.49 |
| 6:H:656:MET:O | 6:H:660:LYS:HG3 | 2.12 | 0.49 |
| 8:I:203:GLY:HA3 | 8:I:223:VAL:HG22 | 1.94 | 0.49 |
| 9:J:441:VAL:O | 9:J:442:ASP:CB | 2.59 | 0.49 |
| 9:K:372:LEU:HD22 | 9:K:404:VAL:HG22 | 1.94 | 0.49 |
| 15:R:208:LEU:HD13 | 15:R:255:VAL:HG21 | 1.93 | 0.49 |
| 17:Y:269:ASP:HB3 | 17:Y:300:LEU:HD21 | 1.94 | 0.49 |
| 1:A:1551:ASN:OD1 | 1:A:1554:PHE:CD2 | 2.65 | 0.49 |
| 6:H:743:ILE:HG22 | 6:H:759:ASN:HD21 | 1.77 | 0.49 |
| 10:L:63:LEU:HD22 | 10:L:138:GLN:HE21 | 1.77 | 0.49 |
| 12:N:249:ARG:HB3 | 12:N:250:LEU:HD23 | 1.94 | 0.49 |
| 3:P:117:LEU:O | 3:P:117:LEU:HD23 | 2.11 | 0.49 |
| 14:Q:430:TYR:CD1 | 14:Q:431:PRO:HA | 2.48 | 0.49 |
| 15:R:430:TYR:CD1 | 15:R:431:PRO:HA | 2.48 | 0.49 |
| 3:C:313:LYS:HG2 | 3:C:343:LEU:HD22 | 1.95 | 0.49 |
| 8:I:639:LEU:HB2 | 8:I:652:VAL:HG12 | 1.93 | 0.49 |
| 13:O:233:PRO:HA | 13:O:263:ARG:HH21 | 1.77 | 0.49 |
| 3:P:303:PHE:C | 3:P:303:PHE:HD1 | 2.14 | 0.49 |
| 15:R:239:ASN:ND2 | 15:R:240:TYR:CE2 | 2.81 | 0.49 |
| 16:S:55:LEU:O | 16:S:59:LYS:HD3 | 2.12 | 0.49 |
| 8:I:116:MET:HE1 | 8:I:211:SER:O | 2.13 | 0.49 |
| 9:J:397:ILE:CG2 | 9:J:398:ALA:H | 2.25 | 0.49 |
| 13:O:707:LYS:CA | 13:O:710:ILE:HG22 | 2.42 | 0.49 |
| 15:R:425:LEU:N | 15:R:425:LEU:HD12 | 2.28 | 0.49 |
| 1:A:248:PHE:CZ | 1:A:250:ASN:HB2 | 2.48 | 0.49 |
| 1:A:78:LYS:HD3 | 1:A:592:HIS:HB2 | 1.94 | 0.49 |
| 3:C:48:LEU:HD21 | 3:C:116:PHE:CZ | 2.47 | 0.49 |
| 6:H:739:VAL:O | 6:H:743:ILE:HG13 | 2.13 | 0.49 |
| 8:I:337:ILE:O | 8:I:341:TYR:CD2 | 2.66 | 0.49 |
| 8:I:207:ALA:CB | 8:I:575:LEU:HD12 | 2.43 | 0.49 |
| 9:J:376:LEU:HD23 | 9:J:407:GLU:HG2 | 1.93 | 0.49 |
| 9:K:256:VAL:O | 9:K:259:GLU:HG2 | 2.12 | 0.49 |
| 9:K:441:VAL:HG13 | 9:K:474:LEU:HD22 | 1.95 | 0.49 |
| 12:N:63:ALA:HB3 | 12:N:64:ALA:CB | 2.42 | 0.49 |
| 13:O:402:LEU:HD13 | 13:O:425:LYS:CG | 2.42 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:509:LEU:HG | 13:O:513:LYS:HE3 | 1.95 | 0.49 |
| 1:A:945:GLU:O | 13:O:599:ILE:HD13 | 2.13 | 0.49 |
| 17:X:376:LEU:HD11 | 17:X:398:GLU:OE2 | 2.13 | 0.49 |
| 17:X:393:ILE:HG22 | 17:X:397:ARG:HD3 | 1.94 | 0.49 |
| 17:X:170:LYS:HA | 17:Y:49:LEU:CD2 | 2.42 | 0.49 |
| 1:A:1086:MET:CE | 1:A:1564:LEU:HD13 | 2.42 | 0.49 |
| 1:A:1160:TYR:HB2 | 13:O:332:GLN:HB3 | 1.93 | 0.49 |
| 1:A:1770:LEU:HD13 | 1:A:1798:ARG:HH22 | 1.78 | 0.49 |
| 9:J:165:GLU:HB2 | 9:K:21:SER:HB2 | 1.94 | 0.49 |
| 7:G:3:ARG:HB2 | 9:J:443:LYS:HZ1 | 1.77 | 0.49 |
| 10:L:24:GLU:HG3 | 10:L:159:TYR:CE1 | 2.48 | 0.49 |
| 12:N:156:MET:O | 12:N:160:VAL:HG23 | 2.12 | 0.49 |
| 12:N:180:PHE:CG | 12:N:299:TRP:HH2 | 2.30 | 0.49 |
| 1:A:455:VAL:HB | 1:A:471:VAL:HG12 | 1.94 | 0.49 |
| 3:C:296:ARG:HD3 | 3:P:101:ARG:HH22 | 1.78 | 0.49 |
| 6:H:145:ASN:HB2 | 6:H:146:PRO:C | 2.34 | 0.49 |
| 8:I:412:LYS:C | 8:I:447:PHE:HZ | 2.15 | 0.49 |
| 8:I:36:ALA:HB2 | 8:I:80:LEU:HD21 | 1.94 | 0.49 |
| 10:L:45:LEU:HD11 | 10:L:156:ILE:HD12 | 1.95 | 0.49 |
| 12:N:545:LEU:O | 12:N:549:PHE:N | 2.46 | 0.49 |
| 1:A:1157:TRP:HA | 13:O:332:GLN:OE1 | 2.12 | 0.49 |
| 13:O:36:ALA:CB | 13:O:75:LEU:HD21 | 2.43 | 0.49 |
| 13:O:669:LYS:HZ1 | 13:O:751:LEU:HD13 | 1.78 | 0.49 |
| 13:O:78:LEU:HD12 | 13:O:78:LEU:O | 2.13 | 0.49 |
| 3:P:119:MET:HG2 | 3:P:158:LEU:HD21 | 1.95 | 0.49 |
| 16:S:21:GLU:O | 16:S:45:LEU:HD21 | 2.06 | 0.49 |
| 1:A:436:LEU:H | 1:A:501:THR:CG2 | 2.26 | 0.48 |
| 8:I:424:ALA:O | 8:I:428:MET:HG2 | 2.13 | 0.48 |
| 12:N:659:VAL:HG22 | 12:N:660:THR:H | 1.77 | 0.48 |
| 3:P:334:CYS:HB3 | 3:P:357:ALA:HB2 | 1.94 | 0.48 |
| 6:F:500:TRP:CB | 6:H:30:ARG:NH2 | 2.74 | 0.48 |
| 9:J:294:LEU:HD12 | 9:K:54:HIS:HE2 | 1.78 | 0.48 |
| 12:N:286:LEU:O | 12:N:288:GLU:N | 2.46 | 0.48 |
| 16:S:68:PHE:HE1 | 16:S:78:TRP:CG | 2.31 | 0.48 |
| 17:X:168:THR:OG1 | 17:X:171:ILE:CD1 | 2.61 | 0.48 |
| 17:Y:376:LEU:HD11 | 17:Y:398:GLU:OE2 | 2.12 | 0.48 |
| 1:A:1644:TYR:O | 1:A:1645:GLU:HG2 | 2.13 | 0.48 |
| 3:C:466:GLU:HG3 | 15:R:82:HIS:CD2 | 2.49 | 0.48 |
| 6:F:537:GLU:CD | 6:F:600:TYR:OH | 2.52 | 0.48 |
| 8:I:446:THR:O | 8:I:449:ALA:HB3 | 2.12 | 0.48 |
| 9:J:20:GLN:HA | 9:J:20:GLN:OE1 | 2.14 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:297:SER:O | 9:J:329:LEU:HD11 | 2.13 | 0.48 |
| 9:J:215:PRO:HB2 | 9:J:435:ILE:HD11 | 1.95 | 0.48 |
| 12:N:281:TYR:CZ | 12:N:284:SER:HB3 | 2.48 | 0.48 |
| 12:N:700:LEU:HD13 | 12:N:707:GLU:HG3 | 1.95 | 0.48 |
| 13:O:422:ILE:O | 13:O:426:THR:HG22 | 2.14 | 0.48 |
| 14:Q:239:ASN:ND2 | 14:Q:240:TYR:CE2 | 2.81 | 0.48 |
| 16:S:38:MET:CE | 18:Z:199:TYR:CE2 | 2.69 | 0.48 |
| 6:F:130:ARG:HG2 | 17:Y:506:GLN:HB2 | 1.96 | 0.48 |
| 18:Z:91:ILE:HG12 | 18:Z:150:SER:HB3 | 1.95 | 0.48 |
| 1:A:1082:VAL:HG22 | 1:A:1138:HIS:CG | 2.48 | 0.48 |
| 1:A:1136:SER:O | 1:A:1139:ASN:HB3 | 2.13 | 0.48 |
| 1:A:612:ILE:O | 1:A:641:TRP:HZ3 | 1.95 | 0.48 |
| 3:C:33:LYS:NZ | 3:C:64:ALA:HA | 2.29 | 0.48 |
| 6:H:102:SER:OG | 6:H:104:ASP:OD1 | 2.17 | 0.48 |
| 6:H:743:ILE:HG22 | 6:H:759:ASN:ND2 | 2.29 | 0.48 |
| 6:F:459:ALA:HB2 | 6:H:7:PRO:HG2 | 1.95 | 0.48 |
| 6:H:736:GLU:OE1 | 10:L:177:PHE:HB2 | 2.13 | 0.48 |
| 12:N:523:LEU:HD22 | 12:N:538:GLU:OE1 | 2.12 | 0.48 |
| 14:Q:208:LEU:CD1 | 14:Q:255:VAL:HG21 | 2.43 | 0.48 |
| 3:C:334:CYS:HB3 | 3:C:357:ALA:HB2 | 1.95 | 0.48 |
| 3:C:413:LYS:O | 3:C:415:PRO:HD3 | 2.14 | 0.48 |
| 6:F:164:PRO:CG | 6:F:471:LYS:HG3 | 2.43 | 0.48 |
| 8:I:300:VAL:HA | 8:I:303:GLU:CD | 2.31 | 0.48 |
| 8:I:290:PHE:CE2 | 8:I:325:LEU:HD12 | 2.47 | 0.48 |
| 8:I:427:ARG:HB2 | 8:I:428:MET:CE | 2.42 | 0.48 |
| 16:S:82:ILE:CD1 | 16:S:102:LEU:HD23 | 2.43 | 0.48 |
| 16:S:58:GLN:C | 16:S:62:PHE:CD2 | 2.84 | 0.48 |
| 1:A:1405:LEU:CD1 | 1:A:1467:GLY:HA2 | 2.41 | 0.48 |
| 3:C:265:ILE:O | 3:C:269:ILE:HG12 | 2.14 | 0.48 |
| 6:H:564:LYS:O | 6:H:565:ASN:HB2 | 2.14 | 0.48 |
| 8:I:290:PHE:HB3 | 8:I:320:LEU:HD11 | 1.95 | 0.48 |
| 9:K:228:GLN:HA | 9:K:233:VAL:HG21 | 1.95 | 0.48 |
| 9:K:458:LEU:HB3 | 9:K:460:LYS:HG3 | 1.95 | 0.48 |
| 12:N:88:SER:O | 12:N:91:PHE:HB3 | 2.13 | 0.48 |
| 12:N:91:PHE:CZ | 12:N:94:ALA:HB2 | 2.49 | 0.48 |
| 15:R:208:LEU:CD1 | 15:R:255:VAL:HG21 | 2.43 | 0.48 |
| 6:F:541:THR:HG23 | 15:R:499:ARG:HG2 | 1.96 | 0.48 |
| 17:X:393:ILE:HG22 | 17:X:397:ARG:HH11 | 1.78 | 0.48 |
| 1:A:1080:LEU:N | 1:A:1081:PRO:HD2 | 2.29 | 0.48 |
| 1:A:1602:HIS:O | 1:A:1603:LEU:HB3 | 2.13 | 0.48 |
| 1:A:772:GLU:HG3 | 1:A:867:CYS:HA | 1.95 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:49:LEU:HD13 | 8:I:730:VAL:HG21 | 1.95 | 0.48 |
| 8:I:269:LEU:HB2 | 8:I:526:LYS:HZ1 | 1.77 | 0.48 |
| 12:N:91:PHE:CE1 | 12:N:94:ALA:HB2 | 2.48 | 0.48 |
| 13:O:281:LEU:HD21 | 13:O:283:LEU:HD12 | 1.95 | 0.48 |
| 13:O:356:ASP:HA | 13:O:357:SER:CB | 2.42 | 0.48 |
| 15:R:105:GLN:O | 15:R:107:PRO:HD3 | 2.14 | 0.48 |
| 16:S:19:GLY:HA3 | 18:Z:134:GLN:CG | 2.44 | 0.48 |
| 17:X:99:LYS:HD3 | 17:X:102:MET:CE | 2.43 | 0.48 |
| 17:X:339:ALA:O | 17:X:343:VAL:HG23 | 2.14 | 0.48 |
| 17:Y:168:THR:OG1 | 17:Y:171:ILE:CD1 | 2.61 | 0.48 |
| 17:Y:338:HIS:O | 17:Y:341:PRO:HD2 | 2.14 | 0.48 |
| 1:A:437:CYS:HA | 1:A:626:LYS:HD2 | 1.96 | 0.48 |
| 1:A:799:LEU:C | 1:A:801:PRO:HD2 | 2.33 | 0.48 |
| 6:F:152:PHE:CE1 | 6:F:162:PRO:HG2 | 2.49 | 0.48 |
| 6:H:486:ASN:O | 6:H:490:HIS:CD2 | 2.67 | 0.48 |
| 8:I:410:SER:O | 8:I:414:PHE:HD2 | 1.95 | 0.48 |
| 12:N:519:TYR:CE1 | 12:N:523:LEU:HD21 | 2.49 | 0.48 |
| 13:O:635:GLY:O | 13:O:637:PRO:HD3 | 2.14 | 0.48 |
| 17:X:436:THR:HG23 | 17:X:437:LEU:HD12 | 1.96 | 0.48 |
| 18:Z:138:THR:HG23 | 18:Z:142:LEU:CD1 | 2.44 | 0.48 |
| 1:A:1201:HIS:CE1 | 1:A:1203:MET:HB2 | 2.49 | 0.48 |
| 1:A:1573:SER:HB2 | 1:A:1617:ARG:HH21 | 1.78 | 0.48 |
| 3:C:521:PHE:HD1 | 3:C:553:ILE:HG22 | 1.74 | 0.48 |
| 8:I:188:TYR:HA | 8:I:193:PHE:O | 2.14 | 0.48 |
| 9:J:413:PHE:CD1 | 9:J:454:VAL:HG12 | 2.49 | 0.48 |
| 10:L:144:ASN:ND2 | 10:L:151:THR:HG23 | 2.29 | 0.48 |
| 12:N:706:ARG:HB2 | 12:N:716:ILE:HD13 | 1.94 | 0.48 |
| 13:O:423:ALA:O | 13:O:426:THR:HG23 | 2.13 | 0.48 |
| 13:O:681:PRO:O | 13:O:682:LYS:HB2 | 2.14 | 0.48 |
| 3:P:437:VAL:HG22 | 3:P:469:ALA:HB2 | 1.96 | 0.48 |
| 15:R:98:GLU:HG2 | 15:R:101:PRO:CG | 2.41 | 0.48 |
| 1:A:174:PRO:HG2 | 1:A:175:PHE:CD2 | 2.49 | 0.48 |
| 3:C:209:LEU:O | 3:C:213:ILE:HG12 | 2.14 | 0.48 |
| 6:F:130:ARG:HH11 | 17:Y:506:GLN:CB | 2.27 | 0.48 |
| 6:F:564:LYS:O | 6:F:565:ASN:HB2 | 2.13 | 0.48 |
| 8:I:294:LYS:CB | 8:I:320:LEU:HD13 | 2.43 | 0.48 |
| 9:J:230:ASN:OD1 | 9:J:231:LEU:N | 2.47 | 0.48 |
| 17:Y:339:ALA:O | 17:Y:343:VAL:HG23 | 2.13 | 0.48 |
| 18:Z:81:VAL:HG21 | 18:Z:155:ILE:HD12 | 1.96 | 0.48 |
| 1:A:1621:PRO:HG3 | 1:A:1653:ALA:CB | 2.44 | 0.47 |
| 3:C:48:LEU:HD21 | 3:C:116:PHE:CE2 | 2.49 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:59:ARG:HH12 | 6:H:562:MET:HB2 | 1.79 | 0.47 |
| 6:F:673:CYS:O | 6:F:677:VAL:HG23 | 2.14 | 0.47 |
| 10:L:75:LYS:HA | 10:L:131:PRO:HB3 | 1.95 | 0.47 |
| 3:C:145:GLN:CG | 13:O:246:PHE:HA | 2.43 | 0.47 |
| 3:P:48:LEU:HD21 | 3:P:116:PHE:CZ | 2.48 | 0.47 |
| 16:S:79:ASP:CB | 16:S:120:ARG:HH11 | 2.27 | 0.47 |
| 17:X:452:LEU:CD2 | 17:X:461:ALA:H | 2.23 | 0.47 |
| 3:C:317:SER:OG | 11:M:27:GLU:HG3 | 2.14 | 0.47 |
| 6:H:121:LEU:HG | 6:H:125:TYR:HE1 | 1.79 | 0.47 |
| 9:J:393:GLN:O | 9:J:396:SER:HB3 | 2.13 | 0.47 |
| 12:N:765:LEU:HA | 12:N:765:LEU:HD23 | 1.70 | 0.47 |
| 3:P:265:ILE:O | 3:P:269:ILE:HG12 | 2.14 | 0.47 |
| 16:S:197:GLN:C | 16:S:200:VAL:HG22 | 2.34 | 0.47 |
| 1:A:1235:LEU:HD21 | 1:A:1257:ILE:CD1 | 2.40 | 0.47 |
| 8:I:673:LEU:HA | 8:I:676:ASN:HB2 | 1.95 | 0.47 |
| 12:N:556:PHE:CZ | 12:N:600:PHE:HA | 2.49 | 0.47 |
| 13:O:411:LYS:HE2 | 13:O:412:HIS:HE1 | 1.74 | 0.47 |
| 13:O:39:VAL:HG11 | 13:O:97:ILE:HG13 | 1.94 | 0.47 |
| 3:P:308:TYR:CD2 | 14:Q:499:ARG:HD2 | 2.49 | 0.47 |
| 16:S:188:ARG:HH12 | 18:Z:147:VAL:CG1 | 2.26 | 0.47 |
| 8:I:206:LEU:HD22 | 8:I:570:PHE:CD2 | 2.50 | 0.47 |
| 9:K:227:LEU:O | 9:K:230:ASN:N | 2.48 | 0.47 |
| 9:K:263:PHE:CZ | 9:K:290:LYS:HG2 | 2.49 | 0.47 |
| 12:N:282:GLU:O | 12:N:284:SER:N | 2.44 | 0.47 |
| 3:P:316:LEU:CD1 | 3:P:340:TYR:HB2 | 2.44 | 0.47 |
| 14:Q:166:ARG:CZ | 14:Q:413:GLU:OE1 | 2.62 | 0.47 |
| 15:R:112:HIS:CE1 | 15:R:116:TRP:HZ3 | 2.31 | 0.47 |
| 16:S:141:TYR:CE1 | 16:S:297:ALA:C | 2.88 | 0.47 |
| 1:A:1172:TYR:CZ | 1:A:1176:LEU:HD23 | 2.49 | 0.47 |
| 3:C:101:ARG:CZ | 3:P:296:ARG:HA | 2.44 | 0.47 |
| 6:F:537:GLU:OE1 | 6:F:600:TYR:CE2 | 2.67 | 0.47 |
| 9:J:272:ILE:HD11 | 9:J:304:ALA:HB2 | 1.97 | 0.47 |
| 9:K:350:HIS:ND1 | 9:K:377:GLU:OE1 | 2.47 | 0.47 |
| 10:L:29:ALA:O | 10:L:31:TRP:CD1 | 2.67 | 0.47 |
| 13:O:91:ASN:O | 13:O:95:ILE:HG12 | 2.14 | 0.47 |
| 3:P:209:LEU:O | 3:P:213:ILE:HG12 | 2.15 | 0.47 |
| 1:A:1078:MET:HB2 | 1:A:1552:TYR:CE1 | 2.50 | 0.47 |
| 1:A:1511:ASN:HD22 | 1:A:1511:ASN:H | 1.60 | 0.47 |
| 3:C:180:ARG:HG3 | 3:C:212:LEU:HD21 | 1.97 | 0.47 |
| 8:I:276:TRP:HA | 8:I:279:ILE:HG22 | 1.96 | 0.47 |
| 9:J:456:ARG:CG | 9:J:488:ILE:HG22 | 2.44 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:69:TYR:O | 9:J:70:GLU:CB | 2.62 | 0.47 |
| 18:Z:80:SER:O | 18:Z:157:THR:HB | 2.14 | 0.47 |
| 1:A:1064:GLU:HA | 1:A:1125:ILE:HD11 | 1.97 | 0.47 |
| 1:A:93:LEU:HD11 | 1:A:151:ILE:HD12 | 1.97 | 0.47 |
| 8:I:442:GLN:HE21 | 13:O:69:GLN:HG2 | 1.80 | 0.47 |
| 9:J:191:SER:O | 9:J:193:LEU:HG | 2.14 | 0.47 |
| 9:J:58:HIS:CD2 | 9:K:262:PRO:HD3 | 2.50 | 0.47 |
| 13:O:129:THR:O | 13:O:130:SER:CB | 2.61 | 0.47 |
| 16:S:25:SER:HB2 | 16:S:45:LEU:HD21 | 1.96 | 0.47 |
| 17:X:349:SER:HA | 17:X:352:SER:OG | 2.15 | 0.47 |
| 1:A:1413:LEU:HD22 | 1:A:1416:TRP:HZ3 | 1.80 | 0.47 |
| 1:A:665:MET:O | 1:A:669:GLY:N | 2.44 | 0.47 |
| 3:C:550:LEU:HD22 | 3:C:553:ILE:HD11 | 1.97 | 0.47 |
| 8:I:291:VAL:HG12 | 8:I:298:THR:HA | 1.96 | 0.47 |
| 13:O:628:ALA:HB2 | 13:O:643:LEU:HD22 | 1.97 | 0.47 |
| 13:O:710:ILE:O | 13:O:713:VAL:HG12 | 2.14 | 0.47 |
| 16:S:21:GLU:O | 16:S:45:LEU:CD1 | 2.62 | 0.47 |
| 3:C:333:THR:O | 3:C:337:ILE:HG12 | 2.15 | 0.47 |
| 6:F:96:VAL:HG12 | 6:F:97:PHE:CD1 | 2.50 | 0.47 |
| 9:J:220:ILE:HG12 | 9:J:240:ARG:NH1 | 2.30 | 0.47 |
| 9:J:475:ILE:HD11 | 9:J:478:ASN:ND2 | 2.28 | 0.47 |
| 9:K:499:VAL:HG11 | 9:K:523:ILE:CD1 | 2.45 | 0.47 |
| 12:N:202:GLU:OE1 | 12:N:202:GLU:O | 2.33 | 0.47 |
| 12:N:542:VAL:HG11 | 12:N:558:GLU:CD | 2.35 | 0.47 |
| 12:N:567:SER:HB2 | 12:N:594:VAL:O | 2.14 | 0.47 |
| 14:Q:196:ASN:ND2 | 14:Q:211:ALA:HB3 | 2.30 | 0.47 |
| 17:Y:42:ARG:CB | 17:Y:82:TYR:OH | 2.63 | 0.47 |
| 2:B:16:TRP:CH2 | 12:N:630:LYS:CE | 2.98 | 0.47 |
| 3:C:119:MET:HG2 | 3:C:158:LEU:HD21 | 1.97 | 0.47 |
| 6:H:146:PRO:CG | 6:H:167:THR:HA | 2.45 | 0.47 |
| 8:I:70:CYS:C | 8:I:71:LEU:HD12 | 2.35 | 0.47 |
| 9:J:78:ARG:NH1 | 9:K:17:GLN:HB3 | 2.29 | 0.47 |
| 12:N:273:MET:CG | 12:N:277:CYS:SG | 2.95 | 0.47 |
| 12:N:577:GLU:HG2 | 12:N:583:ALA:HB2 | 1.97 | 0.47 |
| 12:N:73:GLU:O | 12:N:74:TRP:CB | 2.63 | 0.47 |
| 3:P:274:HIS:O | 3:P:276:ILE:O | 2.33 | 0.47 |
| 3:P:358:LEU:CD1 | 3:P:368:TRP:CE2 | 2.98 | 0.47 |
| 3:P:365:LEU:HB3 | 3:P:395:ASN:HD21 | 1.80 | 0.47 |
| 16:S:83:SER:C | 16:S:87:GLN:HG3 | 2.34 | 0.47 |
| 1:A:162:HIS:HD2 | 1:A:168:ASP:HB3 | 1.79 | 0.47 |
| 1:A:804:ASP:N | 1:A:804:ASP:OD1 | 2.48 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:845:TYR:HB3 | 1:A:1812:TRP:CZ3 | 2.50 | 0.47 |
| 8:I:301:GLN:O | 8:I:304:PHE:N | 2.48 | 0.47 |
| 8:I:578:ASN:ND2 | 8:I:646:ASP:HB3 | 2.30 | 0.47 |
| 9:J:496:GLU:HB2 | 9:J:526:TYR:CE1 | 2.50 | 0.47 |
| 9:K:284:LEU:HD12 | 9:K:311:MET:HE1 | 1.97 | 0.47 |
| 6:H:97:PHE:HA | 9:K:433:LYS:HD3 | 1.97 | 0.47 |
| 9:K:248:LYS:N | 9:K:438:GLU:OE2 | 2.48 | 0.47 |
| 2:B:27:ARG:HD3 | 12:N:813:GLY:HA2 | 1.97 | 0.47 |
| 13:O:123:GLU:N | 13:O:124:PRO:HA | 2.30 | 0.47 |
| 13:O:36:ALA:O | 13:O:39:VAL:HG12 | 2.15 | 0.47 |
| 13:O:425:LYS:HB2 | 13:O:441:GLN:HG2 | 1.96 | 0.47 |
| 14:Q:186:TYR:CE2 | 16:S:27:GLU:HB2 | 2.49 | 0.47 |
| 16:S:141:TYR:CE2 | 16:S:299:PRO:HD3 | 2.50 | 0.47 |
| 3:C:259:PHE:HB3 | 3:C:265:ILE:HD13 | 1.94 | 0.46 |
| 6:F:146:PRO:CG | 6:F:167:THR:HA | 2.46 | 0.46 |
| 6:F:481:CYS:HB2 | 6:F:512:LEU:HD13 | 1.96 | 0.46 |
| 6:H:537:GLU:CD | 6:H:600:TYR:OH | 2.53 | 0.46 |
| 8:I:287:LEU:O | 8:I:291:VAL:HG23 | 2.15 | 0.46 |
| 8:I:399:LYS:HG2 | 8:I:525:VAL:HG21 | 1.98 | 0.46 |
| 9:K:443:LYS:O | 9:K:446:PRO:HD2 | 2.15 | 0.46 |
| 9:J:322:TYR:CZ | 11:M:31:ILE:HD13 | 2.50 | 0.46 |
| 12:N:258:ALA:HA | 12:N:261:VAL:HG22 | 1.97 | 0.46 |
| 3:P:361:ASN:HB3 | 3:P:363:ARG:N | 2.30 | 0.46 |
| 3:P:388:TYR:HB3 | 3:P:405:LEU:HG | 1.98 | 0.46 |
| 14:Q:442:HIS:CE1 | 14:Q:468:ARG:HD2 | 2.51 | 0.46 |
| 15:R:461:ALA:HB2 | 15:R:467:LEU:CD1 | 2.45 | 0.46 |
| 17:Y:349:SER:HA | 17:Y:352:SER:OG | 2.15 | 0.46 |
| 1:A:442:LEU:HB3 | 1:A:455:VAL:HG13 | 1.96 | 0.46 |
| 2:B:16:TRP:CZ2 | 2:B:45:PRO:HA | 2.50 | 0.46 |
| 5:E:99:ILE:HD11 | 5:E:103:LEU:HD13 | 1.98 | 0.46 |
| 6:F:98:ASN:OD1 | 6:F:98:ASN:N | 2.47 | 0.46 |
| 6:H:592:ARG:HA | 6:H:592:ARG:HD3 | 1.66 | 0.46 |
| 8:I:25:PHE:CD1 | 8:I:71:LEU:HD13 | 2.50 | 0.46 |
| 8:I:440:MET:HB3 | 8:I:445:ILE:HD11 | 1.97 | 0.46 |
| 8:I:561:ARG:NH2 | 8:I:589:THR:O | 2.44 | 0.46 |
| 7:G:4:ARG:HB2 | 9:J:373:TYR:HE1 | 1.81 | 0.46 |
| 9:K:280:LYS:HB3 | 9:K:283:GLU:HG2 | 1.97 | 0.46 |
| 6:H:541:THR:CG2 | 10:L:184:ARG:HB3 | 2.45 | 0.46 |
| 12:N:753:LEU:HG | 12:N:757:TYR:HE1 | 1.81 | 0.46 |
| 3:P:405:LEU:HA | 3:P:408:THR:HG22 | 1.97 | 0.46 |
| 17:X:339:ALA:HB2 | 17:X:369:ASN:HB2 | 1.97 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:X:494:ASP:OD1 | 17:X:494:ASP:N | 2.48 | 0.46 |
| 17:Y:494:ASP:OD1 | 17:Y:494:ASP:N | 2.48 | 0.46 |
| 1:A:256:VAL:HB | 1:A:269:TRP:HB2 | 1.98 | 0.46 |
| 1:A:957:ASP:CG | 1:A:1820:PHE:HZ | 2.19 | 0.46 |
| 3:C:477:HIS:CD2 | 3:C:482:GLU:OE1 | 2.64 | 0.46 |
| 6:F:533:VAL:HG23 | 6:F:559:LEU:HD22 | 1.97 | 0.46 |
| 8:I:145:LEU:HD13 | 8:I:267:LEU:HD22 | 1.98 | 0.46 |
| 4:D:5:PHE:CE1 | 13:O:427:ALA:HB1 | 2.51 | 0.46 |
| 15:R:130:ILE:HG23 | 15:R:131:LEU:H | 1.78 | 0.46 |
| 17:X:40:HIS:CB | 17:Y:201:LEU:HD11 | 2.36 | 0.46 |
| 1:A:1477:ALA:HA | 1:A:1525:MET:O | 2.14 | 0.46 |
| 1:A:1621:PRO:HG3 | 1:A:1653:ALA:HB1 | 1.97 | 0.46 |
| 1:A:252:ASP:HB2 | 1:A:253:PRO:HD3 | 1.98 | 0.46 |
| 6:F:164:PRO:HG3 | 6:F:471:LYS:HG3 | 1.98 | 0.46 |
| 5:E:89:LEU:HD11 | 6:H:592:ARG:HB2 | 1.97 | 0.46 |
| 6:H:98:ASN:OD1 | 6:H:98:ASN:N | 2.49 | 0.46 |
| 8:I:414:PHE:CE1 | 8:I:451:PHE:HE1 | 2.31 | 0.46 |
| 8:I:437:LEU:HA | 8:I:438:ASN:C | 2.35 | 0.46 |
| 8:I:413:ASN:C | 8:I:447:PHE:CE1 | 2.89 | 0.46 |
| 9:J:219:VAL:O | 9:J:221:PRO:HD3 | 2.14 | 0.46 |
| 9:K:167:PHE:O | 9:K:171:THR:HG22 | 2.15 | 0.46 |
| 9:K:298:ASN:OD1 | 9:K:300:VAL:HG22 | 2.15 | 0.46 |
| 9:K:496:GLU:HB2 | 9:K:526:TYR:CE1 | 2.50 | 0.46 |
| 9:K:8:LYS:HD2 | 9:K:8:LYS:HA | 1.82 | 0.46 |
| 9:K:93:LEU:HD12 | 9:K:93:LEU:N | 2.31 | 0.46 |
| 15:R:124:ASP:O | 15:R:127:GLU:O | 2.33 | 0.46 |
| 16:S:36:ARG:NH2 | 16:S:90:PRO:O | 2.48 | 0.46 |
| 17:X:146:TYR:CD1 | 17:X:154:ASP:HB2 | 2.50 | 0.46 |
| 17:X:373:VAL:O | 17:X:376:LEU:N | 2.46 | 0.46 |
| 17:X:406:ARG:HB2 | 17:X:409:CYS:SG | 2.56 | 0.46 |
| 17:X:63:MET:SD | 17:Y:235:TRP:NE1 | 2.89 | 0.46 |
| 3:C:358:LEU:O | 3:C:362:PRO:HB3 | 2.15 | 0.46 |
| 8:I:139:LEU:HD21 | 8:I:192:MET:CE | 2.45 | 0.46 |
| 8:I:28:TRP:CD1 | 8:I:723:ALA:HB1 | 2.51 | 0.46 |
| 8:I:238:THR:HG22 | 8:I:548:MET:SD | 2.55 | 0.46 |
| 9:J:185:LEU:HD11 | 9:J:205:PHE:HB2 | 1.96 | 0.46 |
| 9:J:36:GLU:HG2 | 9:J:37:PRO:HD2 | 1.98 | 0.46 |
| 9:K:230:ASN:OD1 | 9:K:231:LEU:N | 2.48 | 0.46 |
| 1:A:1753:TYR:CD2 | 13:O:643:LEU:HD12 | 2.42 | 0.46 |
| 3:P:120:TYR:CE2 | 3:P:124:LEU:HD11 | 2.51 | 0.46 |
| 14:Q:163:LYS:HD3 | 15:R:466:THR:HG22 | 1.97 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:R:190:VAL:HG12 | 15:R:450:THR:HG21 | 1.98 | 0.46 |
| 17:Y:350:PHE:CZ | 17:Y:378:LEU:HD12 | 2.50 | 0.46 |
| 1:A:1294:TYR:CD1 | 1:A:1294:TYR:C | 2.89 | 0.46 |
| 3:C:101:ARG:NH2 | 3:P:296:ARG:HA | 2.31 | 0.46 |
| 3:C:120:TYR:CE2 | 3:C:124:LEU:HD11 | 2.50 | 0.46 |
| 3:C:359:LYS:HG2 | 11:M:14:LEU:HD22 | 1.97 | 0.46 |
| 6:H:58:TYR:OH | 6:H:62:LYS:HD2 | 2.16 | 0.46 |
| 8:I:11:PHE:HD1 | 8:I:746:MET:HA | 1.80 | 0.46 |
| 8:I:142:LEU:HD13 | 8:I:264:TYR:CE2 | 2.51 | 0.46 |
| 8:I:189:ALA:N | 8:I:193:PHE:O | 2.48 | 0.46 |
| 8:I:202:ALA:O | 8:I:221:THR:OG1 | 2.30 | 0.46 |
| 8:I:45:LEU:CD2 | 8:I:54:ARG:NH1 | 2.79 | 0.46 |
| 8:I:513:LEU:HD23 | 13:O:473:LEU:HD11 | 1.98 | 0.46 |
| 8:I:685:PHE:HA | 8:I:701:PRO:HD3 | 1.98 | 0.46 |
| 8:I:73:TRP:CD2 | 8:I:80:LEU:HD13 | 2.50 | 0.46 |
| 9:J:42:TRP:CE3 | 9:J:42:TRP:HA | 2.50 | 0.46 |
| 13:O:126:VAL:HG13 | 13:O:132:VAL:HG12 | 1.98 | 0.46 |
| 13:O:292:GLY:HA3 | 13:O:336:ASP:CB | 2.45 | 0.46 |
| 13:O:621:SER:HB3 | 13:O:651:ILE:HG12 | 1.96 | 0.46 |
| 15:R:196:ASN:ND2 | 15:R:211:ALA:HB3 | 2.31 | 0.46 |
| 15:R:296:ARG:CD | 16:S:272:ILE:HG12 | 2.46 | 0.46 |
| 17:X:87:LEU:HD22 | 17:X:95:ASN:HD22 | 1.80 | 0.46 |
| 1:A:1037:VAL:HA | 1:A:1040:LEU:HB2 | 1.98 | 0.46 |
| 1:A:956:ARG:NH1 | 1:A:1785:GLU:OE1 | 2.48 | 0.46 |
| 1:A:948:PRO:HB3 | 1:A:1813:GLN:CD | 2.36 | 0.46 |
| 9:J:334:GLY:N | 9:J:335:PRO:CD | 2.79 | 0.46 |
| 1:A:40:ARG:HG2 | 13:O:248:PRO:HG2 | 1.98 | 0.46 |
| 17:Y:436:THR:HG23 | 17:Y:437:LEU:HD12 | 1.98 | 0.46 |
| 1:A:1326:TYR:HB2 | 1:A:1386:TRP:CZ2 | 2.50 | 0.46 |
| 1:A:1079:ALA:HB1 | 1:A:1556:LEU:CA | 2.45 | 0.46 |
| 1:A:40:ARG:CZ | 13:O:248:PRO:HB2 | 2.46 | 0.46 |
| 6:F:58:TYR:OH | 6:F:62:LYS:HD2 | 2.16 | 0.46 |
| 6:H:142:LEU:HA | 6:H:146:PRO:HB3 | 1.97 | 0.46 |
| 9:J:147:THR:O | 9:J:150:THR:HG22 | 2.16 | 0.46 |
| 9:J:354:MET:CE | 9:J:374:ILE:HG23 | 2.46 | 0.46 |
| 9:J:46:CYS:O | 9:J:50:THR:OG1 | 2.22 | 0.46 |
| 9:J:93:LEU:N | 9:J:93:LEU:HD12 | 2.31 | 0.46 |
| 9:K:222:GLU:OE1 | 9:K:228:GLN:HG3 | 2.16 | 0.46 |
| 6:H:702:ASN:ND2 | 10:L:180:TYR:CD1 | 2.84 | 0.46 |
| 10:L:87:GLU:CD | 10:L:146:GLN:HE22 | 2.19 | 0.46 |
| 13:O:354:ARG:CD | 13:O:573:LYS:O | 2.63 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:290:ARG:NH2 | 3:P:319:LEU:HD12 | 2.26 | 0.46 |
| 15:R:85:ALA:O | 15:R:88:MET:HB2 | 2.15 | 0.46 |
| 18:Z:159:LYS:HB3 | 18:Z:159:LYS:HE2 | 1.78 | 0.46 |
| 18:Z:158:ASP:C | 18:Z:160:ASP:H | 2.19 | 0.46 |
| 3:C:516:LEU:HD22 | 3:C:520:TYR:CE2 | 2.50 | 0.46 |
| 3:C:66:PRO:O | 3:C:67:LEU:HB3 | 2.16 | 0.46 |
| 6:H:473:TYR:HD2 | 6:H:500:TRP:CZ2 | 2.34 | 0.46 |
| 8:I:286:ARG:O | 8:I:290:PHE:CG | 2.69 | 0.46 |
| 8:I:45:LEU:HG | 8:I:57:SER:HA | 1.98 | 0.46 |
| 9:J:445:GLU:CA | 9:J:474:LEU:HD23 | 2.43 | 0.46 |
| 9:J:514:PHE:O | 9:J:518:MET:HB2 | 2.16 | 0.46 |
| 9:K:502:PHE:CZ | 9:K:518:MET:HG3 | 2.51 | 0.46 |
| 13:O:571:CYS:SG | 13:O:579:MET:HB3 | 2.56 | 0.46 |
| 1:A:1745:PRO:HB3 | 13:O:609:ALA:HB1 | 1.97 | 0.46 |
| 3:P:358:LEU:O | 3:P:362:PRO:HB3 | 2.15 | 0.46 |
| 3:P:365:LEU:HD23 | 3:P:395:ASN:ND2 | 2.31 | 0.46 |
| 15:R:127:GLU:HA | 15:R:128:ALA:HA | 1.70 | 0.46 |
| 16:S:29:VAL:HG11 | 18:Z:140:THR:HB | 1.98 | 0.46 |
| 1:A:1246:PRO:HB2 | 1:A:1249:VAL:HG23 | 1.98 | 0.46 |
| 1:A:776:ASN:HA | 1:A:869:ARG:NE | 2.31 | 0.46 |
| 6:F:563:ASP:OD1 | 6:F:564:LYS:O | 2.34 | 0.46 |
| 6:H:656:MET:SD | 9:K:523:ILE:HG23 | 2.56 | 0.46 |
| 6:H:729:LEU:HD13 | 6:H:739:VAL:HG22 | 1.98 | 0.46 |
| 9:K:180:GLU:O | 9:K:184:LEU:N | 2.35 | 0.46 |
| 12:N:531:PHE:O | 12:N:533:PHE:HA | 2.15 | 0.46 |
| 13:O:159:GLN:O | 13:O:163:GLN:HG2 | 2.15 | 0.46 |
| 3:C:145:GLN:HG3 | 13:O:246:PHE:CG | 2.50 | 0.46 |
| 13:O:274:LEU:HD23 | 13:O:275:LEU:HD12 | 1.98 | 0.46 |
| 3:P:373:HIS:O | 3:P:377:GLU:HG2 | 2.15 | 0.46 |
| 1:A:1230:ILE:HG21 | 15:R:120:LEU:HD23 | 1.98 | 0.46 |
| 17:Y:145:CYS:O | 17:Y:149:LEU:HG | 2.15 | 0.46 |
| 1:A:617:LEU:HD11 | 1:A:782:GLY:CA | 2.46 | 0.45 |
| 8:I:202:ALA:O | 8:I:223:VAL:CG2 | 2.64 | 0.45 |
| 9:K:481:THR:O | 9:K:485:ILE:HG13 | 2.16 | 0.45 |
| 10:L:73:THR:HG22 | 10:L:131:PRO:HB2 | 1.97 | 0.45 |
| 12:N:155:THR:HA | 12:N:158:ARG:HD2 | 1.99 | 0.45 |
| 3:C:390:HIS:CD2 | 13:O:280:ARG:NH2 | 2.84 | 0.45 |
| 3:P:33:LYS:NZ | 3:P:64:ALA:HA | 2.30 | 0.45 |
| 17:X:145:CYS:O | 17:X:149:LEU:HG | 2.15 | 0.45 |
| 1:A:1176:LEU:HA | 1:A:1176:LEU:HD22 | 1.67 | 0.45 |
| 1:A:1522:SER:O | 1:A:1526:VAL:HG13 | 2.17 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1543:HIS:CD2 | 1:A:1559:HIS:HE1 | 2.34 | 0.45 |
| 1:A:94:TYR:HE1 | 1:A:96:ALA:HB2 | 1.81 | 0.45 |
| 1:A:94:TYR:O | 1:A:100:VAL:HA | 2.16 | 0.45 |
| 3:C:93:TYR:CD1 | 3:C:98:GLU:OE2 | 2.69 | 0.45 |
| 3:C:92:ALA:O | 3:C:96:VAL:HG23 | 2.16 | 0.45 |
| 8:I:278:GLU:HA | 8:I:281:MET:SD | 2.55 | 0.45 |
| 8:I:72:ALA:C | 8:I:80:LEU:HD12 | 2.37 | 0.45 |
| 9:J:69:TYR:O | 9:J:70:GLU:HB3 | 2.16 | 0.45 |
| 15:R:261:LEU:N | 15:R:261:LEU:CD1 | 2.79 | 0.45 |
| 17:X:283:ARG:O | 17:X:407:LEU:HD12 | 2.16 | 0.45 |
| 1:A:872:LEU:HD11 | 1:A:939:PHE:CD2 | 2.52 | 0.45 |
| 1:A:957:ASP:OD2 | 1:A:1820:PHE:HZ | 1.99 | 0.45 |
| 5:E:55:CYS:O | 5:E:58:VAL:HG12 | 2.17 | 0.45 |
| 6:F:19:TYR:HE2 | 6:H:50:ARG:CD | 2.28 | 0.45 |
| 8:I:166:LYS:O | 8:I:170:ASP:N | 2.45 | 0.45 |
| 8:I:74:ARG:HD2 | 8:I:174:ASN:HD22 | 1.81 | 0.45 |
| 9:J:332:THR:H | 9:J:363:LEU:HD11 | 1.82 | 0.45 |
| 9:J:334:GLY:HA3 | 9:J:364:MET:SD | 2.57 | 0.45 |
| 12:N:519:TYR:HE1 | 12:N:523:LEU:HD21 | 1.82 | 0.45 |
| 2:B:17:VAL:CG2 | 12:N:634:THR:H | 2.21 | 0.45 |
| 13:O:226:ASP:OD1 | 13:O:227:GLU:N | 2.48 | 0.45 |
| 13:O:62:GLN:O | 13:O:66:PRO:CD | 2.64 | 0.45 |
| 13:O:738:ARG:CZ | 13:O:738:ARG:HB3 | 2.45 | 0.45 |
| 3:P:515:TYR:HA | 3:P:518:GLN:HG2 | 1.99 | 0.45 |
| 14:Q:188:ASN:O | 14:Q:231:SER:HA | 2.16 | 0.45 |
| 15:R:442:HIS:CE1 | 15:R:468:ARG:HD2 | 2.51 | 0.45 |
| 17:X:338:HIS:O | 17:X:341:PRO:HD2 | 2.16 | 0.45 |
| 1:A:1019:MET:HB2 | 1:A:1021:HIS:CE1 | 2.52 | 0.45 |
| 1:A:1086:MET:HG2 | 1:A:1610:TYR:CE1 | 2.52 | 0.45 |
| 1:A:613:ALA:HB1 | 1:A:619:GLN:HB2 | 1.98 | 0.45 |
| 1:A:628:ILE:HG12 | 1:A:765:VAL:HG11 | 1.98 | 0.45 |
| 1:A:860:TYR:CG | 1:A:861:PRO:HD2 | 2.51 | 0.45 |
| 8:I:737:ASN:OD1 | 8:I:738:LEU:N | 2.49 | 0.45 |
| 9:K:248:LYS:HB2 | 9:K:438:GLU:OE2 | 2.17 | 0.45 |
| 13:O:402:LEU:HD13 | 13:O:425:LYS:HE2 | 1.98 | 0.45 |
| 16:S:200:VAL:HG23 | 16:S:201:SER:N | 2.32 | 0.45 |
| 16:S:261:PRO:O | 16:S:263:PRO:N | 2.49 | 0.45 |
| 16:S:58:GLN:O | 16:S:62:PHE:CE2 | 2.65 | 0.45 |
| 17:X:168:THR:OG1 | 17:X:171:ILE:HD12 | 2.17 | 0.45 |
| 17:X:87:LEU:HD22 | 17:X:95:ASN:ND2 | 2.30 | 0.45 |
| 17:Y:316:ALA:HB1 | 17:Y:351:TYR:CZ | 2.52 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:Z:75:TRP:NE1 | 18:Z:161:LEU:HD21 | 2.31 | 0.45 |
| 1:A:1089:LEU:CD1 | 1:A:1611:VAL:HG23 | 2.45 | 0.45 |
| 2:B:42:ASP:O | 2:B:43:ASP:CB | 2.64 | 0.45 |
| 6:F:639:TYR:CD1 | 15:R:498:ILE:HG21 | 2.52 | 0.45 |
| 6:H:515:TYR:CE2 | 6:H:545:HIS:CD2 | 3.03 | 0.45 |
| 9:K:384:SER:HB3 | 9:K:415:ASN:OD1 | 2.16 | 0.45 |
| 10:L:98:VAL:HB | 10:L:134:THR:HG21 | 1.99 | 0.45 |
| 13:O:83:GLU:HG3 | 13:O:90:ALA:CB | 2.47 | 0.45 |
| 3:P:92:ALA:O | 3:P:96:VAL:HG23 | 2.16 | 0.45 |
| 14:Q:261:LEU:N | 14:Q:261:LEU:CD1 | 2.79 | 0.45 |
| 14:Q:498:ILE:O | 14:Q:499:ARG:HB2 | 2.16 | 0.45 |
| 15:R:88:MET:O | 15:R:91:ALA:HB3 | 2.16 | 0.45 |
| 16:S:29:VAL:CG1 | 16:S:36:ARG:CZ | 2.91 | 0.45 |
| 16:S:41:LEU:HD12 | 18:Z:141:PHE:CB | 2.47 | 0.45 |
| 14:Q:179:PRO:HB3 | 16:S:555:ARG:CZ | 2.47 | 0.45 |
| 18:Z:83:LYS:HA | 18:Z:102:PHE:O | 2.17 | 0.45 |
| 1:A:1540:ARG:NH1 | 12:N:486:ASP:O | 2.50 | 0.45 |
| 1:A:617:LEU:HD11 | 1:A:782:GLY:HA3 | 1.97 | 0.45 |
| 5:E:96:PHE:HB2 | 6:H:595:GLN:HE21 | 1.82 | 0.45 |
| 8:I:300:VAL:C | 8:I:303:GLU:HB2 | 2.36 | 0.45 |
| 9:J:376:LEU:CD2 | 9:J:407:GLU:HG2 | 2.47 | 0.45 |
| 12:N:76:VAL:O | 12:N:80:GLN:HB3 | 2.16 | 0.45 |
| 3:P:379:LYS:HD2 | 3:P:379:LYS:HA | 1.75 | 0.45 |
| 14:Q:190:VAL:HG12 | 14:Q:450:THR:HG21 | 1.99 | 0.45 |
| 1:A:1138:HIS:O | 1:A:1141:VAL:N | 2.50 | 0.45 |
| 1:A:42:LEU:HD21 | 3:C:394:VAL:HG13 | 1.99 | 0.45 |
| 8:I:118:VAL:HG12 | 8:I:173:LEU:O | 2.16 | 0.45 |
| 9:J:354:MET:HE2 | 9:J:374:ILE:HG23 | 1.98 | 0.45 |
| 9:K:231:LEU:HA | 9:K:234:VAL:HG22 | 1.98 | 0.45 |
| 12:N:281:TYR:HE2 | 12:N:356:PRO:HB2 | 1.71 | 0.45 |
| 13:O:119:PHE:CZ | 13:O:136:LEU:HD11 | 2.52 | 0.45 |
| 16:S:85:THR:HB | 16:S:98:MET:CE | 2.47 | 0.45 |
| 17:X:442:GLN:CG | 17:X:472:ARG:CG | 2.79 | 0.45 |
| 17:Y:341:PRO:O | 17:Y:344:VAL:HG12 | 2.16 | 0.45 |
| 17:Y:485:LEU:O | 17:Y:489:GLU:HG2 | 2.17 | 0.45 |
| 18:Z:56:THR:HG23 | 18:Z:62:ILE:HG13 | 1.99 | 0.45 |
| 1:A:1145:LEU:HD22 | 1:A:1611:VAL:HG21 | 1.99 | 0.45 |
| 1:A:239:VAL:HG21 | 1:A:409:ILE:HD12 | 1.97 | 0.45 |
| 5:E:89:LEU:HD21 | 6:H:588:LYS:HB3 | 1.98 | 0.45 |
| 6:H:639:TYR:CD1 | 6:H:658:PHE:HE1 | 2.35 | 0.45 |
| 8:I:116:MET:SD | 8:I:210:LEU:CG | 3.02 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:I:304:PHE:CZ | 8:I:448:VAL:HG13 | 2.51 | 0.45 |
| 9:J:418:TRP:CZ3 | 9:J:457:LYS:HG3 | 2.52 | 0.45 |
| 12:N:570:ILE:CD1 | 12:N:633:ARG:NH1 | 2.73 | 0.45 |
| 13:O:604:LEU:HB3 | 13:O:627:LEU:CD2 | 2.46 | 0.45 |
| 3:P:242:GLN:O | 3:P:243:LEU:HB2 | 2.17 | 0.45 |
| 3:P:312:MET:H | 3:P:312:MET:HG2 | 1.62 | 0.45 |
| 3:P:402:TRP:CH2 | 3:P:424:ARG:HG2 | 2.52 | 0.45 |
| 3:P:487:ALA:HB1 | 3:P:519:TYR:HE1 | 1.82 | 0.45 |
| 16:S:85:THR:HB | 16:S:98:MET:HE2 | 1.99 | 0.45 |
| 17:X:134:SER:O | 17:X:138:VAL:HG23 | 2.17 | 0.45 |
| 1:A:1279:ARG:HG2 | 1:A:1280:PRO:HD2 | 1.98 | 0.45 |
| 1:A:93:LEU:HD21 | 1:A:151:ILE:HG13 | 1.99 | 0.45 |
| 2:B:16:TRP:CD1 | 2:B:33:CYS:CA | 2.86 | 0.45 |
| 3:C:494:ILE:HA | 3:C:497:ILE:HD12 | 1.99 | 0.45 |
| 6:H:556:SER:OG | 6:H:573:ALA:HA | 2.17 | 0.45 |
| 8:I:12:ARG:O | 8:I:744:PHE:HA | 2.17 | 0.45 |
| 8:I:224:SER:HB2 | 8:I:230:GLU:H | 1.81 | 0.45 |
| 8:I:276:TRP:CZ2 | 8:I:280:LEU:HD22 | 2.51 | 0.45 |
| 8:I:17:LYS:HE3 | 8:I:51:SER:O | 2.15 | 0.45 |
| 9:K:277:GLU:OE1 | 9:K:277:GLU:HA | 2.16 | 0.45 |
| 13:O:394:THR:HA | 13:O:615:ARG:NH1 | 2.32 | 0.45 |
| 3:P:273:TYR:HB3 | 3:P:282:ALA:HB2 | 1.99 | 0.45 |
| 14:Q:355:GLN:O | 18:Z:136:THR:HG21 | 2.17 | 0.45 |
| 17:Y:532:TYR:CE1 | 17:Y:548:GLY:HA3 | 2.52 | 0.45 |
| 1:A:1189:ALA:HB3 | 1:A:1192:ASN:HD22 | 1.81 | 0.45 |
| 1:A:87:VAL:HG12 | 1:A:88:ASP:N | 2.32 | 0.45 |
| 3:C:550:LEU:O | 3:C:553:ILE:HG12 | 2.17 | 0.45 |
| 6:F:465:LEU:HD22 | 6:F:495:HIS:CE1 | 2.52 | 0.45 |
| 9:J:50:THR:O | 9:J:50:THR:HG22 | 2.16 | 0.45 |
| 9:K:50:THR:O | 9:K:50:THR:HG22 | 2.17 | 0.45 |
| 10:L:24:GLU:HA | 10:L:158:ILE:O | 2.16 | 0.45 |
| 12:N:268:VAL:HA | 12:N:271:GLU:CD | 2.38 | 0.45 |
| 12:N:434:THR:O | 12:N:437:GLN:N | 2.50 | 0.45 |
| 3:P:66:PRO:HD2 | 3:P:68:ALA:O | 2.17 | 0.45 |
| 15:R:84:SER:HB2 | 15:R:87:GLN:HB3 | 1.99 | 0.45 |
| 16:S:134:GLU:C | 16:S:136:LEU:N | 2.68 | 0.45 |
| 17:Y:406:ARG:HB2 | 17:Y:409:CYS:SG | 2.57 | 0.45 |
| 1:A:1781:GLN:HB2 | 1:A:1783:THR:HG22 | 1.98 | 0.44 |
| 6:F:130:ARG:HD2 | 6:F:133:LYS:HD3 | 1.99 | 0.44 |
| 8:I:347:LEU:O | 8:I:351:HIS:HB2 | 2.17 | 0.44 |
| 9:J:468:HIS:HB3 | 9:J:485:ILE:HG23 | 1.99 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:N:400:TYR:CZ | 12:N:404:ILE:HD11 | 2.52 | 0.44 |
| 12:N:574:ILE:HG13 | 12:N:625:LYS:HE2 | 1.99 | 0.44 |
| 12:N:655:LEU:HA | 12:N:724:ARG:O | 2.17 | 0.44 |
| 14:Q:461:ALA:HB2 | 14:Q:467:LEU:CD1 | 2.47 | 0.44 |
| 17:X:134:SER:N | 17:X:137:GLU:OE1 | 2.50 | 0.44 |
| 17:X:235:TRP:NE1 | 17:Y:63:MET:SD | 2.90 | 0.44 |
| 17:X:87:LEU:HD13 | 17:X:95:ASN:ND2 | 2.31 | 0.44 |
| 3:C:89:LEU:HD12 | 3:P:60:PHE:HB2 | 1.99 | 0.44 |
| 3:C:96:VAL:N | 3:C:97:LYS:HA | 2.32 | 0.44 |
| 6:H:689:LEU:HD11 | 6:H:716:ASN:HD21 | 1.81 | 0.44 |
| 12:N:74:TRP:CG | 12:N:75:PHE:N | 2.85 | 0.44 |
| 13:O:99:LEU:C | 13:O:99:LEU:HD12 | 2.37 | 0.44 |
| 16:S:162:TYR:HD2 | 16:S:174:ILE:CD1 | 2.30 | 0.44 |
| 17:Y:168:THR:OG1 | 17:Y:171:ILE:HD12 | 2.18 | 0.44 |
| 1:A:173:LEU:HA | 1:A:174:PRO:HD2 | 1.88 | 0.44 |
| 1:A:268:VAL:O | 1:A:412:LEU:HD23 | 2.17 | 0.44 |
| 3:C:126:GLY:C | 3:C:148:ASN:OD1 | 2.55 | 0.44 |
| 7:G:15:ASP:O | 9:J:487:TYR:OH | 2.34 | 0.44 |
| 6:H:473:TYR:CD2 | 6:H:500:TRP:HZ2 | 2.35 | 0.44 |
| 6:H:703:PRO:CD | 10:L:180:TYR:CD2 | 3.00 | 0.44 |
| 8:I:269:LEU:HD11 | 8:I:522:LEU:HD13 | 1.99 | 0.44 |
| 8:I:410:SER:O | 8:I:413:ASN:HB2 | 2.17 | 0.44 |
| 8:I:276:TRP:CZ3 | 8:I:476:GLY:HA3 | 2.52 | 0.44 |
| 9:J:163:CYS:SG | 9:J:163:CYS:O | 2.75 | 0.44 |
| 9:J:227:LEU:HD22 | 9:J:233:VAL:HG11 | 2.00 | 0.44 |
| 9:J:476:PRO:HB2 | 3:P:148:ASN:ND2 | 2.32 | 0.44 |
| 12:N:550:GLY:HA2 | 12:N:551:GLU:HB2 | 1.99 | 0.44 |
| 12:N:609:LEU:HD22 | 12:N:639:HIS:HD2 | 1.83 | 0.44 |
| 16:S:30:GLN:CB | 16:S:91:GLN:CB | 2.92 | 0.44 |
| 16:S:25:SER:HB2 | 16:S:45:LEU:CG | 2.47 | 0.44 |
| 17:X:485:LEU:O | 17:X:489:GLU:HG2 | 2.17 | 0.44 |
| 17:Y:261:LEU:HD22 | 17:Y:267:LEU:HD23 | 1.99 | 0.44 |
| 17:Y:87:LEU:HD11 | 17:Y:99:LYS:HG3 | 1.99 | 0.44 |
| 1:A:1790:TYR:O | 1:A:1793:MET:HB2 | 2.17 | 0.44 |
| 1:A:482:VAL:HG22 | 1:A:593:ASN:HA | 2.00 | 0.44 |
| 7:G:13:LEU:HA | 7:G:16:ILE:HD12 | 1.98 | 0.44 |
| 8:I:65:GLY:O | 8:I:84:LEU:HD12 | 2.18 | 0.44 |
| 9:K:509:ARG:HG3 | 9:K:512:ASP:HB2 | 2.00 | 0.44 |
| 6:H:545:HIS:HE1 | 10:L:182:SER:O | 2.00 | 0.44 |
| 12:N:478:GLU:H | 12:N:479:ASP:HA | 1.82 | 0.44 |
| 12:N:699:TRP:HB3 | 12:N:705:LEU:HD23 | 2.00 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:286:PHE:HB3 | 3:P:303:PHE:CE2 | 2.53 | 0.44 |
| 16:S:163:GLU:CD | 16:S:196:PHE:CD1 | 2.80 | 0.44 |
| 17:X:410:TYR:O | 17:X:414:ILE:HG22 | 2.17 | 0.44 |
| 17:Y:546:LEU:O | 17:Y:550:GLN:HG2 | 2.17 | 0.44 |
| 1:A:1216:LYS:N | 1:A:1216:LYS:HD2 | 2.32 | 0.44 |
| 1:A:1279:ARG:NH1 | 1:A:1287:TYR:OH | 2.51 | 0.44 |
| 6:F:734:PRO:HB2 | 9:J:144:ASP:HB3 | 1.99 | 0.44 |
| 8:I:224:SER:HB3 | 8:I:229:SER:HA | 1.96 | 0.44 |
| 8:I:430:GLU:HA | 14:Q:429:LYS:HE2 | 1.99 | 0.44 |
| 12:N:186:GLN:O | 12:N:190:LYS:HG3 | 2.18 | 0.44 |
| 13:O:416:GLU:O | 13:O:420:ILE:HG22 | 2.18 | 0.44 |
| 3:P:283:LEU:HD13 | 3:P:306:LEU:HD11 | 2.00 | 0.44 |
| 17:Y:99:LYS:HD3 | 17:Y:102:MET:CE | 2.48 | 0.44 |
| 17:Y:281:TYR:HB3 | 17:Y:290:SER:OG | 2.17 | 0.44 |
| 1:A:1194:HIS:CG | 15:R:121:ASN:HD21 | 2.36 | 0.44 |
| 1:A:1845:LEU:N | 1:A:1846:PRO:HD2 | 2.32 | 0.44 |
| 1:A:872:LEU:HD11 | 1:A:939:PHE:HB2 | 1.99 | 0.44 |
| 4:D:14:GLU:HB2 | 4:D:17:TRP:CZ3 | 2.53 | 0.44 |
| 6:F:26:PHE:CD1 | 6:H:149:TRP:CG | 3.06 | 0.44 |
| 6:H:483:GLU:O | 6:H:487:ILE:HG12 | 2.17 | 0.44 |
| 6:H:703:PRO:HB3 | 6:H:733:VAL:CG2 | 2.47 | 0.44 |
| 8:I:360:LEU:HD12 | 8:I:397:ILE:CD1 | 2.47 | 0.44 |
| 9:K:147:THR:O | 9:K:150:THR:HG22 | 2.18 | 0.44 |
| 9:K:163:CYS:SG | 9:K:163:CYS:O | 2.76 | 0.44 |
| 9:K:404:VAL:O | 9:K:408:VAL:HG23 | 2.18 | 0.44 |
| 14:Q:185:TYR:CD1 | 16:S:27:GLU:CG | 3.01 | 0.44 |
| 14:Q:425:LEU:HB2 | 14:Q:439:LEU:HB2 | 1.99 | 0.44 |
| 17:X:149:LEU:O | 17:X:150:LYS:HB2 | 2.17 | 0.44 |
| 17:X:199:CYS:HA | 17:X:200:PRO:HD2 | 1.81 | 0.44 |
| 17:X:371:ASN:N | 17:X:371:ASN:HD22 | 2.09 | 0.44 |
| 17:Y:305:ILE:HG22 | 17:Y:340:GLU:OE1 | 2.17 | 0.44 |
| 1:A:1136:SER:OG | 1:A:1171:GLU:HB3 | 2.17 | 0.44 |
| 1:A:1599:ASN:HB2 | 1:A:1603:LEU:H | 1.83 | 0.44 |
| 1:A:454:CYS:O | 1:A:471:VAL:HA | 2.18 | 0.44 |
| 6:H:522:PHE:O | 6:H:525:VAL:HB | 2.18 | 0.44 |
| 8:I:44:VAL:C | 8:I:45:LEU:HD12 | 2.37 | 0.44 |
| 9:J:306:GLY:HA3 | 9:J:323:LEU:HD13 | 1.99 | 0.44 |
| 9:K:222:GLU:OE2 | 9:K:228:GLN:HG3 | 2.18 | 0.44 |
| 9:K:337:TRP:HB3 | 9:K:360:ALA:HB2 | 1.98 | 0.44 |
| 12:N:648:VAL:CG1 | 12:N:650:LEU:HG | 2.47 | 0.44 |
| 16:S:30:GLN:CB | 16:S:36:ARG:HH21 | 2.30 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:S:41:LEU:HD21 | 16:S:90:PRO:HB3 | 1.98 | 0.44 |
| 16:S:59:LYS:HA | 16:S:62:PHE:HD2 | 1.82 | 0.44 |
| 16:S:83:SER:O | 16:S:87:GLN:CB | 2.65 | 0.44 |
| 17:X:270:ASN:HA | 17:Y:62:THR:HG21 | 1.99 | 0.44 |
| 17:X:281:TYR:HB3 | 17:X:290:SER:OG | 2.17 | 0.44 |
| 1:A:1671:PRO:HB2 | 1:A:1705:GLN:HE22 | 1.82 | 0.44 |
| 1:A:174:PRO:HG3 | 1:A:356:PHE:CE2 | 2.53 | 0.44 |
| 1:A:42:LEU:HD13 | 3:C:363:ARG:HG3 | 2.00 | 0.44 |
| 3:C:296:ARG:HA | 3:P:101:ARG:NH2 | 2.33 | 0.44 |
| 3:C:60:PHE:CG | 3:P:89:LEU:HD12 | 2.52 | 0.44 |
| 3:C:61:SER:CB | 3:C:262:SER:HB2 | 2.46 | 0.44 |
| 3:C:66:PRO:HD2 | 3:C:68:ALA:O | 2.17 | 0.44 |
| 6:F:483:GLU:O | 6:F:487:ILE:HG12 | 2.17 | 0.44 |
| 6:F:89:GLU:CD | 6:F:130:ARG:NH2 | 2.71 | 0.44 |
| 6:H:621:LEU:HG | 6:H:644:ILE:HG21 | 1.99 | 0.44 |
| 8:I:420:TRP:HB2 | 8:I:440:MET:HE1 | 1.99 | 0.44 |
| 8:I:96:GLU:OE1 | 12:N:427:TYR:HE1 | 2.01 | 0.44 |
| 9:J:477:GLN:O | 9:J:508:LEU:HD13 | 2.17 | 0.44 |
| 9:J:509:ARG:HD2 | 9:J:512:ASP:HB2 | 1.99 | 0.44 |
| 10:L:113:LEU:HD13 | 10:L:120:ILE:HD13 | 1.99 | 0.44 |
| 3:P:402:TRP:HZ3 | 3:P:421:TYR:HD1 | 1.66 | 0.44 |
| 3:P:48:LEU:HD23 | 3:P:48:LEU:N | 2.33 | 0.44 |
| 3:P:96:VAL:N | 3:P:97:LYS:HA | 2.33 | 0.44 |
| 14:Q:411:TYR:CE1 | 14:Q:475:LEU:CD2 | 3.01 | 0.44 |
| 16:S:75:LEU:O | 16:S:75:LEU:HD22 | 2.18 | 0.44 |
| 17:Y:100:TYR:HB2 | 17:Y:142:MET:HG2 | 2.00 | 0.44 |
| 1:A:1194:HIS:CD2 | 15:R:121:ASN:HD21 | 2.36 | 0.44 |
| 1:A:1552:TYR:OH | 1:A:1604:GLN:NE2 | 2.51 | 0.44 |
| 1:A:1571:ARG:NH1 | 1:A:1694:ASP:O | 2.51 | 0.44 |
| 6:F:522:PHE:O | 6:F:525:VAL:HB | 2.18 | 0.44 |
| 9:K:391:PHE:CE2 | 9:K:411:VAL:HG21 | 2.53 | 0.44 |
| 12:N:165:THR:N | 12:N:166:PRO:CA | 2.79 | 0.44 |
| 17:X:316:ALA:HB1 | 17:X:351:TYR:CZ | 2.53 | 0.44 |
| 17:Y:39:ASP:N | 17:Y:39:ASP:OD1 | 2.50 | 0.44 |
| 1:A:1621:PRO:HA | 1:A:1697:LEU:O | 2.18 | 0.43 |
| 2:B:36:ASP:O | 2:B:38:LYS:N | 2.51 | 0.43 |
| 3:C:148:ASN:HB3 | 3:C:151:LEU:CD1 | 2.48 | 0.43 |
| 3:C:358:LEU:O | 3:C:362:PRO:CA | 2.65 | 0.43 |
| 6:F:556:SER:OG | 6:F:573:ALA:HA | 2.18 | 0.43 |
| 6:H:552:LEU:HG | 6:H:576:CYS:SG | 2.57 | 0.43 |
| 5:E:78:ARG:NH2 | 6:H:554:VAL:HG22 | 2.33 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:K:289:HIS:CD2 | 11:M:57:TRP:CE3 | 3.06 | 0.43 |
| 9:K:272:ILE:HG21 | 9:K:303:PHE:CE2 | 2.53 | 0.43 |
| 9:K:372:LEU:HD11 | 9:K:407:GLU:CG | 2.47 | 0.43 |
| 9:K:74:TYR:OH | 9:K:78:ARG:HD2 | 2.17 | 0.43 |
| 12:N:574:ILE:HA | 12:N:625:LYS:HE2 | 2.00 | 0.43 |
| 13:O:386:GLN:HB2 | 13:O:424:GLN:NE2 | 2.32 | 0.43 |
| 15:R:96:SER:O | 15:R:99:ASN:HB2 | 2.18 | 0.43 |
| 16:S:134:GLU:N | 16:S:135:PRO:HD3 | 2.33 | 0.43 |
| 16:S:58:GLN:NE2 | 16:S:62:PHE:CZ | 2.75 | 0.43 |
| 6:H:489:SER:O | 17:X:105:GLN:NE2 | 2.51 | 0.43 |
| 1:A:1041:LEU:HD13 | 1:A:1084:ARG:HA | 2.00 | 0.43 |
| 1:A:1254:VAL:HG11 | 1:A:1298:ALA:CA | 2.44 | 0.43 |
| 1:A:119:VAL:HG11 | 1:A:153:ILE:HG21 | 2.00 | 0.43 |
| 1:A:1637:THR:OG1 | 1:A:1665:GLN:HG3 | 2.18 | 0.43 |
| 1:A:1634:LEU:O | 1:A:1650:GLU:HA | 2.18 | 0.43 |
| 3:C:36:LEU:O | 3:C:39:ILE:HG22 | 2.19 | 0.43 |
| 8:I:294:LYS:CB | 8:I:320:LEU:HD22 | 2.49 | 0.43 |
| 9:J:432:ILE:HD11 | 9:J:444:TRP:CD1 | 2.53 | 0.43 |
| 9:K:167:PHE:CE1 | 9:K:171:THR:HG21 | 2.53 | 0.43 |
| 9:K:178:ALA:HA | 9:K:181:GLU:CD | 2.38 | 0.43 |
| 9:K:146:ARG:CZ | 9:K:332:THR:HG22 | 2.48 | 0.43 |
| 12:N:404:ILE:HA | 12:N:417:LEU:HD11 | 2.00 | 0.43 |
| 3:P:158:LEU:HD11 | 3:P:174:LEU:CD1 | 2.48 | 0.43 |
| 15:R:188:ASN:O | 15:R:231:SER:HA | 2.17 | 0.43 |
| 15:R:425:LEU:HB2 | 15:R:439:LEU:HB2 | 1.99 | 0.43 |
| 16:S:84:TRP:O | 16:S:88:ASN:CG | 2.57 | 0.43 |
| 17:Y:134:SER:N | 17:Y:137:GLU:OE1 | 2.51 | 0.43 |
| 1:A:161:MET:HG3 | 1:A:216:PRO:HB3 | 2.00 | 0.43 |
| 1:A:790:LEU:HD13 | 1:A:806:TYR:OH | 2.18 | 0.43 |
| 2:B:16:TRP:HB3 | 2:B:33:CYS:HB3 | 1.99 | 0.43 |
| 6:H:657:HIS:HA | 6:H:660:LYS:HE3 | 2.00 | 0.43 |
| 6:H:747:TYR:CD2 | 6:H:755:LEU:HB3 | 2.53 | 0.43 |
| 9:J:441:VAL:HG23 | 9:J:442:ASP:N | 2.33 | 0.43 |
| 12:N:560:MET:HA | 12:N:560:MET:HE2 | 2.01 | 0.43 |
| 12:N:602:PRO:N | 12:N:603:PRO:HD2 | 2.32 | 0.43 |
| 3:C:145:GLN:HG2 | 13:O:246:PHE:HA | 1.99 | 0.43 |
| 3:P:242:GLN:NE2 | 3:P:428:LEU:O | 2.51 | 0.43 |
| 3:C:89:LEU:HD12 | 3:P:60:PHE:CB | 2.49 | 0.43 |
| 15:R:84:SER:O | 15:R:88:MET:N | 2.51 | 0.43 |
| 14:Q:185:TYR:CD1 | 16:S:27:GLU:HG3 | 2.53 | 0.43 |
| 16:S:38:MET:HB3 | 18:Z:181:VAL:CG2 | 2.46 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:X:39:ASP:N | 17:X:39:ASP:OD1 | 2.51 | 0.43 |
| 17:Y:100:TYR:CB | 17:Y:142:MET:CG | 2.96 | 0.43 |
| 18:Z:170:SER:OG | 18:Z:171:GLY:N | 2.51 | 0.43 |
| 1:A:409:ILE:HG22 | 1:A:410:ASP:N | 2.33 | 0.43 |
| 2:B:38:LYS:HG2 | 2:B:40:PRO:HG2 | 1.99 | 0.43 |
| 2:B:62:LYS:O | 2:B:69:VAL:HG21 | 2.17 | 0.43 |
| 8:I:430:GLU:CD | 14:Q:429:LYS:CG | 2.86 | 0.43 |
| 9:J:167:PHE:HA | 9:J:170:LEU:HD21 | 1.99 | 0.43 |
| 9:J:242:TYR:HB2 | 9:J:250:CYS:SG | 2.59 | 0.43 |
| 10:L:33:LEU:HD13 | 10:L:54:TRP:CD2 | 2.53 | 0.43 |
| 12:N:527:LEU:HD11 | 12:N:561:LEU:HD22 | 2.00 | 0.43 |
| 13:O:402:LEU:HD13 | 13:O:425:LYS:HG2 | 1.99 | 0.43 |
| 3:P:209:LEU:HB3 | 3:P:233:PHE:HE1 | 1.82 | 0.43 |
| 16:S:162:TYR:CD2 | 16:S:174:ILE:CD1 | 3.01 | 0.43 |
| 17:X:341:PRO:O | 17:X:344:VAL:HG12 | 2.18 | 0.43 |
| 17:Y:149:LEU:O | 17:Y:150:LYS:HB2 | 2.18 | 0.43 |
| 17:Y:437:LEU:CB | 17:Y:444:LEU:HD11 | 2.48 | 0.43 |
| 1:A:1230:ILE:CA | 1:A:1236:LEU:HD13 | 2.49 | 0.43 |
| 1:A:1404:LEU:CD2 | 1:A:1464:ILE:HD11 | 2.46 | 0.43 |
| 1:A:1138:HIS:CE1 | 1:A:1604:GLN:HE21 | 2.26 | 0.43 |
| 1:A:1839:PHE:CD1 | 1:A:1840:MET:HG3 | 2.53 | 0.43 |
| 1:A:777:THR:HB | 1:A:946:THR:O | 2.18 | 0.43 |
| 3:C:356:ARG:NH2 | 11:M:19:TRP:HA | 2.33 | 0.43 |
| 4:D:18:PHE:O | 4:D:18:PHE:CG | 2.71 | 0.43 |
| 4:D:6:PRO:HB2 | 13:O:420:ILE:HG13 | 2.01 | 0.43 |
| 8:I:202:ALA:C | 8:I:223:VAL:HG22 | 2.38 | 0.43 |
| 8:I:312:LYS:CG | 8:I:428:MET:HB3 | 2.45 | 0.43 |
| 9:J:247:PHE:CE2 | 9:J:277:GLU:HG3 | 2.54 | 0.43 |
| 13:O:663:ALA:O | 13:O:667:VAL:HG23 | 2.18 | 0.43 |
| 1:A:1194:HIS:CB | 15:R:121:ASN:HD21 | 2.31 | 0.43 |
| 1:A:1512:LEU:HA | 1:A:1515:CYS:SG | 2.58 | 0.43 |
| 1:A:1618:LEU:HA | 1:A:1656:LEU:HA | 2.01 | 0.43 |
| 1:A:1666:ILE:HG21 | 1:A:1687:LEU:HD11 | 2.01 | 0.43 |
| 1:A:845:TYR:CE1 | 1:A:951:ILE:HD11 | 2.52 | 0.43 |
| 2:B:16:TRP:HB3 | 2:B:33:CYS:CA | 2.48 | 0.43 |
| 6:F:75:LEU:HG | 6:F:91:ILE:HD13 | 2.00 | 0.43 |
| 8:I:231:VAL:CG1 | 8:I:556:LEU:HD12 | 2.48 | 0.43 |
| 9:K:276:VAL:HA | 9:K:311:MET:CE | 2.49 | 0.43 |
| 10:L:125:THR:CA | 10:L:126:ASP:HB3 | 2.49 | 0.43 |
| 8:I:95:VAL:HG12 | 12:N:389:PRO:HG2 | 2.01 | 0.43 |
| 12:N:560:MET:HA | 12:N:560:MET:HE3 | 2.01 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:601:LEU:HB2 | 13:O:602:PRO:HD3 | 2.00 | 0.43 |
| 15:R:179:PRO:HG2 | 16:S:226:THR:HG22 | 2.00 | 0.43 |
| 16:S:88:ASN:ND2 | 16:S:88:ASN:N | 2.67 | 0.43 |
| 17:X:50:HIS:HA | 17:X:53:VAL:HG22 | 1.99 | 0.43 |
| 1:A:1024:MET:HG2 | 1:A:1034:VAL:HG11 | 2.00 | 0.43 |
| 1:A:1110:ARG:HG2 | 1:A:1117:THR:HG22 | 2.00 | 0.43 |
| 1:A:1166:ALA:HA | 1:A:1169:ALA:HB2 | 1.99 | 0.43 |
| 1:A:1170:ASN:HD21 | 1:A:1203:MET:HG3 | 1.83 | 0.43 |
| 1:A:1304:MET:O | 1:A:1307:LEU:HB2 | 2.18 | 0.43 |
| 1:A:1610:TYR:C | 1:A:1610:TYR:CD1 | 2.92 | 0.43 |
| 1:A:501:THR:HB | 1:A:504:VAL:HG22 | 2.01 | 0.43 |
| 1:A:871:ARG:HG3 | 1:A:872:LEU:N | 2.34 | 0.43 |
| 2:B:27:ARG:CB | 12:N:810:TYR:CE2 | 2.96 | 0.43 |
| 6:H:513:SER:HA | 6:H:515:TYR:CE1 | 2.54 | 0.43 |
| 6:H:537:GLU:CD | 6:H:568:GLU:OE1 | 2.57 | 0.43 |
| 9:J:404:VAL:O | 9:J:408:VAL:HG23 | 2.19 | 0.43 |
| 9:J:465:LEU:HD22 | 9:J:469:ARG:HH11 | 1.83 | 0.43 |
| 9:K:268:LEU:N | 9:K:269:PRO:HD2 | 2.34 | 0.43 |
| 9:K:432:ILE:HD11 | 9:K:444:TRP:CD1 | 2.54 | 0.43 |
| 10:L:14:LYS:HA | 10:L:17:GLU:OE1 | 2.19 | 0.43 |
| 13:O:324:LEU:HD22 | 13:O:350:LEU:HD12 | 2.00 | 0.43 |
| 13:O:385:VAL:HG11 | 13:O:402:LEU:HG | 2.01 | 0.43 |
| 3:P:170:PHE:O | 3:P:171:GLY:C | 2.56 | 0.43 |
| 14:Q:163:LYS:NZ | 16:S:224:ARG:HH22 | 2.16 | 0.43 |
| 16:S:64:TYR:HH | 16:S:84:TRP:HD1 | 1.63 | 0.43 |
| 6:F:130:ARG:HD3 | 17:Y:506:GLN:HB2 | 2.00 | 0.43 |
| 1:A:457:PHE:HB3 | 1:A:468:PHE:CE1 | 2.53 | 0.43 |
| 6:H:761:SER:O | 6:H:765:ASP:N | 2.51 | 0.43 |
| 8:I:207:ALA:HB3 | 8:I:220:VAL:HB | 2.00 | 0.43 |
| 8:I:320:LEU:HA | 8:I:320:LEU:HD12 | 1.75 | 0.43 |
| 8:I:497:TRP:HH2 | 8:I:507:LEU:HD13 | 1.81 | 0.43 |
| 9:K:230:ASN:O | 9:K:233:VAL:HG22 | 2.18 | 0.43 |
| 9:K:272:ILE:HG23 | 9:K:307:CYS:SG | 2.59 | 0.43 |
| 9:K:309:TYR:HD2 | 9:K:315:LYS:HB3 | 1.83 | 0.43 |
| 3:P:209:LEU:HB3 | 3:P:233:PHE:CE1 | 2.53 | 0.43 |
| 3:C:67:LEU:HD22 | 3:P:78:GLU:HA | 2.01 | 0.43 |
| 15:R:357:ALA:CB | 16:S:305:GLU:HG3 | 2.48 | 0.43 |
| 15:R:498:ILE:O | 15:R:499:ARG:HB2 | 2.19 | 0.43 |
| 16:S:78:TRP:CD1 | 16:S:109:LEU:HD11 | 2.54 | 0.43 |
| 17:X:267:LEU:CD1 | 17:Y:59:LEU:HD11 | 2.39 | 0.43 |
| 2:B:47:VAL:HG21 | 2:B:82:PHE:CD2 | 2.53 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:46:ARG:HB3 | 3:C:116:PHE:CE2 | 2.53 | 0.43 |
| 3:C:414:MET:HG2 | 13:O:330:ILE:HD13 | 1.95 | 0.43 |
| 6:F:96:VAL:O | 6:F:97:PHE:HB2 | 2.18 | 0.43 |
| 6:H:515:TYR:HD1 | 6:H:515:TYR:H | 1.66 | 0.43 |
| 6:H:673:CYS:O | 6:H:677:VAL:HG23 | 2.19 | 0.43 |
| 8:I:306:HIS:HE1 | 8:I:316:GLU:HB3 | 1.83 | 0.43 |
| 8:I:290:PHE:HE2 | 8:I:325:LEU:HD12 | 1.84 | 0.43 |
| 9:J:268:LEU:N | 9:J:269:PRO:HD2 | 2.33 | 0.43 |
| 12:N:501:ILE:HD13 | 12:N:548:ARG:NH2 | 2.34 | 0.43 |
| 13:O:648:ILE:O | 13:O:652:LEU:HG | 2.19 | 0.43 |
| 16:S:38:MET:HE2 | 18:Z:181:VAL:CB | 2.38 | 0.43 |
| 16:S:66:ILE:O | 16:S:69:TYR:HB2 | 2.19 | 0.43 |
| 16:S:68:PHE:HE1 | 16:S:78:TRP:HA | 1.82 | 0.43 |
| 17:X:222:MET:O | 17:X:226:VAL:HG23 | 2.19 | 0.43 |
| 1:A:1165:HIS:HD2 | 1:A:1167:GLU:H | 1.67 | 0.43 |
| 1:A:1550:MET:SD | 1:A:1558:HIS:HE1 | 2.42 | 0.43 |
| 1:A:1595:HIS:NE2 | 1:A:1598:ASP:HB2 | 2.34 | 0.43 |
| 2:B:26:CYS:HB3 | 2:B:59:CYS:SG | 2.59 | 0.43 |
| 3:C:54:TRP:CE3 | 3:C:203:TRP:HB2 | 2.54 | 0.43 |
| 6:F:142:LEU:HA | 6:F:146:PRO:HB3 | 2.00 | 0.43 |
| 6:H:702:ASN:HA | 6:H:703:PRO:HD3 | 1.91 | 0.43 |
| 8:I:74:ARG:HD2 | 8:I:174:ASN:ND2 | 2.34 | 0.43 |
| 8:I:313:ALA:HB3 | 8:I:317:LEU:CD1 | 2.47 | 0.43 |
| 8:I:427:ARG:HB2 | 8:I:428:MET:HE3 | 2.01 | 0.43 |
| 12:N:556:PHE:CE1 | 12:N:600:PHE:HA | 2.54 | 0.43 |
| 2:B:8:TRP:NE1 | 12:N:644:VAL:HG12 | 2.34 | 0.43 |
| 13:O:56:GLU:HB3 | 13:O:86:CYS:SG | 2.59 | 0.43 |
| 15:R:258:GLN:O | 15:R:258:GLN:HG2 | 2.19 | 0.43 |
| 16:S:200:VAL:O | 16:S:204:THR:HG23 | 2.19 | 0.43 |
| 16:S:70:THR:O | 16:S:74:PRO:CD | 2.65 | 0.43 |
| 7:W:5:LYS:HB3 | 7:W:5:LYS:HE3 | 1.76 | 0.43 |
| 17:Y:134:SER:O | 17:Y:138:VAL:HG23 | 2.18 | 0.43 |
| 1:A:1036:ASP:O | 1:A:1040:LEU:HD13 | 2.19 | 0.42 |
| 1:A:1250:GLN:O | 1:A:1254:VAL:HG23 | 2.19 | 0.42 |
| 8:I:19:LEU:HD13 | 8:I:23:ILE:HG13 | 2.00 | 0.42 |
| 12:N:151:GLU:O | 12:N:155:THR:HG23 | 2.19 | 0.42 |
| 15:R:112:HIS:NE2 | 15:R:116:TRP:CZ3 | 2.80 | 0.42 |
| 7:W:13:LEU:HA | 7:W:16:ILE:HD12 | 2.01 | 0.42 |
| 17:X:430:ALA:HB2 | 17:X:451:CYS:SG | 2.59 | 0.42 |
| 17:Y:170:LYS:HG2 | 17:Y:171:ILE:HD12 | 2.01 | 0.42 |
| 17:Y:222:MET:O | 17:Y:226:VAL:HG23 | 2.18 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Y:410:TYR:O | 17:Y:414:ILE:HG22 | 2.19 | 0.42 |
| 16:S:33:ARG:HA | 18:Z:144:LEU:HG | 2.01 | 0.42 |
| 1:A:1162:LYS:HZ2 | 1:A:1196:TYR:HE1 | 1.65 | 0.42 |
| 1:A:1190:THR:O | 1:A:1193:ILE:HB | 2.19 | 0.42 |
| 1:A:131:PHE:HE1 | 1:A:187:LEU:HB2 | 1.84 | 0.42 |
| 1:A:1813:GLN:O | 1:A:1817:VAL:HG23 | 2.19 | 0.42 |
| 1:A:487:THR:HG22 | 1:A:501:THR:HA | 2.00 | 0.42 |
| 8:I:280:LEU:HG | 8:I:280:LEU:O | 2.19 | 0.42 |
| 9:J:42:TRP:HE3 | 9:J:42:TRP:HA | 1.83 | 0.42 |
| 9:J:482:TYR:CD1 | 9:J:485:ILE:HD11 | 2.54 | 0.42 |
| 9:K:386:LEU:HD12 | 9:K:386:LEU:N | 2.34 | 0.42 |
| 12:N:395:ASP:OD1 | 12:N:398:THR:HG23 | 2.18 | 0.42 |
| 12:N:455:THR:CB | 12:N:501:ILE:HD11 | 2.49 | 0.42 |
| 3:C:414:MET:HG3 | 13:O:330:ILE:HD11 | 1.99 | 0.42 |
| 13:O:40:LEU:HD22 | 13:O:82:ILE:HD12 | 2.00 | 0.42 |
| 16:S:75:LEU:CB | 16:S:115:TYR:OH | 2.62 | 0.42 |
| 18:Z:163:VAL:HA | 18:Z:164:PRO:HD3 | 1.85 | 0.42 |
| 1:A:1360:VAL:HB | 1:A:1364:CYS:HB2 | 2.00 | 0.42 |
| 1:A:250:ASN:HD22 | 1:A:251:THR:N | 2.17 | 0.42 |
| 6:F:135:SER:OG | 6:F:160:GLU:HG3 | 2.18 | 0.42 |
| 6:F:61:LEU:HD23 | 6:F:61:LEU:HA | 1.94 | 0.42 |
| 6:H:49:TYR:HD1 | 6:H:78:CYS:HG | 1.67 | 0.42 |
| 9:J:210:LYS:HE3 | 9:J:212:TYR:CZ | 2.54 | 0.42 |
| 9:K:289:HIS:ND1 | 11:M:57:TRP:CZ3 | 2.87 | 0.42 |
| 12:N:570:ILE:CD1 | 12:N:633:ARG:HH12 | 2.22 | 0.42 |
| 12:N:662:VAL:HB | 12:N:687:MET:SD | 2.58 | 0.42 |
| 14:Q:258:GLN:HG2 | 14:Q:258:GLN:O | 2.19 | 0.42 |
| 3:P:399:TYR:CE2 | 14:Q:498:ILE:CG2 | 3.02 | 0.42 |
| 16:S:82:ILE:HG21 | 16:S:127:LYS:HD3 | 2.02 | 0.42 |
| 17:Y:465:LEU:HD23 | 17:Y:485:LEU:HD11 | 2.01 | 0.42 |
| 1:A:280:ASN:C | 1:A:346:ASN:N | 2.71 | 0.42 |
| 1:A:877:ILE:HG23 | 1:A:881:ILE:HD12 | 2.00 | 0.42 |
| 3:C:402:TRP:HZ3 | 3:C:421:TYR:HD1 | 1.66 | 0.42 |
| 6:F:621:LEU:HG | 6:F:644:ILE:HG21 | 2.00 | 0.42 |
| 6:H:703:PRO:CD | 10:L:180:TYR:CE2 | 3.02 | 0.42 |
| 8:I:285:SER:O | 8:I:289:LYS:HG2 | 2.19 | 0.42 |
| 8:I:474:ARG:O | 8:I:477:GLN:HG3 | 2.19 | 0.42 |
| 10:L:83:TYR:N | 10:L:116:PRO:O | 2.53 | 0.42 |
| 12:N:574:ILE:CD1 | 12:N:625:LYS:HG2 | 2.34 | 0.42 |
| 12:N:669:TYR:CZ | 12:N:684:ALA:HB1 | 2.53 | 0.42 |
| 3:P:151:LEU:HB3 | 3:P:182:LEU:HD11 | 2.02 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:60:PHE:CB | 3:P:89:LEU:HD12 | 2.49 | 0.42 |
| 17:X:270:ASN:HB2 | 17:X:273:LEU:HB2 | 2.01 | 0.42 |
| 1:A:1316:MET:O | 1:A:1319:LEU:O | 2.38 | 0.42 |
| 1:A:1322:PRO:CG | 1:A:1375:TYR:OH | 2.54 | 0.42 |
| 1:A:802:TYR:CZ | 1:A:841:PRO:HA | 2.54 | 0.42 |
| 6:F:134:GLY:O | 6:F:137:CYS:HB3 | 2.19 | 0.42 |
| 6:H:473:TYR:CD2 | 6:H:500:TRP:CZ2 | 3.08 | 0.42 |
| 9:J:18:GLN:NE2 | 9:K:134:LEU:CD1 | 2.83 | 0.42 |
| 9:K:251:TYR:HA | 9:K:254:THR:HG22 | 2.01 | 0.42 |
| 11:M:32:PRO:C | 11:M:34:ASN:H | 2.22 | 0.42 |
| 12:N:506:VAL:O | 12:N:510:GLY:HA3 | 2.19 | 0.42 |
| 12:N:772:ARG:HB3 | 12:N:776:MET:HE1 | 2.01 | 0.42 |
| 13:O:594:SER:O | 13:O:595:SER:HB3 | 2.19 | 0.42 |
| 3:P:417:TYR:O | 3:P:421:TYR:CD2 | 2.72 | 0.42 |
| 1:A:1194:HIS:NE2 | 15:R:117:ALA:HA | 2.35 | 0.42 |
| 14:Q:420:PHE:HB3 | 16:S:31:PRO:HD2 | 2.02 | 0.42 |
| 17:X:465:LEU:HD23 | 17:X:485:LEU:HD11 | 2.02 | 0.42 |
| 1:A:1249:VAL:O | 1:A:1252:ALA:HB3 | 2.20 | 0.42 |
| 1:A:1307:LEU:HD21 | 1:A:1579:SER:HA | 2.01 | 0.42 |
| 1:A:93:LEU:HB2 | 1:A:128:TRP:CH2 | 2.54 | 0.42 |
| 3:C:158:LEU:HD11 | 3:C:174:LEU:CD1 | 2.49 | 0.42 |
| 9:J:497:ASN:OD1 | 9:J:497:ASN:N | 2.53 | 0.42 |
| 9:J:61:ARG:HG2 | 9:J:61:ARG:NH1 | 2.34 | 0.42 |
| 11:M:31:ILE:HG22 | 11:M:33:LEU:HD22 | 2.02 | 0.42 |
| 12:N:523:LEU:O | 12:N:527:LEU:HG | 2.20 | 0.42 |
| 13:O:434:ARG:HA | 13:O:434:ARG:HD2 | 1.75 | 0.42 |
| 13:O:493:LEU:HD13 | 13:O:507:TRP:HB2 | 2.01 | 0.42 |
| 3:P:244:ILE:HD11 | 3:P:276:ILE:HD11 | 2.02 | 0.42 |
| 3:P:297:ILE:HD11 | 3:P:333:THR:HB | 2.01 | 0.42 |
| 15:R:193:SER:HB3 | 15:R:234:TRP:CD2 | 2.55 | 0.42 |
| 16:S:30:GLN:CB | 16:S:36:ARG:NH2 | 2.83 | 0.42 |
| 17:Y:391:GLU:O | 17:Y:394:ILE:HG12 | 2.19 | 0.42 |
| 1:A:971:PRO:HG2 | 1:A:974:VAL:HG23 | 2.01 | 0.42 |
| 3:C:515:TYR:HA | 3:C:518:GLN:HG2 | 2.00 | 0.42 |
| 6:F:762:TRP:NE1 | 9:J:362:GLN:HB2 | 2.35 | 0.42 |
| 8:I:398:LEU:HD23 | 13:O:444:MET:HG3 | 2.01 | 0.42 |
| 9:J:482:TYR:HD1 | 9:J:485:ILE:HD11 | 1.85 | 0.42 |
| 3:C:554:LEU:HD12 | 9:K:386:LEU:HD11 | 2.01 | 0.42 |
| 12:N:180:PHE:CG | 12:N:299:TRP:CH2 | 3.05 | 0.42 |
| 13:O:256:LEU:HA | 13:O:256:LEU:HD23 | 1.85 | 0.42 |
| 13:O:508:MET:HA | 13:O:511:ASP:OD2 | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:547:LYS:HG3 | 13:O:563:LEU:HD21 | 2.02 | 0.42 |
| 3:P:151:LEU:HD22 | 3:P:178:VAL:HG13 | 2.01 | 0.42 |
| 3:P:424:ARG:HG3 | 3:P:424:ARG:NH1 | 2.33 | 0.42 |
| 14:Q:193:SER:HB3 | 14:Q:234:TRP:CD2 | 2.55 | 0.42 |
| 17:X:452:LEU:HD22 | 17:X:461:ALA:CA | 2.47 | 0.42 |
| 18:Z:13:LEU:HD22 | 18:Z:111:LYS:HB3 | 2.00 | 0.42 |
| 1:A:857:MET:CB | 1:A:858:PRO:CD | 2.95 | 0.42 |
| 3:C:262:SER:O | 3:C:266:VAL:HG23 | 2.20 | 0.42 |
| 6:H:481:CYS:O | 6:H:485:ILE:HG12 | 2.19 | 0.42 |
| 8:I:370:ALA:HB2 | 8:I:386:ILE:HD12 | 2.01 | 0.42 |
| 8:I:586:LEU:HD12 | 8:I:587:LEU:N | 2.34 | 0.42 |
| 12:N:556:PHE:HA | 12:N:600:PHE:CD1 | 2.55 | 0.42 |
| 13:O:350:LEU:HA | 13:O:350:LEU:HD23 | 1.86 | 0.42 |
| 13:O:568:LEU:HD13 | 13:O:583:VAL:HG13 | 2.02 | 0.42 |
| 13:O:711:ARG:HH12 | 13:O:745:PRO:HB3 | 1.84 | 0.42 |
| 3:P:127:GLU:OE2 | 3:P:127:GLU:HA | 2.20 | 0.42 |
| 17:Y:230:VAL:HA | 17:Y:231:PRO:HD2 | 1.88 | 0.42 |
| 18:Z:48:LYS:HG3 | 18:Z:49:TYR:CD2 | 2.55 | 0.42 |
| 18:Z:81:VAL:CG2 | 18:Z:155:ILE:HD12 | 2.49 | 0.42 |
| 1:A:1638:TYR:CD1 | 1:A:1638:TYR:N | 2.88 | 0.42 |
| 1:A:1739:SER:N | 1:A:1740:ALA:HB3 | 2.35 | 0.42 |
| 5:E:102:LEU:HD13 | 6:H:594:ILE:HG22 | 2.01 | 0.42 |
| 6:F:699:ASP:CB | 6:F:702:ASN:HD21 | 2.31 | 0.42 |
| 6:H:515:TYR:CD1 | 6:H:515:TYR:N | 2.88 | 0.42 |
| 8:I:403:LEU:HG | 8:I:407:ILE:HD11 | 2.02 | 0.42 |
| 9:J:19:TYR:CD1 | 9:J:49:LEU:CD1 | 2.97 | 0.42 |
| 9:J:230:ASN:O | 9:J:233:VAL:HG22 | 2.20 | 0.42 |
| 9:K:289:HIS:CG | 11:M:57:TRP:CZ3 | 3.08 | 0.42 |
| 9:K:497:ASN:OD1 | 9:K:497:ASN:N | 2.52 | 0.42 |
| 9:K:499:VAL:HG11 | 9:K:523:ILE:HD11 | 2.02 | 0.42 |
| 12:N:414:MET:SD | 12:N:498:SER:N | 2.93 | 0.42 |
| 13:O:648:ILE:HA | 13:O:651:ILE:HD12 | 2.02 | 0.42 |
| 3:C:434:ARG:HH11 | 15:R:80:ILE:HD13 | 1.85 | 0.42 |
| 16:S:272:ILE:HG13 | 16:S:273:THR:N | 2.35 | 0.42 |
| 17:X:242:ALA:O | 17:X:246:VAL:HG23 | 2.20 | 0.42 |
| 3:C:170:PHE:O | 3:C:171:GLY:C | 2.57 | 0.42 |
| 3:C:89:LEU:HD21 | 3:C:93:TYR:CE2 | 2.55 | 0.42 |
| 6:H:130:ARG:NH1 | 9:K:473:VAL:CG2 | 2.82 | 0.42 |
| 8:I:556:LEU:HD11 | 8:I:586:LEU:HD21 | 2.02 | 0.42 |
| 9:J:17:GLN:HB3 | 9:K:78:ARG:NH1 | 2.34 | 0.42 |
| 9:K:284:LEU:HD11 | 9:K:307:CYS:SG | 2.60 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:K:422:GLU:OE1 | 9:K:458:LEU:HD22 | 2.20 | 0.42 |
| 9:K:491:LEU:HA | 7:W:22:ILE:HG21 | 2.02 | 0.42 |
| 10:L:14:LYS:HB3 | 10:L:18:ARG:CZ | 2.50 | 0.42 |
| 12:N:152:GLU:O | 12:N:156:MET:HG2 | 2.19 | 0.42 |
| 13:O:707:LYS:HA | 13:O:710:ILE:CG2 | 2.49 | 0.42 |
| 3:P:123:TYR:CE1 | 3:P:151:LEU:HD21 | 2.55 | 0.42 |
| 3:P:303:PHE:CE1 | 3:P:307:LEU:HD22 | 2.54 | 0.42 |
| 17:X:261:LEU:HD22 | 17:X:267:LEU:HD23 | 2.02 | 0.42 |
| 17:Y:513:ARG:NH1 | 17:Y:544:LYS:HB3 | 2.34 | 0.42 |
| 1:A:1191:LEU:HD23 | 1:A:1191:LEU:H | 1.84 | 0.41 |
| 1:A:1424:LYS:HA | 1:A:1427:ASP:OD2 | 2.20 | 0.41 |
| 6:F:550:VAL:HG21 | 9:K:289:HIS:CB | 2.43 | 0.41 |
| 6:F:726:LEU:HD21 | 6:F:742:LEU:HD22 | 2.02 | 0.41 |
| 8:I:86:ASP:OD1 | 8:I:87:THR:N | 2.53 | 0.41 |
| 9:K:20:GLN:CA | 9:K:20:GLN:HE21 | 2.32 | 0.41 |
| 9:K:258:MET:HA | 9:K:261:ASP:O | 2.20 | 0.41 |
| 9:K:444:TRP:CZ3 | 7:W:6:PRO:HG2 | 2.54 | 0.41 |
| 11:M:32:PRO:O | 11:M:33:LEU:HB2 | 2.20 | 0.41 |
| 3:P:251:TYR:HH | 3:P:268:GLN:HG3 | 1.81 | 0.41 |
| 6:F:130:ARG:NH1 | 17:Y:506:GLN:HB3 | 2.35 | 0.41 |
| 1:A:269:TRP:CZ3 | 1:A:411:HIS:HB2 | 2.55 | 0.41 |
| 3:C:48:LEU:HD23 | 3:C:48:LEU:N | 2.35 | 0.41 |
| 9:J:24:PHE:CE1 | 9:J:28:LYS:CE | 3.00 | 0.41 |
| 9:J:354:MET:HE1 | 9:J:377:GLU:HB2 | 2.01 | 0.41 |
| 9:J:397:ILE:O | 9:J:398:ALA:C | 2.59 | 0.41 |
| 10:L:40:PHE:CA | 10:L:44:GLN:OE1 | 2.64 | 0.41 |
| 12:N:286:LEU:O | 12:N:287:ARG:C | 2.57 | 0.41 |
| 12:N:528:LEU:HD11 | 12:N:641:LEU:HD13 | 2.01 | 0.41 |
| 12:N:681:LEU:HD23 | 12:N:692:LEU:HD21 | 2.01 | 0.41 |
| 13:O:629:PHE:CE1 | 13:O:755:LEU:C | 2.94 | 0.41 |
| 3:P:290:ARG:HD3 | 3:P:300:MET:HE2 | 2.02 | 0.41 |
| 17:X:391:GLU:O | 17:X:394:ILE:HG12 | 2.20 | 0.41 |
| 1:A:1371:LEU:HA | 1:A:1371:LEU:HD23 | 1.86 | 0.41 |
| 1:A:1574:LEU:HG | 1:A:1574:LEU:H | 1.61 | 0.41 |
| 1:A:1814:ILE:O | 1:A:1818:LEU:HD12 | 2.19 | 0.41 |
| 1:A:129:CYS:SG | 1:A:187:LEU:HD13 | 2.60 | 0.41 |
| 1:A:860:TYR:CD1 | 1:A:861:PRO:HD2 | 2.55 | 0.41 |
| 6:H:32:TYR:CE1 | 6:H:41:LEU:HB2 | 2.55 | 0.41 |
| 6:H:624:PHE:O | 6:H:628:ILE:HG12 | 2.21 | 0.41 |
| 8:I:28:TRP:HZ3 | 8:I:33:ASP:O | 2.04 | 0.41 |
| 9:J:290:LYS:O | 9:J:294:LEU:HD23 | 2.19 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:J:323:LEU:HA | 9:J:323:LEU:HD12 | 1.88 | 0.41 |
| 9:J:340:TYR:HE1 | 9:J:344:PHE:CE2 | 2.38 | 0.41 |
| 9:J:21:SER:HB2 | 9:K:165:GLU:HG3 | 2.02 | 0.41 |
| 12:N:149:LEU:HB3 | 12:N:150:ARG:H | 1.60 | 0.41 |
| 14:Q:163:LYS:HE2 | 15:R:464:ASP:O | 2.21 | 0.41 |
| 17:Y:244:ALA:O | 17:Y:248:THR:HG23 | 2.20 | 0.41 |
| 1:A:1236:LEU:HA | 1:A:1237:PRO:HD3 | 1.89 | 0.41 |
| 1:A:780:GLY:C | 1:A:782:GLY:H | 2.23 | 0.41 |
| 3:C:415:PRO:HG3 | 3:C:445:LYS:HB2 | 2.03 | 0.41 |
| 6:F:457:ALA:HA | 6:F:460:GLU:OE1 | 2.21 | 0.41 |
| 6:F:502:LEU:HA | 6:F:505:ILE:HD12 | 2.02 | 0.41 |
| 6:H:502:LEU:HA | 6:H:505:ILE:HD12 | 2.03 | 0.41 |
| 6:H:689:LEU:O | 6:H:693:ASN:HB2 | 2.20 | 0.41 |
| 8:I:330:LEU:C | 8:I:330:LEU:HD13 | 2.41 | 0.41 |
| 8:I:73:TRP:CH2 | 8:I:80:LEU:HD22 | 2.55 | 0.41 |
| 9:J:231:LEU:HA | 9:J:234:VAL:HG22 | 2.01 | 0.41 |
| 9:J:386:LEU:HD12 | 9:J:386:LEU:H | 1.85 | 0.41 |
| 9:K:203:PHE:HE1 | 9:K:218:THR:HB | 1.85 | 0.41 |
| 9:K:203:PHE:CD1 | 9:K:221:PRO:CG | 3.04 | 0.41 |
| 9:J:28:LYS:HD3 | 9:K:230:ASN:ND2 | 2.35 | 0.41 |
| 9:J:322:TYR:CE1 | 11:M:36:LEU:HD11 | 2.54 | 0.41 |
| 1:A:616:GLU:HB2 | 13:O:556:GLN:HA | 2.03 | 0.41 |
| 3:P:97:LYS:HG3 | 3:P:99:TYR:CZ | 2.55 | 0.41 |
| 14:Q:498:ILE:O | 14:Q:498:ILE:HG22 | 2.21 | 0.41 |
| 16:S:20:ASP:O | 16:S:24:LEU:HG | 2.19 | 0.41 |
| 17:X:170:LYS:HG2 | 17:X:171:ILE:HD12 | 2.01 | 0.41 |
| 17:X:437:LEU:CB | 17:X:444:LEU:HD11 | 2.48 | 0.41 |
| 18:Z:146:GLU:CD | 18:Z:146:GLU:N | 2.72 | 0.41 |
| 1:A:1364:CYS:N | 1:A:1365:PRO:HD2 | 2.36 | 0.41 |
| 1:A:811:PRO:HG3 | 1:A:1806:SER:HB3 | 2.01 | 0.41 |
| 3:C:389:ARG:HD3 | 3:C:389:ARG:HA | 1.65 | 0.41 |
| 6:F:45:ALA:CB | 6:F:61:LEU:HD11 | 2.51 | 0.41 |
| 7:G:3:ARG:HB2 | 9:J:443:LYS:HZ3 | 1.86 | 0.41 |
| 8:I:231:VAL:HG12 | 8:I:232:SER:N | 2.35 | 0.41 |
| 8:I:290:PHE:HB3 | 8:I:320:LEU:HD21 | 2.01 | 0.41 |
| 8:I:333:LEU:HG | 8:I:337:ILE:HD12 | 2.02 | 0.41 |
| 9:K:20:GLN:HA | 9:K:20:GLN:HE21 | 1.86 | 0.41 |
| 13:O:541:ILE:O | 13:O:544:VAL:HG22 | 2.20 | 0.41 |
| 3:P:248:LEU:O | 3:P:252:GLN:HG2 | 2.20 | 0.41 |
| 16:S:134:GLU:O | 16:S:135:PRO:C | 2.57 | 0.41 |
| 17:X:434:TYR:HA | 17:X:444:LEU:HD22 | 2.03 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:Y:70:LEU:HD13 | 17:Y:70:LEU:O | 2.20 | 0.41 |
| 1:A:1251:VAL:HG12 | 1:A:1294:TYR:HA | 2.03 | 0.41 |
| 1:A:1325:LEU:HD23 | 1:A:1371:LEU:CD2 | 2.50 | 0.41 |
| 1:A:1387:LEU:HD12 | 1:A:1407:ARG:HG3 | 2.03 | 0.41 |
| 1:A:957:ASP:HA | 1:A:1839:PHE:HE2 | 1.85 | 0.41 |
| 2:B:28:MET:HG2 | 2:B:33:CYS:O | 2.20 | 0.41 |
| 3:C:307:LEU:HD21 | 3:C:316:LEU:HB2 | 2.02 | 0.41 |
| 6:F:666:PRO:O | 6:F:667:GLN:HG3 | 2.21 | 0.41 |
| 8:I:306:HIS:NE2 | 8:I:313:ALA:O | 2.53 | 0.41 |
| 8:I:34:LEU:HD13 | 12:N:390:GLY:HA3 | 2.03 | 0.41 |
| 9:J:447:LEU:O | 9:J:451:LEU:HD23 | 2.20 | 0.41 |
| 12:N:386:LEU:HD12 | 12:N:387:LEU:HG | 2.02 | 0.41 |
| 12:N:389:PRO:HA | 12:N:431:ARG:HH22 | 1.85 | 0.41 |
| 12:N:501:ILE:CD1 | 12:N:501:ILE:H | 2.29 | 0.41 |
| 2:B:16:TRP:HZ3 | 12:N:633:ARG:HG3 | 1.85 | 0.41 |
| 13:O:604:LEU:HB3 | 13:O:627:LEU:HD21 | 2.02 | 0.41 |
| 3:P:389:ARG:HA | 3:P:392:ILE:HG22 | 2.02 | 0.41 |
| 3:P:396:LYS:HD3 | 3:P:396:LYS:HA | 1.88 | 0.41 |
| 1:A:107:LYS:HB2 | 1:A:110:ALA:HB3 | 2.03 | 0.41 |
| 1:A:1750:PHE:HD2 | 1:A:1775:LEU:HD12 | 1.86 | 0.41 |
| 1:A:773:LEU:HB2 | 1:A:783:ILE:HD12 | 2.01 | 0.41 |
| 3:C:206:TRP:O | 3:C:209:LEU:HB2 | 2.21 | 0.41 |
| 6:F:705:CYS:SG | 6:F:706:LYS:N | 2.93 | 0.41 |
| 8:I:237:GLU:CG | 8:I:607:ILE:HD13 | 2.51 | 0.41 |
| 9:K:297:SER:O | 9:K:329:LEU:HD21 | 2.20 | 0.41 |
| 9:K:35:GLU:HB3 | 9:K:40:ILE:HD11 | 2.03 | 0.41 |
| 9:K:66:ASP:OD1 | 9:K:67:LYS:N | 2.54 | 0.41 |
| 12:N:321:LEU:HD22 | 12:N:324:TRP:CD2 | 2.56 | 0.41 |
| 13:O:143:TYR:CD1 | 13:O:143:TYR:C | 2.94 | 0.41 |
| 13:O:266:ASP:CB | 13:O:269:SER:HB3 | 2.51 | 0.41 |
| 13:O:592:TRP:CH2 | 13:O:630:ALA:HA | 2.55 | 0.41 |
| 3:P:358:LEU:O | 3:P:362:PRO:CA | 2.65 | 0.41 |
| 15:R:430:TYR:CG | 15:R:431:PRO:HA | 2.56 | 0.41 |
| 1:A:1645:GLU:CG | 1:A:1646:GLN:H | 2.27 | 0.41 |
| 1:A:1702:ARG:HD3 | 1:A:1782:GLU:CD | 2.41 | 0.41 |
| 3:C:276:ILE:O | 3:C:276:ILE:HG22 | 2.21 | 0.41 |
| 6:F:559:LEU:O | 6:F:562:MET:HG3 | 2.21 | 0.41 |
| 8:I:101:LEU:HD23 | 8:I:102:HIS:N | 2.36 | 0.41 |
| 8:I:184:PHE:HB2 | 8:I:198:VAL:O | 2.20 | 0.41 |
| 8:I:231:VAL:HG21 | 8:I:557:TYR:CE2 | 2.56 | 0.41 |
| 8:I:32:ARG:HD2 | 8:I:34:LEU:HD21 | 2.03 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:719:ALA:HA | 8:I:735:SER:HA | 2.02 | 0.41 |
| 9:J:485:ILE:O | 9:J:488:ILE:HG12 | 2.21 | 0.41 |
| 12:N:235:GLN:HA | 12:N:238:GLU:CD | 2.41 | 0.41 |
| 12:N:427:TYR:O | 12:N:430:THR:HB | 2.21 | 0.41 |
| 13:O:208:SER:HB3 | 13:O:211:GLN:NE2 | 2.36 | 0.41 |
| 3:P:434:ARG:NH1 | 14:Q:498:ILE:HD13 | 2.35 | 0.41 |
| 14:Q:139:ASN:O | 14:Q:140:ALA:CB | 2.68 | 0.41 |
| 15:R:461:ALA:CA | 15:R:467:LEU:HD12 | 2.51 | 0.41 |
| 16:S:73:ASP:HB3 | 16:S:74:PRO:HD3 | 2.02 | 0.41 |
| 17:X:442:GLN:CD | 17:X:472:ARG:CG | 2.89 | 0.41 |
| 1:A:1039:ARG:O | 1:A:1042:GLN:HG3 | 2.21 | 0.41 |
| 1:A:1525:MET:HA | 1:A:1528:ALA:HB2 | 2.03 | 0.41 |
| 1:A:154:LEU:HD13 | 1:A:159:ILE:HG12 | 2.02 | 0.41 |
| 1:A:1658:PRO:HG2 | 1:A:1663:LEU:HD13 | 2.03 | 0.41 |
| 1:A:439:GLN:NE2 | 1:A:456:LYS:HG3 | 2.35 | 0.41 |
| 1:A:767:HIS:O | 1:A:770:TYR:HB3 | 2.20 | 0.41 |
| 3:C:150:ALA:O | 3:C:154:LEU:HD13 | 2.21 | 0.41 |
| 9:J:180:GLU:CA | 9:J:180:GLU:OE1 | 2.69 | 0.41 |
| 9:K:418:TRP:HB3 | 9:K:458:LEU:HD12 | 2.02 | 0.41 |
| 9:K:445:GLU:HA | 9:K:474:LEU:HD12 | 2.03 | 0.41 |
| 12:N:330:ARG:HB2 | 12:N:334:ARG:NH2 | 2.36 | 0.41 |
| 12:N:457:GLN:HA | 12:N:544:LEU:HD11 | 2.02 | 0.41 |
| 12:N:63:ALA:HB3 | 12:N:64:ALA:HB3 | 2.02 | 0.41 |
| 13:O:62:GLN:O | 13:O:66:PRO:HD2 | 2.21 | 0.41 |
| 14:Q:496:GLN:HA | 14:Q:497:GLY:HA2 | 1.78 | 0.41 |
| 15:R:174:ARG:HH11 | 16:S:257:GLY:N | 2.19 | 0.41 |
| 17:X:335:SER:HB2 | 17:X:338:HIS:CD2 | 2.56 | 0.41 |
| 17:Y:45:ALA:HB3 | 17:Y:82:TYR:HE2 | 1.79 | 0.41 |
| 1:A:1036:ASP:O | 1:A:1039:ARG:HB3 | 2.20 | 0.41 |
| 1:A:628:ILE:HD11 | 1:A:762:ILE:HD13 | 2.03 | 0.41 |
| 2:B:13:THR:O | 2:B:15:LEU:HD23 | 2.20 | 0.41 |
| 6:F:462:LEU:HD13 | 6:F:465:LEU:HD23 | 2.02 | 0.41 |
| 6:F:703:PRO:HB3 | 6:F:733:VAL:CG2 | 2.50 | 0.41 |
| 8:I:224:SER:OG | 8:I:228:ALA:O | 2.29 | 0.41 |
| 8:I:440:MET:HA | 8:I:440:MET:HE3 | 2.03 | 0.41 |
| 9:J:441:VAL:CG2 | 9:J:444:TRP:CD1 | 2.91 | 0.41 |
| 12:N:139:GLY:C | 12:N:141:LEU:N | 2.70 | 0.41 |
| 12:N:550:GLY:HA2 | 12:N:551:GLU:CB | 2.51 | 0.41 |
| 13:O:678:TYR:O | 13:O:683:LYS:HB2 | 2.20 | 0.41 |
| 13:O:682:LYS:O | 13:O:685:GLU:HB3 | 2.20 | 0.41 |
| 3:P:46:ARG:HG3 | 3:P:116:PHE:CD2 | 2.55 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:91:LYS:O | 3:P:94:PHE:HB3 | 2.21 | 0.41 |
| 16:S:279:ALA:N | 16:S:280:ASP:HA | 2.36 | 0.41 |
| 9:K:243:TYR:HA | 7:W:3:ARG:HH22 | 1.85 | 0.41 |
| 17:X:244:ALA:O | 17:X:248:THR:HG23 | 2.21 | 0.41 |
| 17:Y:100:TYR:CD1 | 17:Y:138:VAL:HG13 | 2.55 | 0.41 |
| 17:Y:242:ALA:O | 17:Y:246:VAL:HG23 | 2.20 | 0.41 |
| 17:Y:434:TYR:HA | 17:Y:444:LEU:HD22 | 2.03 | 0.41 |
| 1:A:1787:LEU:O | 1:A:1791:ILE:HG12 | 2.21 | 0.41 |
| 1:A:629:LEU:C | 1:A:629:LEU:HD12 | 2.42 | 0.41 |
| 1:A:845:TYR:HB3 | 1:A:1812:TRP:CE3 | 2.56 | 0.41 |
| 3:C:185:VAL:HG13 | 3:C:212:LEU:HD22 | 2.02 | 0.41 |
| 6:F:507:ARG:HD3 | 6:F:538:ILE:CD1 | 2.42 | 0.41 |
| 9:J:168:ASP:HA | 9:J:171:THR:HG22 | 2.03 | 0.41 |
| 9:J:165:GLU:OE2 | 9:K:20:GLN:HB2 | 2.21 | 0.41 |
| 12:N:580:LYS:HB3 | 12:N:582:PRO:HD2 | 2.03 | 0.41 |
| 12:N:595:ILE:CD1 | 12:N:626:TYR:OH | 2.69 | 0.41 |
| 13:O:321:GLU:HA | 13:O:350:LEU:HD13 | 2.02 | 0.41 |
| 13:O:592:TRP:HH2 | 13:O:630:ALA:HA | 1.86 | 0.41 |
| 13:O:688:GLU:O | 13:O:691:ILE:HG22 | 2.21 | 0.41 |
| 3:P:251:TYR:CZ | 3:P:268:GLN:HG3 | 2.55 | 0.41 |
| 14:Q:461:ALA:CA | 14:Q:467:LEU:HD12 | 2.51 | 0.41 |
| 17:X:316:ALA:HB1 | 17:X:351:TYR:CE1 | 2.56 | 0.41 |
| 14:Q:352:THR:CB | 18:Z:51:LEU:HA | 2.51 | 0.41 |
| 1:A:1031:ASP:OD1 | 12:N:489:PRO:N | 2.54 | 0.40 |
| 1:A:1131:MET:O | 1:A:1132:THR:HB | 2.21 | 0.40 |
| 1:A:1619:LEU:HD23 | 1:A:1634:LEU:HD11 | 2.02 | 0.40 |
| 3:C:217:GLU:O | 3:C:221:PHE:HD1 | 2.03 | 0.40 |
| 3:C:416:PHE:CB | 3:C:446:LEU:HD11 | 2.47 | 0.40 |
| 6:F:702:ASN:HB2 | 6:F:705:CYS:SG | 2.61 | 0.40 |
| 6:H:163:ASP:HA | 6:H:164:PRO:HD2 | 1.98 | 0.40 |
| 6:H:639:TYR:CZ | 6:H:643:MET:HG3 | 2.57 | 0.40 |
| 8:I:209:CYS:HG | 8:I:584:HIS:CG | 2.22 | 0.40 |
| 8:I:578:ASN:C | 8:I:578:ASN:OD1 | 2.60 | 0.40 |
| 8:I:585:TYR:CE1 | 8:I:602:ARG:HD3 | 2.56 | 0.40 |
| 9:K:276:VAL:HA | 9:K:311:MET:HE2 | 2.03 | 0.40 |
| 10:L:119:TRP:HH2 | 10:L:155:GLN:HG2 | 1.86 | 0.40 |
| 10:L:79:ILE:HG13 | 10:L:156:ILE:HG12 | 2.03 | 0.40 |
| 12:N:595:ILE:HD12 | 12:N:626:TYR:OH | 2.21 | 0.40 |
| 13:O:127:HIS:O | 13:O:128:LYS:CB | 2.61 | 0.40 |
| 13:O:375:TYR:CE1 | 13:O:417:LEU:HD23 | 2.56 | 0.40 |
| 3:P:58:LEU:HD13 | 3:P:259:PHE:HE2 | 1.86 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:276:ILE:CG2 | 3:P:277:ARG:H | 2.22 | 0.40 |
| 16:S:75:LEU:HA | 16:S:115:TYR:OH | 2.21 | 0.40 |
| 16:S:82:ILE:HD13 | 16:S:102:LEU:HD21 | 2.02 | 0.40 |
| 17:X:442:GLN:CD | 17:X:472:ARG:HG3 | 2.41 | 0.40 |
| 18:Z:78:LYS:HB2 | 18:Z:78:LYS:HE3 | 1.96 | 0.40 |
| 1:A:1071:LEU:O | 1:A:1074:CYS:HB2 | 2.22 | 0.40 |
| 1:A:1208:LEU:O | 1:A:1212:VAL:HG23 | 2.21 | 0.40 |
| 1:A:1227:LEU:O | 1:A:1231:HIS:ND1 | 2.55 | 0.40 |
| 1:A:1359:ASN:HB3 | 10:L:30:VAL:HG11 | 2.04 | 0.40 |
| 1:A:1694:ASP:OD1 | 1:A:1696:VAL:HB | 2.21 | 0.40 |
| 1:A:1867:CYS:CB | 1:A:1881:GLN:NE2 | 2.83 | 0.40 |
| 1:A:799:LEU:O | 1:A:801:PRO:HD2 | 2.21 | 0.40 |
| 3:C:412:LEU:O | 3:C:413:LYS:HB2 | 2.20 | 0.40 |
| 6:F:32:TYR:CE1 | 6:F:41:LEU:HB2 | 2.56 | 0.40 |
| 6:H:158:ILE:HG22 | 6:H:159:GLY:N | 2.36 | 0.40 |
| 6:H:162:PRO:HD2 | 6:H:474:LEU:HD13 | 2.03 | 0.40 |
| 6:H:557:LYS:HB3 | 6:H:557:LYS:HE2 | 1.93 | 0.40 |
| 8:I:618:ILE:HD12 | 8:I:705:MET:HE1 | 2.02 | 0.40 |
| 9:J:289:HIS:C | 9:J:289:HIS:CD2 | 2.94 | 0.40 |
| 9:J:337:TRP:O | 9:J:340:TYR:HB3 | 2.21 | 0.40 |
| 9:J:397:ILE:CG2 | 9:J:398:ALA:N | 2.84 | 0.40 |
| 9:K:244:ASN:O | 9:K:245:CYS:HB2 | 2.21 | 0.40 |
| 12:N:596:LEU:HD13 | 12:N:601:TRP:CZ2 | 2.56 | 0.40 |
| 12:N:611:VAL:HG11 | 12:N:637:TRP:CH2 | 2.56 | 0.40 |
| 13:O:351:GLY:O | 13:O:352:GLN:HG3 | 2.21 | 0.40 |
| 13:O:516:PHE:HB2 | 13:O:535:ILE:HD11 | 2.02 | 0.40 |
| 13:O:65:LEU:HB3 | 13:O:66:PRO:HD3 | 2.03 | 0.40 |
| 16:S:19:GLY:O | 16:S:23:GLU:HG3 | 2.20 | 0.40 |
| 17:X:164:SER:HA | 17:X:167:ARG:NE | 2.37 | 0.40 |
| 17:Y:301:ASP:HA | 17:Y:302:PRO:HD2 | 1.95 | 0.40 |
| 17:Y:350:PHE:CE2 | 17:Y:378:LEU:HD12 | 2.56 | 0.40 |
| 3:C:116:PHE:HE1 | 3:C:174:LEU:HB2 | 1.86 | 0.40 |
| 3:C:312:MET:H | 3:C:312:MET:HG2 | 1.60 | 0.40 |
| 6:F:624:PHE:O | 6:F:628:ILE:HG12 | 2.21 | 0.40 |
| 6:H:698:ILE:HG13 | 6:H:699:ASP:N | 2.36 | 0.40 |
| 6:H:765:ASP:O | 17:X:397:ARG:CZ | 2.68 | 0.40 |
| 8:I:266:ASN:HA | 8:I:526:LYS:HZ3 | 1.85 | 0.40 |
| 8:I:279:ILE:HD12 | 8:I:279:ILE:HA | 1.92 | 0.40 |
| 9:K:413:PHE:HD1 | 9:K:454:VAL:HG23 | 1.86 | 0.40 |
| 9:K:19:TYR:CE1 | 9:K:49:LEU:HD13 | 2.56 | 0.40 |
| 12:N:803:VAL:HG21 | 12:N:810:TYR:HB2 | 2.03 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:340:LEU:HA | 13:O:340:LEU:HD23 | 1.93 | 0.40 |
| 3:P:464:ASP:OD2 | 3:P:469:ALA:HB3 | 2.20 | 0.40 |
| 3:P:66:PRO:O | 3:P:67:LEU:HB3 | 2.20 | 0.40 |
| 14:Q:163:LYS:HD3 | 15:R:466:THR:CG2 | 2.51 | 0.40 |
| 14:Q:430:TYR:CG | 14:Q:431:PRO:HA | 2.56 | 0.40 |
| 15:R:346:VAL:HA | 15:R:347:PRO:HD3 | 1.98 | 0.40 |
| 16:S:41:LEU:HD11 | 18:Z:141:PHE:CB | 2.44 | 0.40 |
| 17:Y:452:LEU:HD22 | 17:Y:461:ALA:CA | 2.47 | 0.40 |
| 17:Y:60:LEU:HB3 | 17:Y:79:LEU:HD11 | 2.04 | 0.40 |
| 14:Q:128:ALA:HB1 | 18:Z:156:TYR:CZ | 2.50 | 0.40 |
| 1:A:181:TRP:HA | 1:A:182:PRO:HD3 | 2.01 | 0.40 |
| 1:A:941:LEU:HB2 | 1:A:977:LEU:HA | 2.03 | 0.40 |
| 3:C:62:LEU:HB3 | 3:C:63:PRO:HD2 | 2.03 | 0.40 |
| 5:E:60:SER:O | 5:E:63:VAL:HG12 | 2.21 | 0.40 |
| 6:F:550:VAL:HG13 | 6:F:551:ALA:N | 2.37 | 0.40 |
| 9:J:342:HIS:CD2 | 9:J:357:TYR:OH | 2.74 | 0.40 |
| 9:K:190:LEU:O | 9:K:198:GLN:NE2 | 2.54 | 0.40 |
| 9:K:63:ARG:HB2 | 9:K:65:LEU:HD13 | 2.01 | 0.40 |
| 12:N:354:SER:O | 12:N:357:ALA:HB3 | 2.22 | 0.40 |
| 12:N:556:PHE:CG | 12:N:600:PHE:HD1 | 2.39 | 0.40 |
| 12:N:596:LEU:HD22 | 12:N:601:TRP:CZ2 | 2.56 | 0.40 |
| 3:P:54:TRP:CE3 | 3:P:203:TRP:HB2 | 2.56 | 0.40 |
| 14:Q:128:ALA:HB3 | 18:Z:156:TYR:CE2 | 2.39 | 0.40 |
| 17:X:154:ASP:N | 17:X:154:ASP:OD1 | 2.54 | 0.40 |
| 17:X:71:PHE:O | 17:X:76:LYS:HE3 | 2.22 | 0.40 |
| 17:Y:164:SER:HA | 17:Y:167:ARG:NE | 2.36 | 0.40 |
| 1:A:1800:LEU:HD11 | 1:A:1811:LEU:HD21 | 2.03 | 0.40 |
| 1:A:223:LEU:HA | 1:A:223:LEU:HD12 | 1.98 | 0.40 |
| 1:A:474:ILE:HD11 | 1:A:490:VAL:HG21 | 2.03 | 0.40 |
| 1:A:808:ARG:NH2 | 1:A:1894:VAL:O | 2.54 | 0.40 |
| 2:B:16:TRP:O | 2:B:31:ASN:O | 2.39 | 0.40 |
| 3:C:91:LYS:O | 3:C:94:PHE:HB3 | 2.22 | 0.40 |
| 6:F:689:LEU:O | 6:F:693:ASN:HB2 | 2.22 | 0.40 |
| 6:H:726:LEU:HD21 | 6:H:742:LEU:HD22 | 2.03 | 0.40 |
| 6:H:765:ASP:O | 17:X:397:ARG:NE | 2.54 | 0.40 |
| 8:I:14:VAL:N | 8:I:743:VAL:O | 2.54 | 0.40 |
| 9:K:250:CYS:SG | 9:K:274:THR:HG23 | 2.55 | 0.40 |
| 10:L:86:ASP:HB3 | 10:L:89:TYR:CB | 2.40 | 0.40 |
| 12:N:202:GLU:HB2 | 12:N:282:GLU:CD | 2.40 | 0.40 |
| 12:N:370:GLN:HE21 | 12:N:373:GLN:HB3 | 1.87 | 0.40 |
| 13:O:267:VAL:O | 13:O:271:THR:HG22 | 2.21 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:544:VAL:HG23 | 13:O:567:LEU:CG | 2.45 | 0.40 |
| 3:P:115:TYR:CD1 | 3:P:115:TYR:C | 2.95 | 0.40 |
| 16:S:29:VAL:C | 16:S:36:ARG:NH2 | 2.62 | 0.40 |
| 16:S:65:GLU:C | 16:S:69:TYR:CD2 | 2.94 | 0.40 |
| 16:S:20:ASP:H | 18:Z:134:GLN:NE2 | 2.12 | 0.40 |
| 18:Z:179:GLU:HG2 | 18:Z:201:ILE:HG12 | 2.02 | 0.40 |
| 16:S:20:ASP:CG | 18:Z:184:ARG:HD2 | 2.32 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 1397/1944 (72%) | 1267 (91%) | 106 (8%) | 24 (2%) | 11 | 56 |
| 2 | B | 75/84 (89%) | 62 (83%) | 8 (11%) | 5 (7%) | 1 | 25 |
| 3 | C | 520/597 (87%) | 498 (96%) | 20 (4%) | 2 (0%) | 39 | 79 |
| 3 | P | 485/597 (81%) | 465 (96%) | 20 (4%) | 0 | 100 | 100 |
| 4 | D | 16/121 (13%) | 14 (88%) | 2 (12%) | 0 | 100 | 100 |
| 5 | E | 54/110 (49%) | 53 (98%) | 1 (2%) | 0 | 100 | 100 |
| 6 | F | 479/824 (58%) | 458 (96%) | 13 (3%) | 8 (2%) | 11 | 56 |
| 6 | H | 479/824 (58%) | 459 (96%) | 14 (3%) | 6 (1%) | 15 | 60 |
| 7 | G | 23/85 (27%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 7 | W | 23/85 (27%) | 23 (100%) | 0 | 0 | 100 | 100 |
| 8 | I | 725/808 (90%) | 683 (94%) | 35 (5%) | 7 (1%) | 19 | 65 |
| 9 | J | 500/620 (81%) | 467 (93%) | 29 (6%) | 4 (1%) | 24 | 69 |
| 9 | K | 489/620 (79%) | 456 (93%) | 27 (6%) | 6 (1%) | 16 | 62 |
| 10 | L | 180/185 (97%) | 165 (92%) | 14 (8%) | 1 (1%) | 30 | 73 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 11 | M | 55/74 (74%) | 46 (84%) | 9 (16%) | 0 | 100 | 100 |
| 12 | N | 679/822 (83%) | 557 (82%) | 68 (10%) | 54 (8%) | 1 | 19 |
| 13 | O | 677/755 (90%) | 640 (94%) | 29 (4%) | 8 (1%) | 16 | 62 |
| 14 | Q | 348/374 (93%) | 317 (91%) | 21 (6%) | 10 (3%) | 6 | 46 |
| 15 | R | 377/499 (76%) | 344 (91%) | 26 (7%) | 7 (2%) | 10 | 54 |
| 16 | S | 267/342 (78%) | 237 (89%) | 18 (7%) | 12 (4%) | 3 | 34 |
| 17 | X | 480/599 (80%) | 464 (97%) | 13 (3%) | 3 (1%) | 30 | 73 |
| 17 | Y | 492/599 (82%) | 474 (96%) | 13 (3%) | 5 (1%) | 19 | 65 |
| 18 | Z | 193/205 (94%) | 186 (96%) | 6 (3%) | 1 (0%) | 34 | 76 |
| All | All | 9013/11773 (77%) | 8358 (93%) | 492 (6%) | 163 (2%) | 15 | 55 |

All (163) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 274 | VAL |
| 1 | A | 630 | PRO |
| 1 | A | 857 | MET |
| 1 | A | 1125 | ILE |
| 1 | A | 1358 | ILE |
| 2 | B | 15 | LEU |
| 2 | B | 37 | CYS |
| 2 | B | 43 | ASP |
| 2 | B | 67 | GLN |
| 8 | I | 431 | ASP |
| 8 | I | 489 | PRO |
| 8 | I | 503 | ASN |
| 9 | J | 221 | PRO |
| 9 | K | 211 | LYS |
| 9 | K | 215 | PRO |
| 12 | N | 74 | TRP |
| 12 | N | 75 | PHE |
| 12 | N | 78 | VAL |
| 12 | N | 79 | LEU |
| 12 | N | 91 | PHE |
| 12 | N | 126 | LEU |
| 12 | N | 140 | LEU |
| 12 | N | 203 | LEU |
| 12 | N | 234 | ARG |
| 12 | N | 252 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 12 | N | 286 | LEU |
| 12 | N | 287 | ARG |
| 12 | N | 290 | HIS |
| 12 | N | 350 | ASP |
| 12 | N | 368 | THR |
| 12 | N | 395 | ASP |
| 12 | N | 412 | PRO |
| 12 | N | 477 | PRO |
| 12 | N | 488 | ASP |
| 12 | N | 489 | PRO |
| 12 | N | 492 | SER |
| 12 | N | 497 | ARG |
| 12 | N | 530 | GLN |
| 12 | N | 606 | ASP |
| 12 | N | 632 | MET |
| 12 | N | 674 | ALA |
| 12 | N | 716 | ILE |
| 14 | Q | 140 | ALA |
| 14 | Q | 141 | PRO |
| 14 | Q | 476 | ASP |
| 14 | Q | 477 | PRO |
| 14 | Q | 478 | ALA |
| 14 | Q | 479 | ARG |
| 15 | R | 106 | THR |
| 16 | S | 77 | VAL |
| 16 | S | 135 | PRO |
| 16 | S | 222 | PRO |
| 16 | S | 230 | LEU |
| 16 | S | 262 | PHE |
| 16 | S | 274 | VAL |
| 17 | X | 213 | SER |
| 17 | Y | 201 | LEU |
| 17 | Y | 213 | SER |
| 18 | Z | 159 | LYS |
| 1 | A | 87 | VAL |
| 1 | A | 860 | TYR |
| 1 | A | 1099 | PRO |
| 1 | A | 1164 | LYS |
| 1 | A | 1307 | LEU |
| 1 | A | 1925 | VAL |
| 3 | C | 27 | SER |
| 6 | F | 129 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 6 | F | 147 | PHE |
| 6 | F | 165 | ASP |
| 6 | F | 493 | SER |
| 6 | H | 129 | ASP |
| 6 | H | 147 | PHE |
| 6 | H | 493 | SER |
| 8 | I | 296 | THR |
| 8 | I | 433 | VAL |
| 9 | J | 70 | GLU |
| 12 | N | 63 | ALA |
| 12 | N | 64 | ALA |
| 12 | N | 101 | SER |
| 12 | N | 278 | ARG |
| 12 | N | 289 | PHE |
| 12 | N | 531 | PHE |
| 12 | N | 550 | GLY |
| 13 | O | 505 | GLN |
| 14 | Q | 137 | PRO |
| 14 | Q | 266 | SER |
| 15 | R | 101 | PRO |
| 15 | R | 266 | SER |
| 15 | R | 494 | ILE |
| 16 | S | 74 | PRO |
| 16 | S | 235 | LYS |
| 17 | X | 202 | ALA |
| 17 | Y | 202 | ALA |
| 1 | A | 1100 | LEU |
| 1 | A | 1283 | PRO |
| 1 | A | 1314 | ILE |
| 6 | F | 103 | HIS |
| 8 | I | 487 | VAL |
| 9 | J | 397 | ILE |
| 9 | K | 129 | LYS |
| 9 | K | 228 | GLN |
| 10 | L | 174 | THR |
| 12 | N | 77 | GLU |
| 12 | N | 144 | THR |
| 12 | N | 280 | GLU |
| 12 | N | 480 | TRP |
| 12 | N | 500 | ASP |
| 12 | N | 629 | LEU |
| 12 | N | 672 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 13 | O | 707 | LYS |
| 15 | R | 108 | THR |
| 16 | S | 559 | ALA |
| 17 | Y | 456 | VAL |
| 1 | A | 253 | PRO |
| 1 | A | 1055 | PRO |
| 1 | A | 1822 | SER |
| 2 | B | 65 | HIS |
| 6 | F | 145 | ASN |
| 6 | H | 145 | ASN |
| 9 | J | 382 | ASN |
| 9 | K | 86 | HIS |
| 12 | N | 219 | PRO |
| 12 | N | 283 | ARG |
| 12 | N | 352 | PRO |
| 12 | N | 353 | ASP |
| 12 | N | 482 | PRO |
| 12 | N | 484 | PRO |
| 12 | N | 595 | ILE |
| 13 | O | 462 | ASN |
| 13 | O | 540 | SER |
| 13 | O | 657 | ILE |
| 13 | O | 745 | PRO |
| 17 | X | 456 | VAL |
| 1 | A | 1356 | ASP |
| 1 | A | 1603 | LEU |
| 6 | F | 96 | VAL |
| 6 | H | 97 | PHE |
| 12 | N | 282 | GLU |
| 12 | N | 499 | SER |
| 13 | O | 126 | VAL |
| 15 | R | 498 | ILE |
| 16 | S | 301 | PRO |
| 1 | A | 502 | GLY |
| 1 | A | 590 | PRO |
| 1 | A | 781 | GLU |
| 1 | A | 1239 | THR |
| 3 | C | 229 | MET |
| 6 | F | 97 | PHE |
| 6 | H | 96 | VAL |
| 12 | N | 142 | MET |
| 12 | N | 551 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14 | Q | 161 | SER |
| 15 | R | 76 | GLY |
| 9 | K | 399 | PRO |
| 16 | S | 257 | GLY |
| 8 | I | 291 | VAL |
| 16 | S | 294 | PRO |
| 1 | A | 858 | PRO |
| 12 | N | 490 | GLY |
| 14 | Q | 498 | ILE |
| 17 | Y | 200 | PRO |
| 12 | N | 166 | PRO |
| 13 | O | 124 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1 | A | 1151/1720 (67%) | 1011 (88%) | 140 (12%) | 6 | 33 |
| 2 | B | 71/75 (95%) | 59 (83%) | 12 (17%) | 2 | 20 |
| 3 | C | 452/520 (87%) | 390 (86%) | 62 (14%) | 4 | 29 |
| 3 | P | 422/520 (81%) | 374 (89%) | 48 (11%) | 7 | 36 |
| 4 | D | 18/115 (16%) | 15 (83%) | 3 (17%) | 3 | 21 |
| 5 | E | 47/89 (53%) | 37 (79%) | 10 (21%) | 1 | 11 |
| 6 | F | 407/727 (56%) | 361 (89%) | 46 (11%) | 7 | 37 |
| 6 | H | 408/727 (56%) | 368 (90%) | 40 (10%) | 10 | 43 |
| 7 | G | 23/77 (30%) | 20 (87%) | 3 (13%) | 5 | 31 |
| 7 | W | 23/77 (30%) | 21 (91%) | 2 (9%) | 13 | 48 |
| 8 | I | 617/730 (84%) | 579 (94%) | 38 (6%) | 23 | 62 |
| 9 | J | 424/548 (77%) | 373 (88%) | 51 (12%) | 6 | 33 |
| 9 | K | 423/548 (77%) | 383 (90%) | 40 (10%) | 11 | 45 |
| 10 | L | 155/170 (91%) | 137 (88%) | 18 (12%) | 7 | 36 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|-----------|-------------|----|
| 11 | M | 55/67 (82%) | 45 (82%) | 10 (18%) | 2 | 16 |
| 12 | N | 518/724 (72%) | 448 (86%) | 70 (14%) | 5 | 30 |
| 13 | O | 577/650 (89%) | 503 (87%) | 74 (13%) | 5 | 31 |
| 14 | Q | 271/310 (87%) | 264 (97%) | 7 (3%) | 54 | 81 |
| 15 | R | 311/411 (76%) | 293 (94%) | 18 (6%) | 25 | 64 |
| 16 | S | 186/293 (64%) | 181 (97%) | 5 (3%) | 52 | 80 |
| 17 | X | 407/513 (79%) | 376 (92%) | 31 (8%) | 16 | 55 |
| 17 | Y | 418/513 (82%) | 381 (91%) | 37 (9%) | 12 | 48 |
| 18 | Z | 181/190 (95%) | 170 (94%) | 11 (6%) | 23 | 63 |
| All | All | 7565/10314 (73%) | 6789 (90%) | 776 (10%) | 13 | 40 |

All (776) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 31 | HIS |
| 1 | A | 36 | ASN |
| 1 | A | 37 | LEU |
| 1 | A | 39 | LEU |
| 1 | A | 47 | GLU |
| 1 | A | 88 | ASP |
| 1 | A | 90 | ASP |
| 1 | A | 92 | GLU |
| 1 | A | 98 | ASN |
| 1 | A | 99 | MET |
| 1 | A | 118 | THR |
| 1 | A | 120 | ASP |
| 1 | A | 127 | LEU |
| 1 | A | 128 | TRP |
| 1 | A | 133 | ILE |
| 1 | A | 151 | ILE |
| 1 | A | 159 | ILE |
| 1 | A | 172 | SER |
| 1 | A | 180 | VAL |
| 1 | A | 210 | MET |
| 1 | A | 212 | SER |
| 1 | A | 216 | PRO |
| 1 | A | 249 | LEU |
| 1 | A | 250 | ASN |
| 1 | A | 271 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 429 | LYS |
| 1 | A | 430 | VAL |
| 1 | A | 437 | CYS |
| 1 | A | 439 | GLN |
| 1 | A | 444 | PHE |
| 1 | A | 449 | GLN |
| 1 | A | 450 | LEU |
| 1 | A | 459 | GLU |
| 1 | A | 474 | ILE |
| 1 | A | 491 | LEU |
| 1 | A | 497 | LEU |
| 1 | A | 508 | LYS |
| 1 | A | 583 | TYR |
| 1 | A | 584 | ILE |
| 1 | A | 614 | THR |
| 1 | A | 638 | LEU |
| 1 | A | 640 | LYS |
| 1 | A | 664 | LEU |
| 1 | A | 766 | LEU |
| 1 | A | 772 | GLU |
| 1 | A | 774 | LYS |
| 1 | A | 781 | GLU |
| 1 | A | 796 | ASP |
| 1 | A | 808 | ARG |
| 1 | A | 871 | ARG |
| 1 | A | 934 | MET |
| 1 | A | 953 | LEU |
| 1 | A | 962 | CYS |
| 1 | A | 964 | GLU |
| 1 | A | 980 | ARG |
| 1 | A | 1016 | MET |
| 1 | A | 1043 | SER |
| 1 | A | 1075 | GLN |
| 1 | A | 1076 | ARG |
| 1 | A | 1089 | LEU |
| 1 | A | 1100 | LEU |
| 1 | A | 1107 | LEU |
| 1 | A | 1118 | VAL |
| 1 | A | 1120 | LEU |
| 1 | A | 1146 | LYS |
| 1 | A | 1168 | LEU |
| 1 | A | 1170 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1176 | LEU |
| 1 | A | 1177 | MET |
| 1 | A | 1179 | LEU |
| 1 | A | 1181 | LEU |
| 1 | A | 1184 | HIS |
| 1 | A | 1202 | GLU |
| 1 | A | 1216 | LYS |
| 1 | A | 1217 | LEU |
| 1 | A | 1220 | MET |
| 1 | A | 1230 | ILE |
| 1 | A | 1232 | ILE |
| 1 | A | 1235 | LEU |
| 1 | A | 1243 | LEU |
| 1 | A | 1273 | LEU |
| 1 | A | 1279 | ARG |
| 1 | A | 1292 | GLU |
| 1 | A | 1312 | ASN |
| 1 | A | 1313 | LEU |
| 1 | A | 1319 | LEU |
| 1 | A | 1323 | GLU |
| 1 | A | 1325 | LEU |
| 1 | A | 1327 | GLN |
| 1 | A | 1359 | ASN |
| 1 | A | 1369 | LEU |
| 1 | A | 1386 | TRP |
| 1 | A | 1400 | LYS |
| 1 | A | 1404 | LEU |
| 1 | A | 1405 | LEU |
| 1 | A | 1409 | LEU |
| 1 | A | 1424 | LYS |
| 1 | A | 1455 | GLU |
| 1 | A | 1482 | LEU |
| 1 | A | 1487 | CYS |
| 1 | A | 1511 | ASN |
| 1 | A | 1536 | LEU |
| 1 | A | 1538 | LEU |
| 1 | A | 1539 | CYS |
| 1 | A | 1540 | ARG |
| 1 | A | 1562 | LEU |
| 1 | A | 1564 | LEU |
| 1 | A | 1573 | SER |
| 1 | A | 1574 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1586 | CYS |
| 1 | A | 1588 | LEU |
| 1 | A | 1597 | THR |
| 1 | A | 1603 | LEU |
| 1 | A | 1607 | ARG |
| 1 | A | 1611 | VAL |
| 1 | A | 1638 | TYR |
| 1 | A | 1646 | GLN |
| 1 | A | 1650 | GLU |
| 1 | A | 1656 | LEU |
| 1 | A | 1662 | LEU |
| 1 | A | 1667 | LYS |
| 1 | A | 1672 | ARG |
| 1 | A | 1674 | TRP |
| 1 | A | 1687 | LEU |
| 1 | A | 1693 | LYS |
| 1 | A | 1694 | ASP |
| 1 | A | 1706 | LEU |
| 1 | A | 1731 | ARG |
| 1 | A | 1742 | THR |
| 1 | A | 1748 | LEU |
| 1 | A | 1749 | SER |
| 1 | A | 1770 | LEU |
| 1 | A | 1785 | GLU |
| 1 | A | 1798 | ARG |
| 1 | A | 1805 | MET |
| 1 | A | 1851 | THR |
| 1 | A | 1854 | ASN |
| 1 | A | 1858 | GLN |
| 1 | A | 1869 | HIS |
| 1 | A | 1882 | LEU |
| 2 | B | 11 | VAL |
| 2 | B | 14 | TRP |
| 2 | B | 15 | LEU |
| 2 | B | 16 | TRP |
| 2 | B | 23 | CYS |
| 2 | B | 34 | CYS |
| 2 | B | 40 | PRO |
| 2 | B | 42 | ASP |
| 2 | B | 62 | LYS |
| 2 | B | 63 | TRP |
| 2 | B | 71 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | B | 79 | GLU |
| 3 | C | 26 | PHE |
| 3 | C | 42 | LEU |
| 3 | C | 44 | ARG |
| 3 | C | 49 | LEU |
| 3 | C | 57 | GLU |
| 3 | C | 70 | LEU |
| 3 | C | 77 | THR |
| 3 | C | 78 | GLU |
| 3 | C | 85 | ASP |
| 3 | C | 89 | LEU |
| 3 | C | 97 | LYS |
| 3 | C | 100 | ASP |
| 3 | C | 101 | ARG |
| 3 | C | 122 | ARG |
| 3 | C | 127 | GLU |
| 3 | C | 128 | LYS |
| 3 | C | 136 | ASP |
| 3 | C | 138 | LEU |
| 3 | C | 147 | LYS |
| 3 | C | 157 | GLU |
| 3 | C | 160 | LYS |
| 3 | C | 172 | LEU |
| 3 | C | 182 | LEU |
| 3 | C | 197 | HIS |
| 3 | C | 201 | LEU |
| 3 | C | 234 | LEU |
| 3 | C | 237 | ILE |
| 3 | C | 239 | THR |
| 3 | C | 244 | ILE |
| 3 | C | 268 | GLN |
| 3 | C | 280 | ASP |
| 3 | C | 289 | LEU |
| 3 | C | 300 | MET |
| 3 | C | 302 | THR |
| 3 | C | 307 | LEU |
| 3 | C | 310 | ARG |
| 3 | C | 312 | MET |
| 3 | C | 313 | LYS |
| 3 | C | 315 | GLU |
| 3 | C | 324 | CYS |
| 3 | C | 334 | CYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 343 | LEU |
| 3 | C | 359 | LYS |
| 3 | C | 361 | ASN |
| 3 | C | 376 | MET |
| 3 | C | 379 | LYS |
| 3 | C | 381 | THR |
| 3 | C | 386 | GLN |
| 3 | C | 389 | ARG |
| 3 | C | 397 | ARG |
| 3 | C | 414 | MET |
| 3 | C | 418 | CYS |
| 3 | C | 424 | ARG |
| 3 | C | 428 | LEU |
| 3 | C | 432 | ASP |
| 3 | C | 435 | MET |
| 3 | C | 441 | GLU |
| 3 | C | 451 | GLU |
| 3 | C | 516 | LEU |
| 3 | C | 518 | GLN |
| 3 | C | 524 | LYS |
| 3 | C | 542 | THR |
| 4 | D | 11 | ARG |
| 4 | D | 12 | VAL |
| 4 | D | 16 | LEU |
| 5 | E | 56 | GLU |
| 5 | E | 57 | SER |
| 5 | E | 58 | VAL |
| 5 | E | 60 | SER |
| 5 | E | 61 | TYR |
| 5 | E | 66 | THR |
| 5 | E | 69 | GLN |
| 5 | E | 85 | LEU |
| 5 | E | 87 | GLU |
| 5 | E | 99 | ILE |
| 6 | F | 22 | ARG |
| 6 | F | 27 | LEU |
| 6 | F | 43 | LEU |
| 6 | F | 70 | GLN |
| 6 | F | 78 | CYS |
| 6 | F | 90 | GLN |
| 6 | F | 98 | ASN |
| 6 | F | 104 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | F | 118 | LEU |
| 6 | F | 121 | LEU |
| 6 | F | 141 | SER |
| 6 | F | 143 | SER |
| 6 | F | 145 | ASN |
| 6 | F | 165 | ASP |
| 6 | F | 462 | LEU |
| 6 | F | 477 | CYS |
| 6 | F | 494 | HIS |
| 6 | F | 503 | CYS |
| 6 | F | 507 | ARG |
| 6 | F | 520 | ARG |
| 6 | F | 521 | ILE |
| 6 | F | 527 | ARG |
| 6 | F | 530 | ASN |
| 6 | F | 536 | MET |
| 6 | F | 538 | ILE |
| 6 | F | 549 | ASP |
| 6 | F | 562 | MET |
| 6 | F | 564 | LYS |
| 6 | F | 576 | CYS |
| 6 | F | 578 | SER |
| 6 | F | 588 | LYS |
| 6 | F | 614 | THR |
| 6 | F | 616 | GLU |
| 6 | F | 618 | ASP |
| 6 | F | 623 | CYS |
| 6 | F | 625 | ARG |
| 6 | F | 655 | GLU |
| 6 | F | 656 | MET |
| 6 | F | 667 | GLN |
| 6 | F | 701 | LYS |
| 6 | F | 705 | CYS |
| 6 | F | 720 | LYS |
| 6 | F | 721 | SER |
| 6 | F | 729 | LEU |
| 6 | F | 748 | LYS |
| 6 | F | 757 | LEU |
| 7 | G | 4 | ARG |
| 7 | G | 5 | LYS |
| 7 | G | 23 | ARG |
| 6 | H | 27 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6 | H | 43 | LEU |
| 6 | H | 61 | LEU |
| 6 | H | 78 | CYS |
| 6 | H | 90 | GLN |
| 6 | H | 98 | ASN |
| 6 | H | 141 | SER |
| 6 | H | 143 | SER |
| 6 | H | 462 | LEU |
| 6 | H | 477 | CYS |
| 6 | H | 480 | ASN |
| 6 | H | 494 | HIS |
| 6 | H | 503 | CYS |
| 6 | H | 507 | ARG |
| 6 | H | 515 | TYR |
| 6 | H | 520 | ARG |
| 6 | H | 521 | ILE |
| 6 | H | 530 | ASN |
| 6 | H | 536 | MET |
| 6 | H | 562 | MET |
| 6 | H | 563 | ASP |
| 6 | H | 564 | LYS |
| 6 | H | 571 | CYS |
| 6 | H | 582 | GLU |
| 6 | H | 584 | ASP |
| 6 | H | 588 | LYS |
| 6 | H | 592 | ARG |
| 6 | H | 599 | ASN |
| 6 | H | 618 | ASP |
| 6 | H | 623 | CYS |
| 6 | H | 655 | GLU |
| 6 | H | 667 | GLN |
| 6 | H | 702 | ASN |
| 6 | H | 709 | ARG |
| 6 | H | 720 | LYS |
| 6 | H | 729 | LEU |
| 6 | H | 755 | LEU |
| 6 | H | 757 | LEU |
| 6 | H | 761 | SER |
| 6 | H | 762 | TRP |
| 8 | I | 26 | LEU |
| 8 | I | 34 | LEU |
| 8 | I | 37 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8 | I | 71 | LEU |
| 8 | I | 75 | PRO |
| 8 | I | 89 | LYS |
| 8 | I | 92 | LEU |
| 8 | I | 101 | LEU |
| 8 | I | 218 | SER |
| 8 | I | 224 | SER |
| 8 | I | 232 | SER |
| 8 | I | 259 | SER |
| 8 | I | 266 | ASN |
| 8 | I | 267 | LEU |
| 8 | I | 269 | LEU |
| 8 | I | 273 | CYS |
| 8 | I | 304 | PHE |
| 8 | I | 322 | MET |
| 8 | I | 325 | LEU |
| 8 | I | 349 | ILE |
| 8 | I | 352 | LEU |
| 8 | I | 353 | GLN |
| 8 | I | 359 | LEU |
| 8 | I | 360 | LEU |
| 8 | I | 361 | TYR |
| 8 | I | 371 | SER |
| 8 | I | 372 | TRP |
| 8 | I | 382 | ASP |
| 8 | I | 447 | PHE |
| 8 | I | 452 | LEU |
| 8 | I | 477 | GLN |
| 8 | I | 522 | LEU |
| 8 | I | 564 | ASP |
| 8 | I | 571 | LYS |
| 8 | I | 588 | PHE |
| 8 | I | 688 | THR |
| 8 | I | 718 | LYS |
| 8 | I | 736 | SER |
| 9 | J | 9 | ARG |
| 9 | J | 23 | LEU |
| 9 | J | 42 | TRP |
| 9 | J | 61 | ARG |
| 9 | J | 69 | TYR |
| 9 | J | 134 | LEU |
| 9 | J | 141 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | J | 157 | LEU |
| 9 | J | 163 | CYS |
| 9 | J | 164 | PHE |
| 9 | J | 169 | LEU |
| 9 | J | 180 | GLU |
| 9 | J | 185 | LEU |
| 9 | J | 188 | LEU |
| 9 | J | 202 | ARG |
| 9 | J | 206 | GLU |
| 9 | J | 214 | LYS |
| 9 | J | 248 | LYS |
| 9 | J | 254 | THR |
| 9 | J | 256 | VAL |
| 9 | J | 259 | GLU |
| 9 | J | 267 | CYS |
| 9 | J | 287 | LEU |
| 9 | J | 290 | LYS |
| 9 | J | 298 | ASN |
| 9 | J | 307 | CYS |
| 9 | J | 323 | LEU |
| 9 | J | 329 | LEU |
| 9 | J | 331 | LYS |
| 9 | J | 340 | TYR |
| 9 | J | 343 | SER |
| 9 | J | 351 | ASP |
| 9 | J | 354 | MET |
| 9 | J | 363 | LEU |
| 9 | J | 385 | LYS |
| 9 | J | 395 | LEU |
| 9 | J | 400 | GLU |
| 9 | J | 423 | LYS |
| 9 | J | 429 | LEU |
| 9 | J | 439 | VAL |
| 9 | J | 445 | GLU |
| 9 | J | 448 | LEU |
| 9 | J | 451 | LEU |
| 9 | J | 465 | LEU |
| 9 | J | 472 | LEU |
| 9 | J | 485 | ILE |
| 9 | J | 488 | ILE |
| 9 | J | 497 | ASN |
| 9 | J | 518 | MET |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | J | 525 | MET |
| 9 | J | 527 | ILE |
| 9 | K | 9 | ARG |
| 9 | K | 20 | GLN |
| 9 | K | 45 | GLN |
| 9 | K | 52 | GLN |
| 9 | K | 63 | ARG |
| 9 | K | 134 | LEU |
| 9 | K | 141 | ASP |
| 9 | K | 146 | ARG |
| 9 | K | 148 | LEU |
| 9 | K | 154 | LYS |
| 9 | K | 157 | LEU |
| 9 | K | 163 | CYS |
| 9 | K | 164 | PHE |
| 9 | K | 169 | LEU |
| 9 | K | 184 | LEU |
| 9 | K | 188 | LEU |
| 9 | K | 190 | LEU |
| 9 | K | 254 | THR |
| 9 | K | 267 | CYS |
| 9 | K | 284 | LEU |
| 9 | K | 287 | LEU |
| 9 | K | 289 | HIS |
| 9 | K | 331 | LYS |
| 9 | K | 340 | TYR |
| 9 | K | 343 | SER |
| 9 | K | 351 | ASP |
| 9 | K | 359 | THR |
| 9 | K | 363 | LEU |
| 9 | K | 370 | PRO |
| 9 | K | 376 | LEU |
| 9 | K | 400 | GLU |
| 9 | K | 423 | LYS |
| 9 | K | 429 | LEU |
| 9 | K | 432 | ILE |
| 9 | K | 454 | VAL |
| 9 | K | 492 | MET |
| 9 | K | 497 | ASN |
| 9 | K | 506 | LEU |
| 9 | K | 510 | ARG |
| 9 | K | 522 | CYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10 | L | 12 | ASP |
| 10 | L | 23 | ARG |
| 10 | L | 25 | ILE |
| 10 | L | 32 | SER |
| 10 | L | 48 | ASP |
| 10 | L | 65 | ASN |
| 10 | L | 67 | GLN |
| 10 | L | 77 | LEU |
| 10 | L | 92 | SER |
| 10 | L | 98 | VAL |
| 10 | L | 101 | ASN |
| 10 | L | 113 | LEU |
| 10 | L | 132 | THR |
| 10 | L | 151 | THR |
| 10 | L | 154 | ARG |
| 10 | L | 162 | VAL |
| 10 | L | 177 | PHE |
| 10 | L | 184 | ARG |
| 11 | M | 7 | ARG |
| 11 | M | 12 | LEU |
| 11 | M | 17 | ASP |
| 11 | M | 29 | VAL |
| 11 | M | 35 | GLU |
| 11 | M | 50 | VAL |
| 11 | M | 51 | LYS |
| 11 | M | 55 | MET |
| 11 | M | 59 | ASP |
| 11 | M | 64 | TYR |
| 12 | N | 74 | TRP |
| 12 | N | 75 | PHE |
| 12 | N | 76 | VAL |
| 12 | N | 77 | GLU |
| 12 | N | 79 | LEU |
| 12 | N | 80 | GLN |
| 12 | N | 150 | ARG |
| 12 | N | 162 | PHE |
| 12 | N | 163 | PHE |
| 12 | N | 170 | GLN |
| 12 | N | 180 | PHE |
| 12 | N | 181 | LEU |
| 12 | N | 202 | GLU |
| 12 | N | 206 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | N | 243 | LEU |
| 12 | N | 250 | LEU |
| 12 | N | 251 | SER |
| 12 | N | 256 | VAL |
| 12 | N | 271 | GLU |
| 12 | N | 277 | CYS |
| 12 | N | 278 | ARG |
| 12 | N | 281 | TYR |
| 12 | N | 285 | PHE |
| 12 | N | 322 | ARG |
| 12 | N | 334 | ARG |
| 12 | N | 340 | ARG |
| 12 | N | 351 | PHE |
| 12 | N | 355 | ARG |
| 12 | N | 364 | CYS |
| 12 | N | 365 | LEU |
| 12 | N | 366 | GLU |
| 12 | N | 372 | GLN |
| 12 | N | 373 | GLN |
| 12 | N | 379 | LYS |
| 12 | N | 386 | LEU |
| 12 | N | 388 | HIS |
| 12 | N | 392 | ASN |
| 12 | N | 394 | CYS |
| 12 | N | 398 | THR |
| 12 | N | 425 | ARG |
| 12 | N | 433 | ASP |
| 12 | N | 435 | VAL |
| 12 | N | 503 | SER |
| 12 | N | 504 | LEU |
| 12 | N | 507 | SER |
| 12 | N | 513 | ASP |
| 12 | N | 517 | ASN |
| 12 | N | 519 | TYR |
| 12 | N | 531 | PHE |
| 12 | N | 544 | LEU |
| 12 | N | 557 | CYS |
| 12 | N | 561 | LEU |
| 12 | N | 566 | ASP |
| 12 | N | 570 | ILE |
| 12 | N | 571 | ASN |
| 12 | N | 592 | TYR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | N | 594 | VAL |
| 12 | N | 604 | PHE |
| 12 | N | 609 | LEU |
| 12 | N | 613 | GLU |
| 12 | N | 622 | TYR |
| 12 | N | 625 | LYS |
| 12 | N | 626 | TYR |
| 12 | N | 632 | MET |
| 12 | N | 638 | LYS |
| 12 | N | 640 | THR |
| 12 | N | 670 | PHE |
| 12 | N | 678 | LEU |
| 12 | N | 695 | ARG |
| 12 | N | 699 | TRP |
| 13 | O | 38 | LEU |
| 13 | O | 40 | LEU |
| 13 | O | 43 | GLU |
| 13 | O | 44 | MET |
| 13 | O | 62 | GLN |
| 13 | O | 78 | LEU |
| 13 | O | 96 | ARG |
| 13 | O | 98 | LYS |
| 13 | O | 99 | LEU |
| 13 | O | 104 | GLU |
| 13 | O | 106 | LYS |
| 13 | O | 129 | THR |
| 13 | O | 136 | LEU |
| 13 | O | 166 | GLU |
| 13 | O | 207 | LEU |
| 13 | O | 266 | ASP |
| 13 | O | 280 | ARG |
| 13 | O | 319 | GLN |
| 13 | O | 328 | ILE |
| 13 | O | 344 | LEU |
| 13 | O | 347 | LEU |
| 13 | O | 381 | ILE |
| 13 | O | 387 | GLN |
| 13 | O | 396 | ASN |
| 13 | O | 398 | LEU |
| 13 | O | 404 | ASP |
| 13 | O | 408 | LEU |
| 13 | O | 411 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | O | 414 | LEU |
| 13 | O | 417 | LEU |
| 13 | O | 419 | ASP |
| 13 | O | 420 | ILE |
| 13 | O | 424 | GLN |
| 13 | O | 426 | THR |
| 13 | O | 434 | ARG |
| 13 | O | 435 | SER |
| 13 | O | 441 | GLN |
| 13 | O | 444 | MET |
| 13 | O | 448 | MET |
| 13 | O | 449 | ASN |
| 13 | O | 496 | ARG |
| 13 | O | 506 | LEU |
| 13 | O | 510 | CYS |
| 13 | O | 511 | ASP |
| 13 | O | 533 | THR |
| 13 | O | 567 | LEU |
| 13 | O | 575 | LYS |
| 13 | O | 579 | MET |
| 13 | O | 581 | ILE |
| 13 | O | 586 | SER |
| 13 | O | 608 | LEU |
| 13 | O | 610 | LEU |
| 13 | O | 616 | LEU |
| 13 | O | 618 | TYR |
| 13 | O | 619 | LEU |
| 13 | O | 623 | THR |
| 13 | O | 625 | LEU |
| 13 | O | 626 | ASN |
| 13 | O | 632 | LEU |
| 13 | O | 636 | ILE |
| 13 | O | 641 | LEU |
| 13 | O | 643 | LEU |
| 13 | O | 646 | MET |
| 13 | O | 649 | GLU |
| 13 | O | 657 | ILE |
| 13 | O | 685 | GLU |
| 13 | O | 691 | ILE |
| 13 | O | 693 | ASN |
| 13 | O | 694 | LEU |
| 13 | O | 706 | CYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | O | 713 | VAL |
| 13 | O | 719 | ARG |
| 13 | O | 723 | THR |
| 13 | O | 735 | MET |
| 3 | P | 38 | LEU |
| 3 | P | 42 | LEU |
| 3 | P | 70 | LEU |
| 3 | P | 77 | THR |
| 3 | P | 78 | GLU |
| 3 | P | 85 | ASP |
| 3 | P | 89 | LEU |
| 3 | P | 97 | LYS |
| 3 | P | 100 | ASP |
| 3 | P | 122 | ARG |
| 3 | P | 160 | LYS |
| 3 | P | 172 | LEU |
| 3 | P | 182 | LEU |
| 3 | P | 234 | LEU |
| 3 | P | 239 | THR |
| 3 | P | 244 | ILE |
| 3 | P | 268 | GLN |
| 3 | P | 289 | LEU |
| 3 | P | 299 | ASN |
| 3 | P | 300 | MET |
| 3 | P | 302 | THR |
| 3 | P | 303 | PHE |
| 3 | P | 310 | ARG |
| 3 | P | 312 | MET |
| 3 | P | 313 | LYS |
| 3 | P | 321 | HIS |
| 3 | P | 324 | CYS |
| 3 | P | 325 | GLU |
| 3 | P | 334 | CYS |
| 3 | P | 335 | CYS |
| 3 | P | 343 | LEU |
| 3 | P | 346 | GLN |
| 3 | P | 358 | LEU |
| 3 | P | 365 | LEU |
| 3 | P | 373 | HIS |
| 3 | P | 379 | LYS |
| 3 | P | 381 | THR |
| 3 | P | 395 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | P | 412 | LEU |
| 3 | P | 423 | ARG |
| 3 | P | 424 | ARG |
| 3 | P | 428 | LEU |
| 3 | P | 435 | MET |
| 3 | P | 441 | GLU |
| 3 | P | 451 | GLU |
| 3 | P | 472 | LYS |
| 3 | P | 479 | GLN |
| 3 | P | 524 | LYS |
| 14 | Q | 133 | LEU |
| 14 | Q | 173 | ASP |
| 14 | Q | 316 | ARG |
| 14 | Q | 401 | GLN |
| 14 | Q | 414 | LEU |
| 14 | Q | 494 | ILE |
| 14 | Q | 499 | ARG |
| 15 | R | 77 | ASP |
| 15 | R | 78 | ARG |
| 15 | R | 79 | TYR |
| 15 | R | 83 | ARG |
| 15 | R | 89 | GLU |
| 15 | R | 94 | LEU |
| 15 | R | 97 | LYS |
| 15 | R | 109 | LYS |
| 15 | R | 110 | LYS |
| 15 | R | 116 | TRP |
| 15 | R | 121 | ASN |
| 15 | R | 126 | GLU |
| 15 | R | 127 | GLU |
| 15 | R | 173 | ASP |
| 15 | R | 316 | ARG |
| 15 | R | 401 | GLN |
| 15 | R | 496 | GLN |
| 15 | R | 499 | ARG |
| 16 | S | 30 | GLN |
| 16 | S | 101 | LEU |
| 16 | S | 106 | VAL |
| 16 | S | 280 | ASP |
| 16 | S | 555 | ARG |
| 7 | W | 5 | LYS |
| 7 | W | 14 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | X | 39 | ASP |
| 17 | X | 49 | LEU |
| 17 | X | 79 | LEU |
| 17 | X | 110 | LEU |
| 17 | X | 184 | GLN |
| 17 | X | 193 | LYS |
| 17 | X | 201 | LEU |
| 17 | X | 204 | ASP |
| 17 | X | 255 | ILE |
| 17 | X | 292 | LEU |
| 17 | X | 299 | MET |
| 17 | X | 300 | LEU |
| 17 | X | 301 | ASP |
| 17 | X | 303 | TYR |
| 17 | X | 323 | ASP |
| 17 | X | 366 | ILE |
| 17 | X | 371 | ASN |
| 17 | X | 386 | MET |
| 17 | X | 401 | ARG |
| 17 | X | 414 | ILE |
| 17 | X | 423 | ILE |
| 17 | X | 452 | LEU |
| 17 | X | 453 | GLU |
| 17 | X | 460 | LYS |
| 17 | X | 465 | LEU |
| 17 | X | 475 | TYR |
| 17 | X | 487 | SER |
| 17 | X | 503 | LEU |
| 17 | X | 506 | GLN |
| 17 | X | 515 | LEU |
| 17 | X | 523 | ASN |
| 17 | Y | 39 | ASP |
| 17 | Y | 49 | LEU |
| 17 | Y | 54 | ARG |
| 17 | Y | 70 | LEU |
| 17 | Y | 79 | LEU |
| 17 | Y | 94 | ARG |
| 17 | Y | 154 | ASP |
| 17 | Y | 184 | GLN |
| 17 | Y | 193 | LYS |
| 17 | Y | 199 | CYS |
| 17 | Y | 204 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | Y | 255 | ILE |
| 17 | Y | 292 | LEU |
| 17 | Y | 294 | PHE |
| 17 | Y | 299 | MET |
| 17 | Y | 300 | LEU |
| 17 | Y | 301 | ASP |
| 17 | Y | 303 | TYR |
| 17 | Y | 323 | ASP |
| 17 | Y | 366 | ILE |
| 17 | Y | 371 | ASN |
| 17 | Y | 386 | MET |
| 17 | Y | 401 | ARG |
| 17 | Y | 405 | CYS |
| 17 | Y | 423 | ILE |
| 17 | Y | 452 | LEU |
| 17 | Y | 453 | GLU |
| 17 | Y | 460 | LYS |
| 17 | Y | 465 | LEU |
| 17 | Y | 475 | TYR |
| 17 | Y | 487 | SER |
| 17 | Y | 503 | LEU |
| 17 | Y | 506 | GLN |
| 17 | Y | 515 | LEU |
| 17 | Y | 523 | ASN |
| 17 | Y | 551 | LYS |
| 17 | Y | 552 | MET |
| 18 | Z | 57 | THR |
| 18 | Z | 66 | ASN |
| 18 | Z | 72 | LEU |
| 18 | Z | 91 | ILE |
| 18 | Z | 106 | CYS |
| 18 | Z | 138 | THR |
| 18 | Z | 146 | GLU |
| 18 | Z | 157 | THR |
| 18 | Z | 160 | ASP |
| 18 | Z | 166 | LYS |
| 18 | Z | 196 | MET |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 38 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 124 | GLN |
| 1 | A | 125 | GLN |
| 1 | A | 162 | HIS |
| 1 | A | 176 | GLN |
| 1 | A | 179 | ASN |
| 1 | A | 215 | HIS |
| 1 | A | 242 | HIS |
| 1 | A | 250 | ASN |
| 1 | A | 266 | HIS |
| 1 | A | 439 | GLN |
| 1 | A | 593 | ASN |
| 1 | A | 776 | ASN |
| 1 | A | 792 | GLN |
| 1 | A | 965 | GLN |
| 1 | A | 1138 | HIS |
| 1 | A | 1161 | ASN |
| 1 | A | 1165 | HIS |
| 1 | A | 1170 | ASN |
| 1 | A | 1184 | HIS |
| 1 | A | 1192 | ASN |
| 1 | A | 1266 | HIS |
| 1 | A | 1380 | ASN |
| 1 | A | 1511 | ASN |
| 1 | A | 1543 | HIS |
| 1 | A | 1558 | HIS |
| 1 | A | 1559 | HIS |
| 1 | A | 1591 | HIS |
| 1 | A | 1604 | GLN |
| 1 | A | 1813 | GLN |
| 1 | A | 1892 | HIS |
| 2 | B | 9 | ASN |
| 2 | B | 31 | ASN |
| 2 | B | 50 | GLN |
| 2 | B | 71 | GLN |
| 3 | C | 71 | GLN |
| 3 | C | 163 | GLN |
| 3 | C | 202 | HIS |
| 3 | C | 287 | ASN |
| 3 | C | 299 | ASN |
| 3 | C | 305 | ASN |
| 3 | C | 373 | HIS |
| 3 | C | 386 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 390 | HIS |
| 3 | C | 477 | HIS |
| 3 | C | 479 | GLN |
| 5 | E | 75 | GLN |
| 6 | F | 70 | GLN |
| 6 | F | 495 | HIS |
| 6 | F | 634 | HIS |
| 6 | F | 636 | ASN |
| 6 | F | 667 | GLN |
| 6 | H | 480 | ASN |
| 6 | H | 494 | HIS |
| 6 | H | 495 | HIS |
| 6 | H | 545 | HIS |
| 6 | H | 595 | GLN |
| 6 | H | 634 | HIS |
| 6 | H | 648 | GLN |
| 6 | H | 657 | HIS |
| 6 | H | 716 | ASN |
| 6 | H | 754 | HIS |
| 6 | H | 759 | ASN |
| 8 | I | 18 | GLN |
| 8 | I | 257 | HIS |
| 8 | I | 266 | ASN |
| 8 | I | 323 | ASN |
| 8 | I | 345 | GLN |
| 8 | I | 362 | HIS |
| 8 | I | 442 | GLN |
| 8 | I | 496 | GLN |
| 8 | I | 535 | GLN |
| 9 | J | 16 | GLN |
| 9 | J | 17 | GLN |
| 9 | J | 18 | GLN |
| 9 | J | 58 | HIS |
| 9 | J | 173 | HIS |
| 9 | J | 271 | HIS |
| 9 | J | 289 | HIS |
| 9 | J | 316 | ASN |
| 9 | J | 342 | HIS |
| 9 | J | 382 | ASN |
| 9 | J | 393 | GLN |
| 9 | J | 406 | HIS |
| 9 | J | 503 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9 | K | 20 | GLN |
| 9 | K | 45 | GLN |
| 9 | K | 86 | HIS |
| 9 | K | 264 | HIS |
| 9 | K | 271 | HIS |
| 9 | K | 316 | ASN |
| 9 | K | 352 | GLN |
| 9 | K | 449 | ASN |
| 9 | K | 477 | GLN |
| 10 | L | 49 | ASN |
| 10 | L | 146 | GLN |
| 10 | L | 152 | HIS |
| 12 | N | 370 | GLN |
| 12 | N | 388 | HIS |
| 12 | N | 571 | ASN |
| 12 | N | 639 | HIS |
| 12 | N | 663 | GLN |
| 12 | N | 671 | GLN |
| 12 | N | 702 | GLN |
| 12 | N | 726 | ASN |
| 13 | O | 61 | ASN |
| 13 | O | 69 | GLN |
| 13 | O | 91 | ASN |
| 13 | O | 211 | GLN |
| 13 | O | 219 | GLN |
| 13 | O | 242 | ASN |
| 13 | O | 247 | ASN |
| 13 | O | 318 | GLN |
| 13 | O | 319 | GLN |
| 13 | O | 387 | GLN |
| 13 | O | 412 | HIS |
| 13 | O | 441 | GLN |
| 13 | O | 449 | ASN |
| 13 | O | 462 | ASN |
| 13 | O | 472 | HIS |
| 13 | O | 539 | ASN |
| 13 | O | 693 | ASN |
| 13 | O | 717 | GLN |
| 3 | P | 50 | HIS |
| 3 | P | 71 | GLN |
| 3 | P | 148 | ASN |
| 3 | P | 287 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | P | 305 | ASN |
| 3 | P | 321 | HIS |
| 3 | P | 361 | ASN |
| 3 | P | 488 | GLN |
| 3 | P | 495 | GLN |
| 15 | R | 99 | ASN |
| 15 | R | 121 | ASN |
| 16 | S | 87 | GLN |
| 16 | S | 88 | ASN |
| 16 | S | 133 | ASN |
| 16 | S | 145 | GLN |
| 16 | S | 192 | GLN |
| 16 | S | 195 | GLN |
| 16 | S | 278 | ASN |
| 16 | S | 306 | ASN |
| 17 | X | 50 | HIS |
| 17 | X | 78 | GLN |
| 17 | X | 89 | HIS |
| 17 | X | 95 | ASN |
| 17 | X | 106 | GLN |
| 17 | X | 151 | GLN |
| 17 | X | 337 | GLN |
| 17 | X | 338 | HIS |
| 17 | X | 371 | ASN |
| 17 | X | 471 | GLN |
| 17 | X | 506 | GLN |
| 17 | Y | 296 | GLN |
| 17 | Y | 337 | GLN |
| 17 | Y | 371 | ASN |
| 17 | Y | 506 | GLN |
| 17 | Y | 541 | ASN |
| 18 | Z | 66 | ASN |
| 18 | Z | 125 | GLN |
| 18 | Z | 134 | GLN |
| 18 | Z | 173 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 12 | N | 2 |
| 8 | I | 1 |
| 16 | S | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | S | 310:ALA | C | 529:SER | N | 39.42 |
| 1 | N | 92:TRP | C | 93:ASN | N | 3.29 |
| 1 | N | 563:ASP | C | 564:MET | N | 2.78 |
| 1 | I | 302:ASP | C | 303:GLU | N | 2.26 |