



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 12:34 pm BST

PDB ID : 1XCK
Title : Crystal structure of apo GroEL
Authors : Bartolucci, C.; Lamba, D.; Grazulis, S.; Manakova, E.; Heumann, H.
Deposited on : 2004-09-02
Resolution : 2.92 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

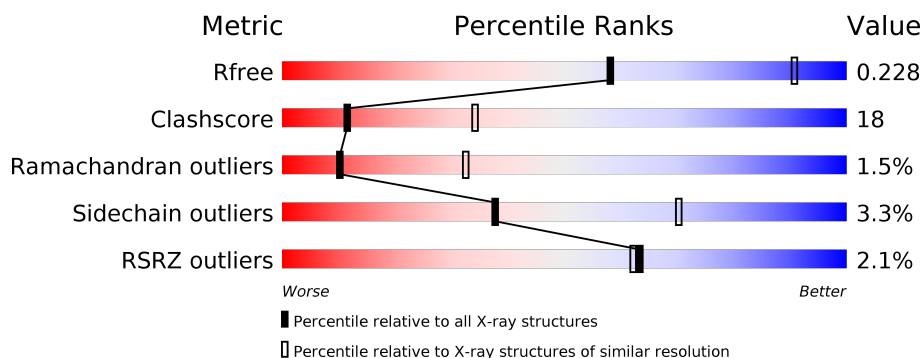
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 Å.

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










| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 2307 (2.94-2.90) |
| Clashscore | 141614 | 2531 (2.94-2.90) |
| Ramachandran outliers | 138981 | 2462 (2.94-2.90) |
| Sidechain outliers | 138945 | 2464 (2.94-2.90) |
| RSRZ outliers | 127900 | 2248 (2.94-2.90) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 547 | <div> <div>%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>• •</div> </div> </div> |
| 1 | B | 547 | <div> <div>3%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>• •</div> </div> </div> |
| 1 | C | 547 | <div> <div>2%</div> <div> <div></div> <div>63%</div> <div>30%</div> <div>• •</div> </div> </div> |
| 1 | D | 547 | <div> <div>%</div> <div> <div></div> <div>65%</div> <div>29%</div> <div>• •</div> </div> </div> |
| 1 | E | 547 | <div> <div>%</div> <div> <div></div> <div>65%</div> <div>28%</div> <div>• •</div> </div> </div> |
| 1 | F | 547 | <div> <div>%</div> <div> <div></div> <div>66%</div> <div>27%</div> <div>• •</div> </div> </div> |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | G | 547 |  |
| 1 | H | 547 |  |
| 1 | I | 547 |  |
| 1 | J | 547 |  |
| 1 | K | 547 |  |
| 1 | L | 547 |  |
| 1 | M | 547 |  |
| 1 | N | 547 |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2 | SO4 | A | 1115 | - | - | - | X |
| 2 | SO4 | B | 1136 | - | - | X | - |
| 2 | SO4 | L | 1117 | - | - | - | X |
| 4 | MPD | N | 1526 | - | - | - | X |

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 55301 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60 kDa chaperonin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |
| 1 | B | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |
| 1 | C | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |
| 1 | D | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |
| 1 | E | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |
| 1 | F | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |
| 1 | G | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |
| 1 | H | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |
| 1 | I | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |
| 1 | J | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |
| 1 | K | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |
| 1 | L | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |
| 1 | M | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |
| 1 | N | 524 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3855 | 2397 | 665 | 773 | 20 | | | |

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | G | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | G | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | G | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | H | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | H | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | H | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | I | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | I | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | J | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | J | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | J | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | J | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | K | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | K | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | L | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | L | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | M | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | M | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | M | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | N | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | N | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

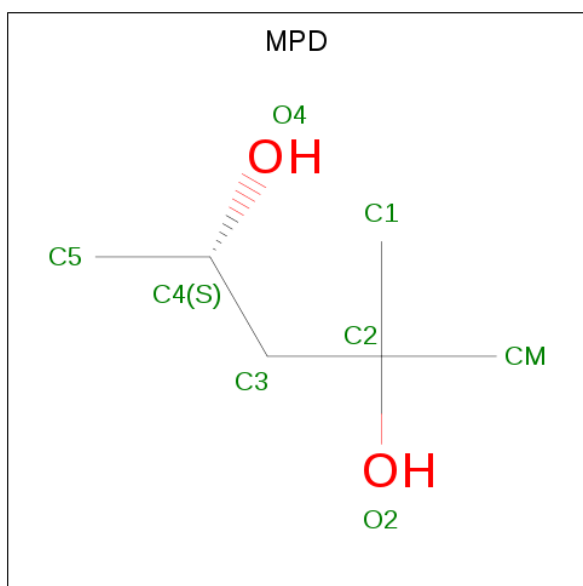
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3 | G | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | J | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | D | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | K | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | E | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | H | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | B | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | I | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | C | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | A | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | N | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3 | L | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | F | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | M | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4 | A | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | A | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | B | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | B | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | B | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | B | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | C | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | D | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |

Continued on next page...

Continued from previous page...

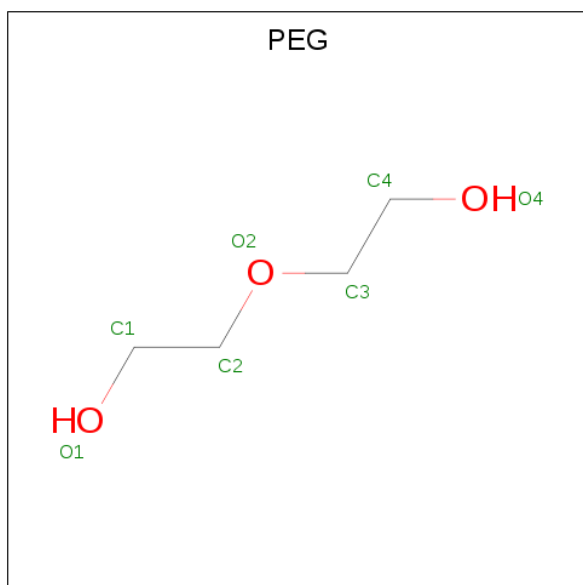
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4 | E | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | E | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | E | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | E | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | E | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | F | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | F | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | F | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | G | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | G | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | H | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | H | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | I | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | I | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | I | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | J | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | K | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | K | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | L | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | M | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | N | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4 | N | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |
| 4 | N | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 6 | 2 | | |

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5 | E | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6 | A | 60 | Total | O | 0 | 0 |
| | | | 60 | 60 | | |
| 6 | B | 76 | Total | O | 0 | 0 |
| | | | 76 | 76 | | |
| 6 | C | 55 | Total | O | 0 | 0 |
| | | | 55 | 55 | | |
| 6 | D | 79 | Total | O | 0 | 0 |
| | | | 79 | 79 | | |
| 6 | E | 64 | Total | O | 0 | 0 |
| | | | 64 | 64 | | |
| 6 | F | 65 | Total | O | 0 | 0 |
| | | | 65 | 65 | | |

Continued on next page...

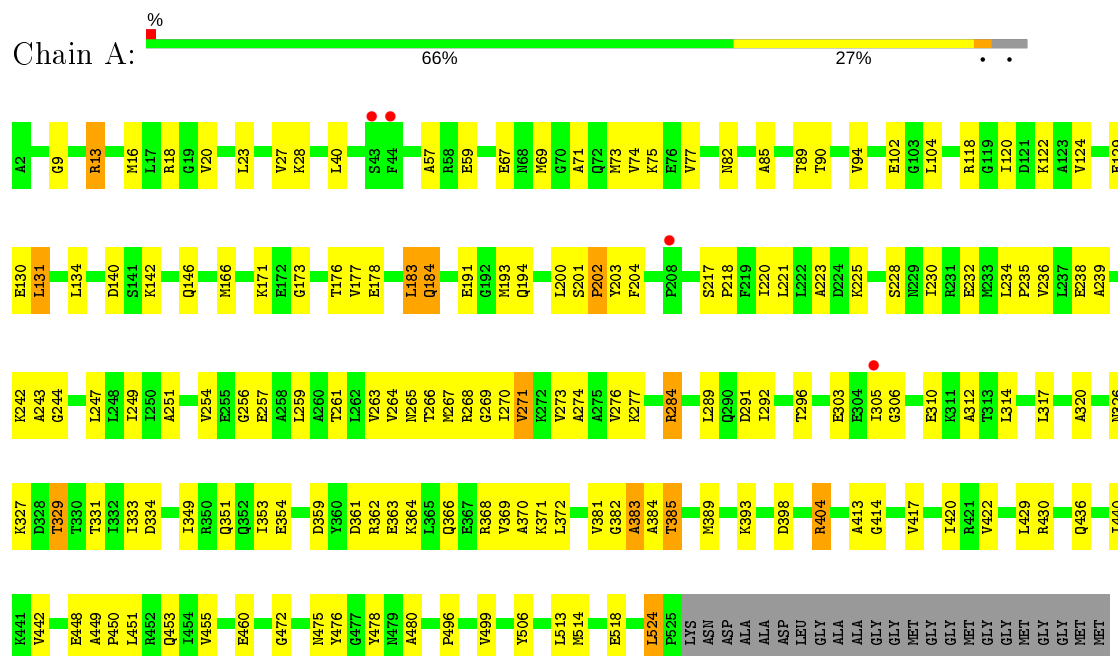
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 6 | G | 84 | Total 84 | O 84 | 0 | 0 |
| 6 | H | 61 | Total 61 | O 61 | 0 | 0 |
| 6 | I | 63 | Total 63 | O 63 | 0 | 0 |
| 6 | J | 45 | Total 45 | O 45 | 0 | 0 |
| 6 | K | 52 | Total 52 | O 52 | 0 | 0 |
| 6 | L | 32 | Total 32 | O 32 | 0 | 0 |
| 6 | M | 49 | Total 49 | O 49 | 0 | 0 |
| 6 | N | 62 | Total 62 | O 62 | 0 | 0 |

3 Residue-property plots

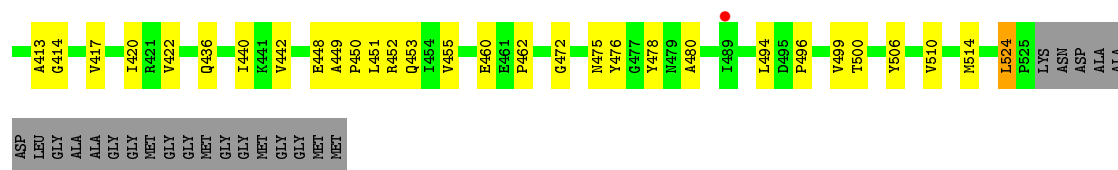
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 60 kDa chaperonin

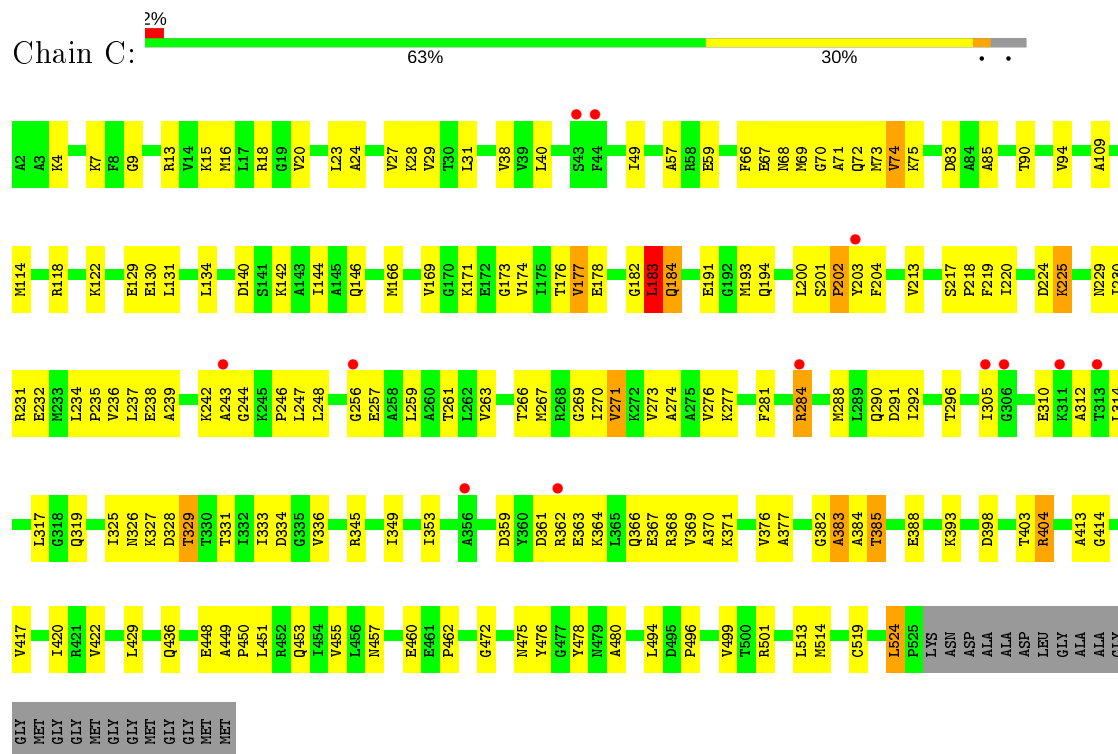


- Molecule 1: 60 kDa chaperonin

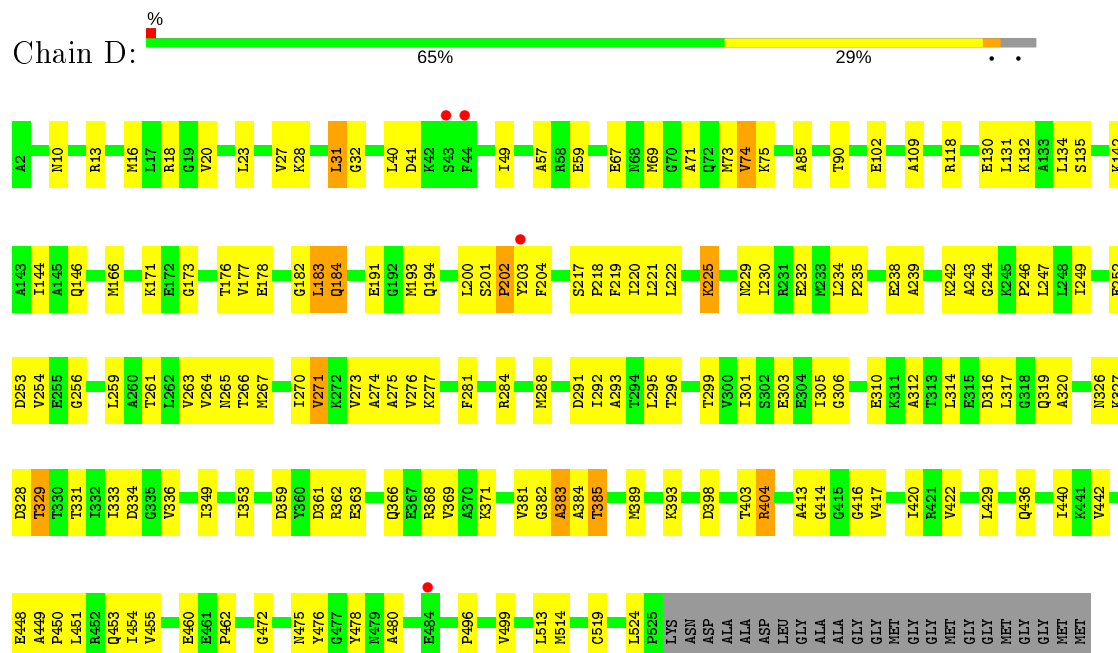




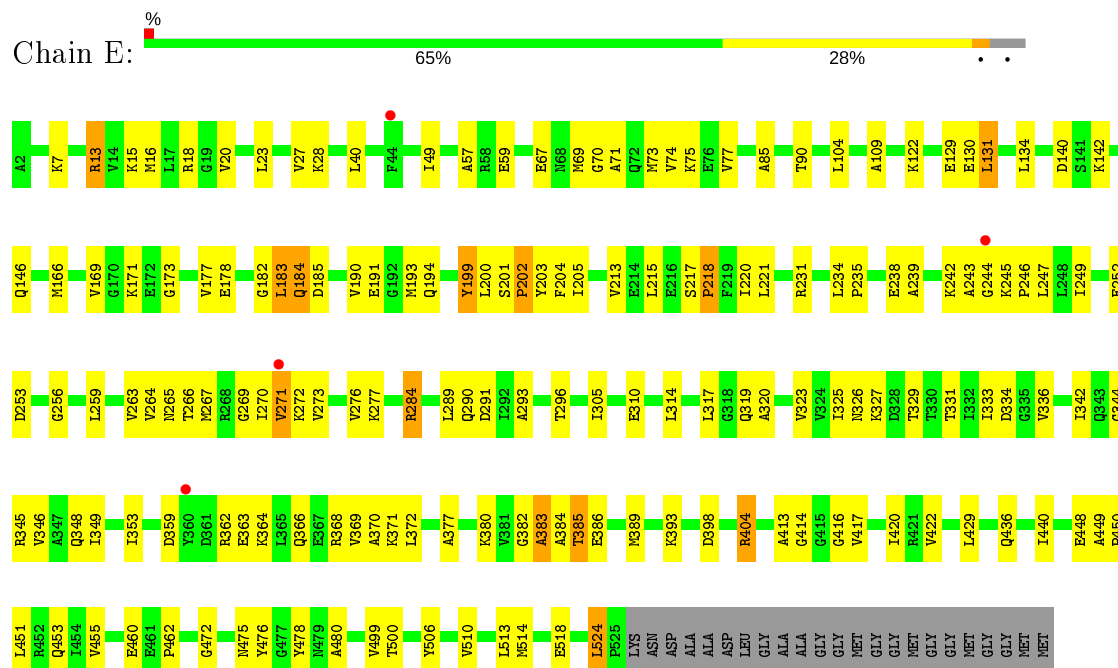
- Molecule 1: 60 kDa chaperonin



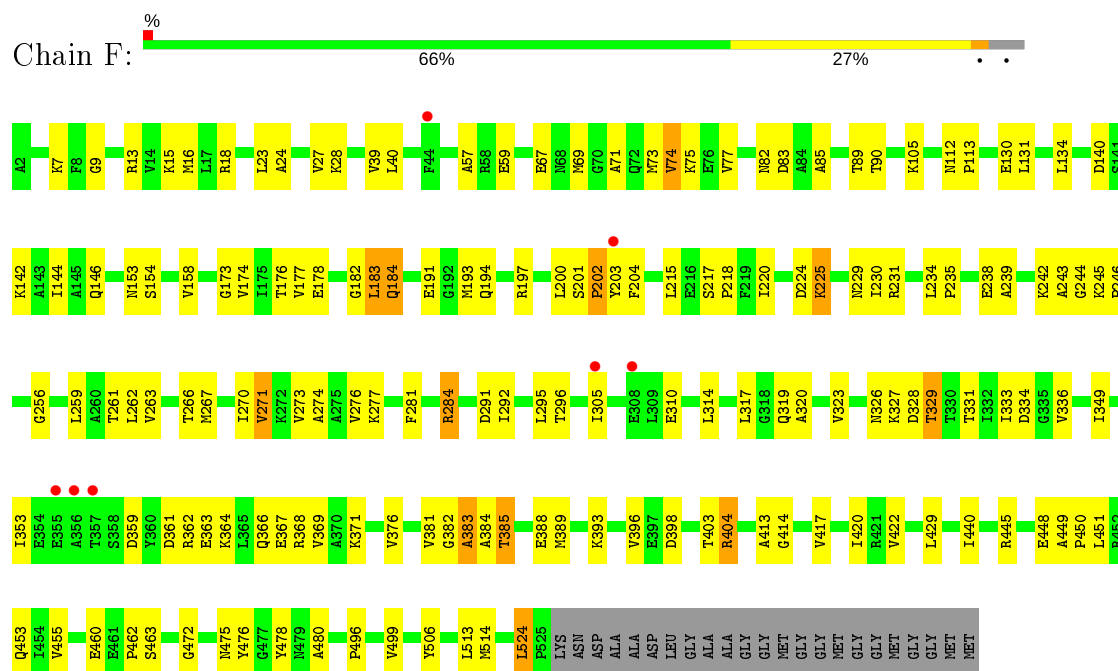
- Molecule 1: 60 kDa chaperonin



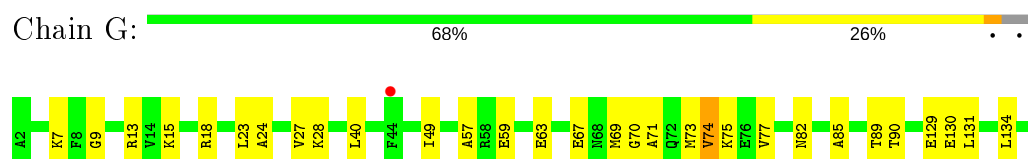
- Molecule 1: 60 kDa chaperonin

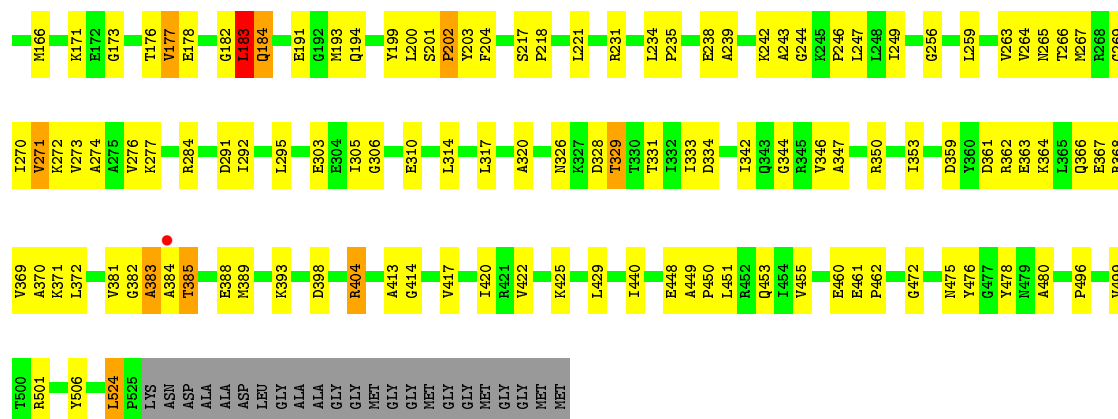


- Molecule 1: 60 kDa chaperonin

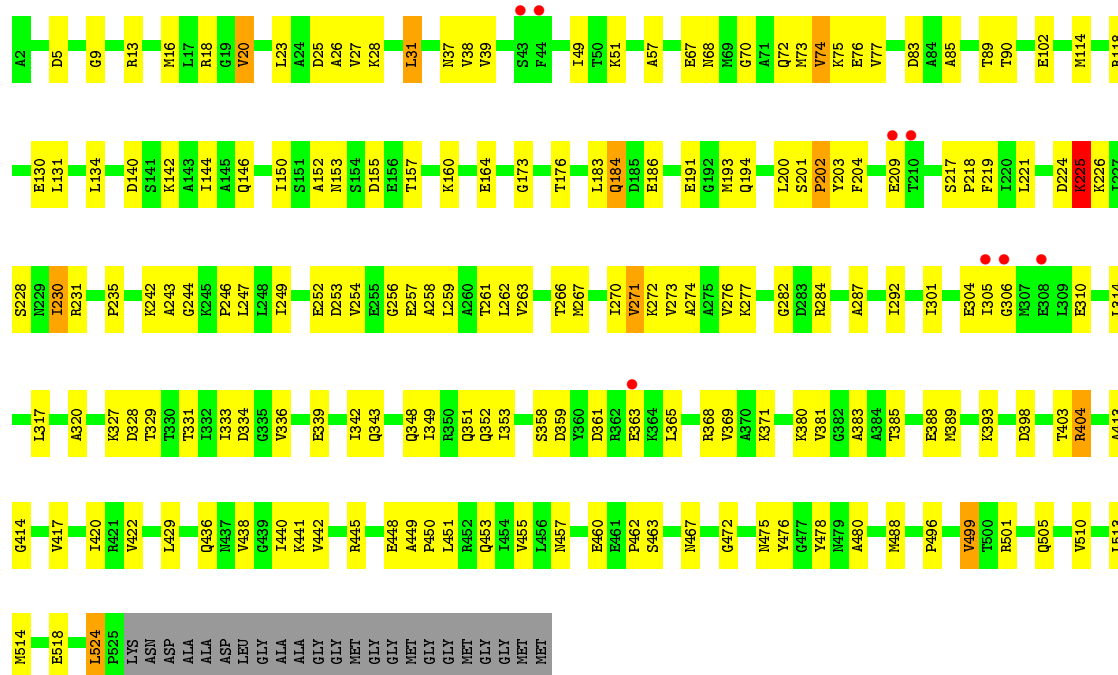


- Molecule 1: 60 kDa chaperonin

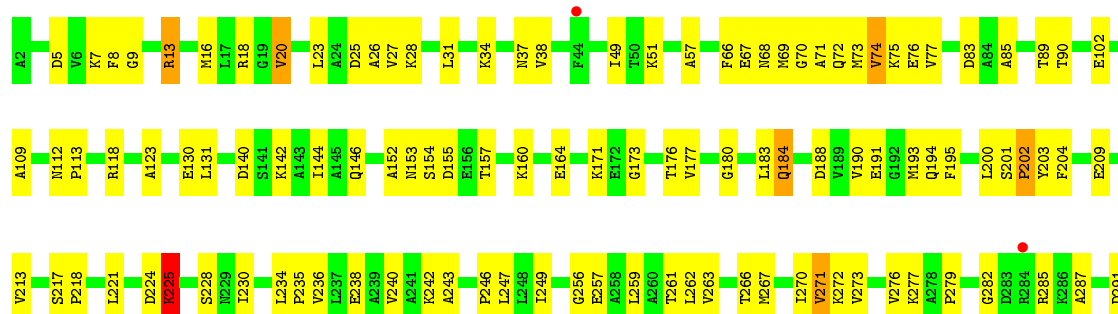


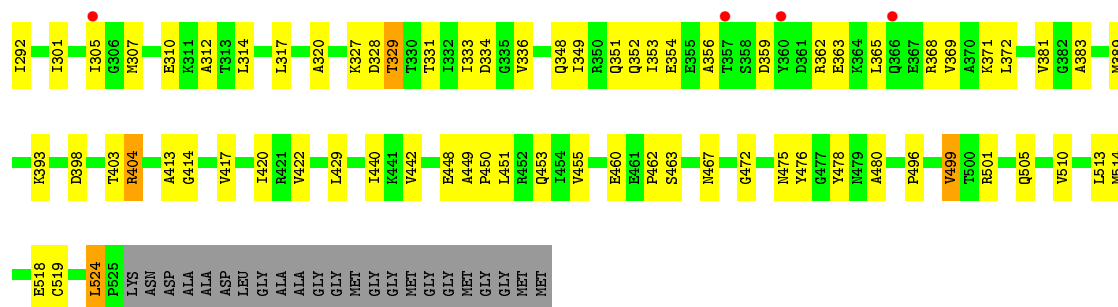


• Molecule 1: 60 kDa chaperonin

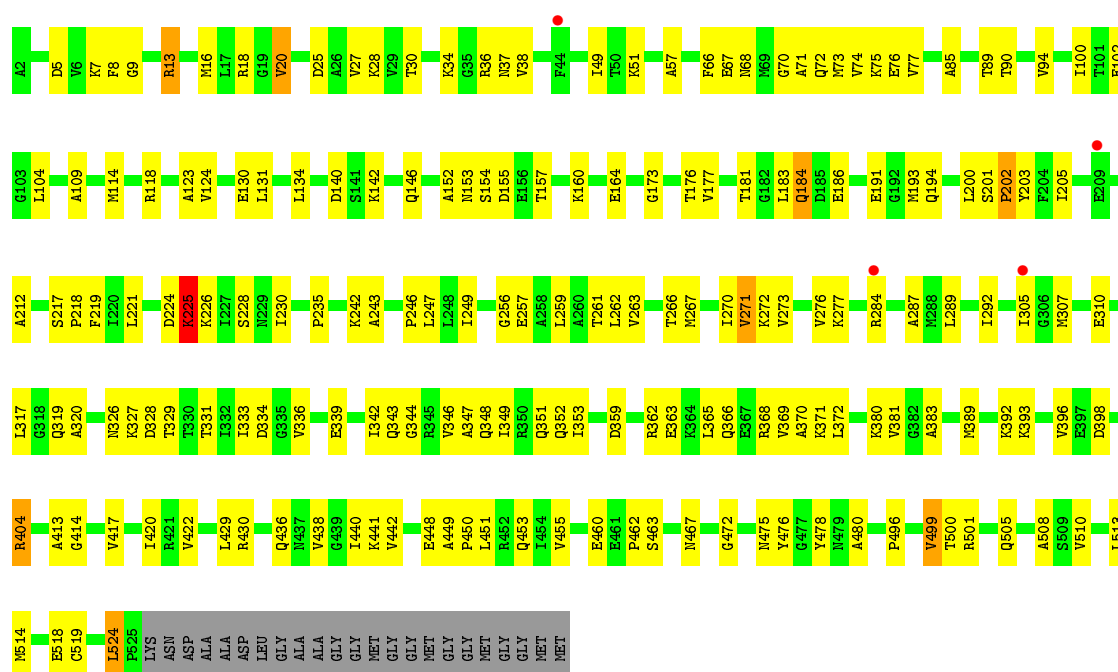


• Molecule 1: 60 kDa chaperonin

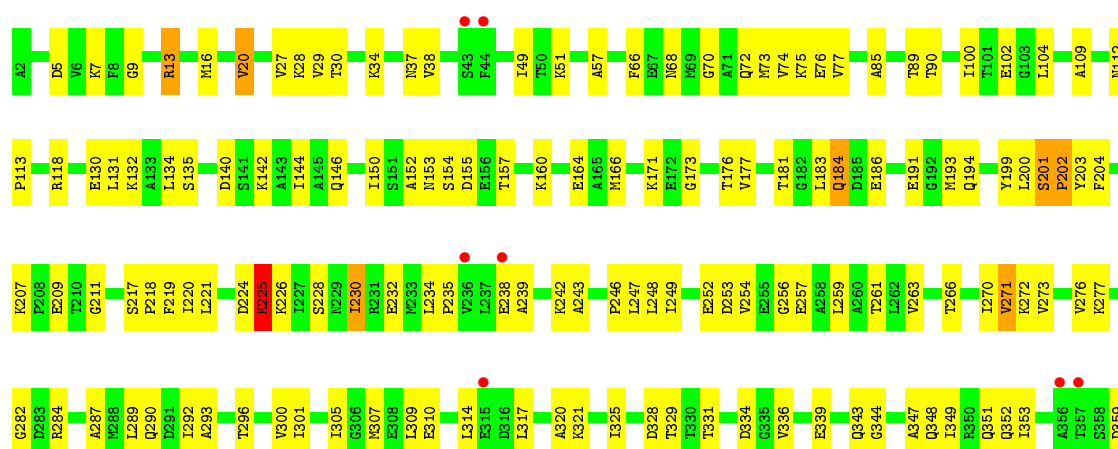


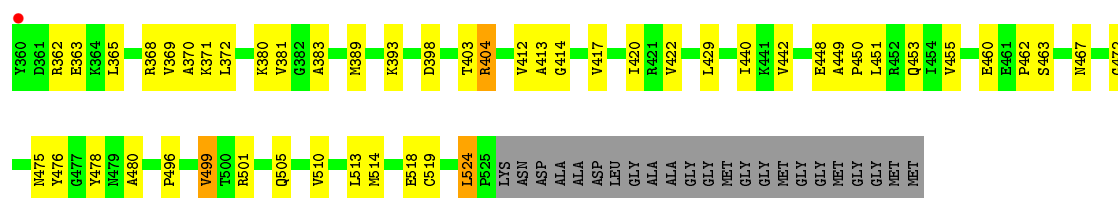


• Molecule 1: 60 kDa chaperonin

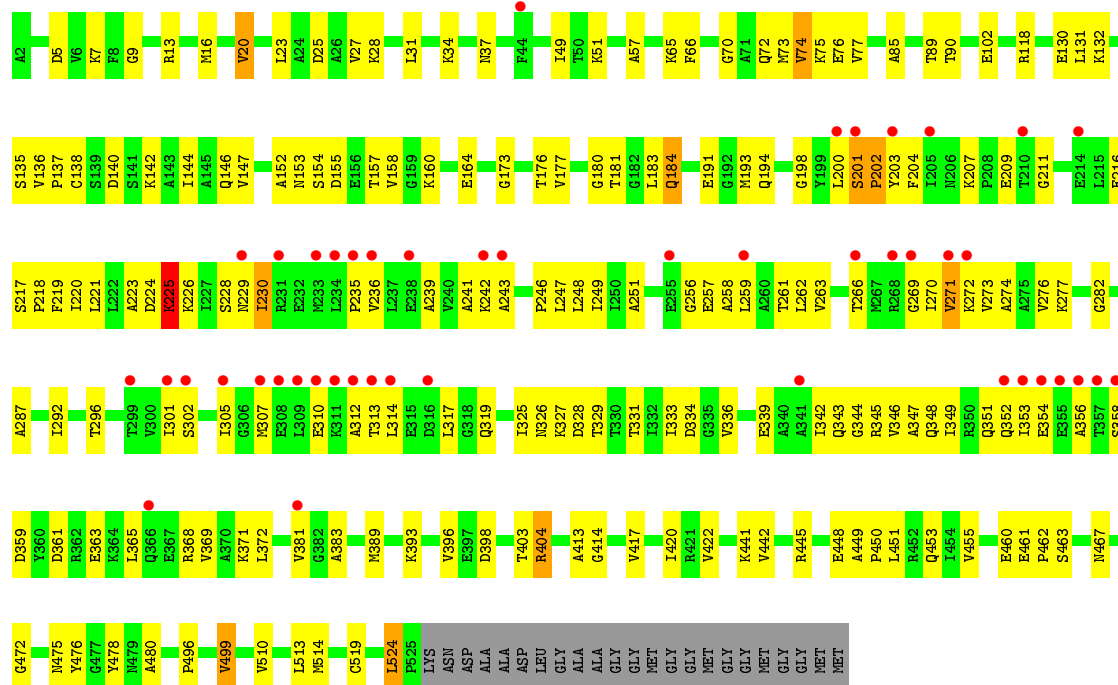


• Molecule 1: 60 kDa chaperonin

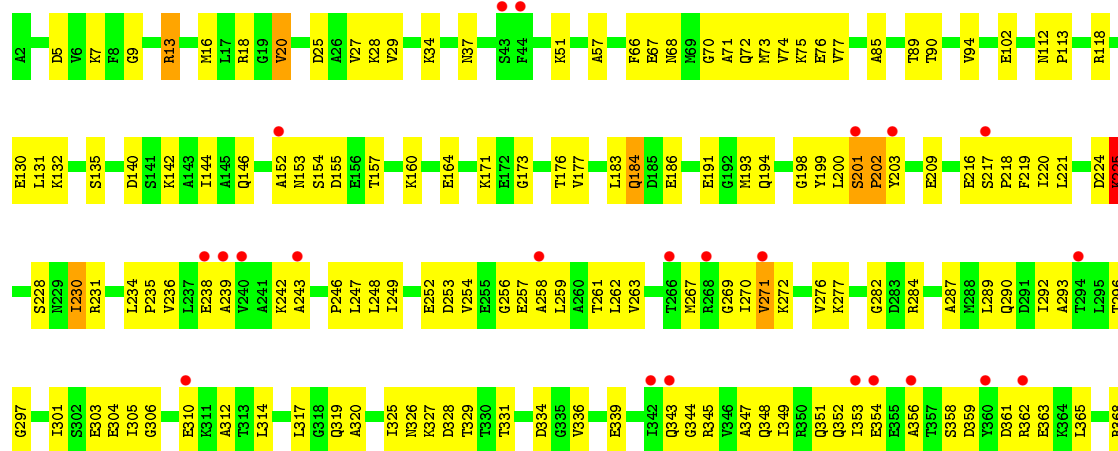


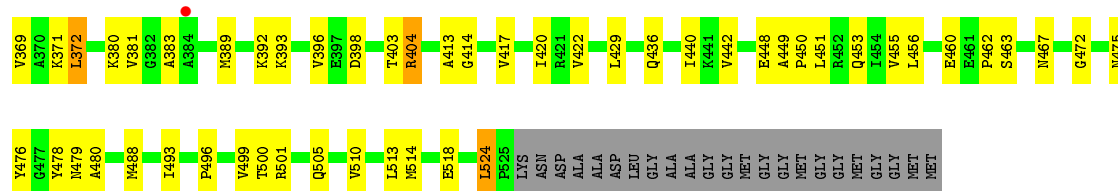


- Molecule 1: 60 kDa chaperonin

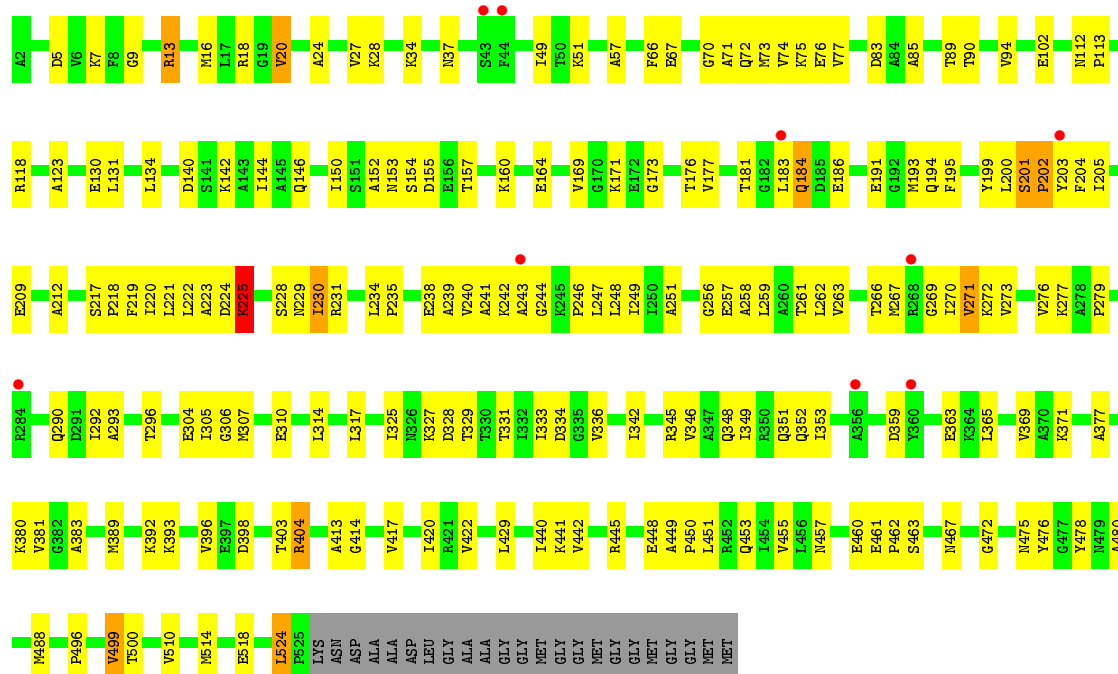


- Molecule 1: 60 kDa chaperonin





• Molecule 1: 60 kDa chaperonin



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 262.80 Å 283.60 Å 135.72 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 33.71 – 2.92 33.65 – 2.92 | Depositor EDS |
| % Data completeness (in resolution range) | 83.8 (33.71-2.92) 83.9 (33.65-2.92) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.04 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 5.43 (at 2.90 Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, R_{free} | 0.203 , 0.235 0.197 , 0.228 | Depositor DCC |
| R_{free} test set | 18290 reflections (9.93%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 53.1 | Xtriage |
| Anisotropy | 0.625 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.31 , 42.3 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 55301 | wwPDB-VP |
| Average B, all atoms (Å ²) | 48.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, PEG, K, SO4

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-----------------|
| | | RMSZ | # $ Z > 5$ | RMSZ | # $ Z > 5$ |
| 1 | A | 0.40 | 0/3883 | 0.69 | 3/5243 (0.1%) |
| 1 | B | 0.40 | 0/3883 | 0.64 | 2/5243 (0.0%) |
| 1 | C | 0.39 | 0/3883 | 0.64 | 1/5243 (0.0%) |
| 1 | D | 0.40 | 0/3883 | 0.64 | 3/5243 (0.1%) |
| 1 | E | 0.39 | 0/3883 | 0.69 | 3/5243 (0.1%) |
| 1 | F | 0.39 | 0/3883 | 0.64 | 2/5243 (0.0%) |
| 1 | G | 0.40 | 0/3883 | 0.64 | 2/5243 (0.0%) |
| 1 | H | 0.37 | 0/3883 | 0.66 | 3/5243 (0.1%) |
| 1 | I | 0.37 | 0/3883 | 0.61 | 2/5243 (0.0%) |
| 1 | J | 0.37 | 0/3883 | 0.61 | 2/5243 (0.0%) |
| 1 | K | 0.37 | 0/3883 | 0.61 | 2/5243 (0.0%) |
| 1 | L | 0.38 | 0/3883 | 0.66 | 3/5243 (0.1%) |
| 1 | M | 0.37 | 0/3883 | 0.61 | 2/5243 (0.0%) |
| 1 | N | 0.36 | 0/3883 | 0.60 | 2/5243 (0.0%) |
| All | All | 0.38 | 0/54362 | 0.64 | 32/73402 (0.0%) |

There are no bond length outliers.

All (32) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | E | 13 | ARG | NE-CZ-NH2 | -14.67 | 112.97 | 120.30 |
| 1 | H | 13 | ARG | NE-CZ-NH2 | -14.55 | 113.03 | 120.30 |
| 1 | A | 13 | ARG | NE-CZ-NH2 | -13.99 | 113.31 | 120.30 |
| 1 | E | 13 | ARG | NE-CZ-NH1 | 13.46 | 127.03 | 120.30 |
| 1 | L | 13 | ARG | NE-CZ-NH2 | -13.45 | 113.58 | 120.30 |
| 1 | H | 13 | ARG | NE-CZ-NH1 | 13.21 | 126.91 | 120.30 |
| 1 | L | 13 | ARG | NE-CZ-NH1 | 13.16 | 126.88 | 120.30 |
| 1 | A | 13 | ARG | NE-CZ-NH1 | 12.65 | 126.63 | 120.30 |
| 1 | H | 13 | ARG | CD-NE-CZ | 6.64 | 132.89 | 123.60 |
| 1 | L | 13 | ARG | CD-NE-CZ | 6.52 | 132.72 | 123.60 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | J | 13 | ARG | NE-CZ-NH1 | -6.38 | 117.11 | 120.30 |
| 1 | N | 13 | ARG | NE-CZ-NH1 | -6.35 | 117.12 | 120.30 |
| 1 | C | 13 | ARG | NE-CZ-NH1 | -6.34 | 117.13 | 120.30 |
| 1 | E | 13 | ARG | CD-NE-CZ | 6.03 | 132.05 | 123.60 |
| 1 | B | 13 | ARG | NE-CZ-NH1 | -5.97 | 117.31 | 120.30 |
| 1 | K | 13 | ARG | NE-CZ-NH1 | -5.84 | 117.38 | 120.30 |
| 1 | F | 13 | ARG | NE-CZ-NH1 | -5.82 | 117.39 | 120.30 |
| 1 | A | 13 | ARG | CD-NE-CZ | 5.64 | 131.50 | 123.60 |
| 1 | I | 13 | ARG | NE-CZ-NH1 | -5.54 | 117.53 | 120.30 |
| 1 | M | 13 | ARG | NE-CZ-NH2 | 5.53 | 123.07 | 120.30 |
| 1 | G | 295 | LEU | CA-CB-CG | 5.51 | 127.98 | 115.30 |
| 1 | M | 13 | ARG | NE-CZ-NH1 | -5.50 | 117.55 | 120.30 |
| 1 | N | 13 | ARG | NE-CZ-NH2 | 5.37 | 122.98 | 120.30 |
| 1 | D | 295 | LEU | CA-CB-CG | 5.35 | 127.61 | 115.30 |
| 1 | J | 13 | ARG | NE-CZ-NH2 | 5.33 | 122.96 | 120.30 |
| 1 | D | 31 | LEU | N-CA-C | 5.31 | 125.34 | 111.00 |
| 1 | K | 13 | ARG | NE-CZ-NH2 | 5.27 | 122.93 | 120.30 |
| 1 | D | 13 | ARG | NE-CZ-NH1 | -5.18 | 117.71 | 120.30 |
| 1 | G | 13 | ARG | NE-CZ-NH1 | -5.09 | 117.75 | 120.30 |
| 1 | B | 13 | ARG | NE-CZ-NH2 | 5.04 | 122.82 | 120.30 |
| 1 | I | 13 | ARG | NE-CZ-NH2 | 5.02 | 122.81 | 120.30 |
| 1 | F | 13 | ARG | NE-CZ-NH2 | 5.01 | 122.81 | 120.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3855 | 0 | 3976 | 121 | 0 |
| 1 | B | 3855 | 0 | 3976 | 146 | 0 |
| 1 | C | 3855 | 0 | 3976 | 155 | 0 |
| 1 | D | 3855 | 0 | 3976 | 126 | 0 |
| 1 | E | 3855 | 0 | 3976 | 139 | 0 |
| 1 | F | 3855 | 0 | 3976 | 127 | 0 |
| 1 | G | 3855 | 0 | 3976 | 117 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | H | 3855 | 0 | 3976 | 150 | 0 |
| 1 | I | 3855 | 0 | 3976 | 152 | 0 |
| 1 | J | 3855 | 0 | 3976 | 146 | 0 |
| 1 | K | 3855 | 0 | 3976 | 154 | 0 |
| 1 | L | 3855 | 0 | 3976 | 163 | 0 |
| 1 | M | 3855 | 0 | 3976 | 175 | 0 |
| 1 | N | 3855 | 0 | 3976 | 175 | 0 |
| 2 | A | 20 | 0 | 0 | 0 | 0 |
| 2 | B | 25 | 0 | 0 | 2 | 0 |
| 2 | C | 20 | 0 | 0 | 0 | 0 |
| 2 | D | 25 | 0 | 0 | 0 | 0 |
| 2 | E | 10 | 0 | 0 | 0 | 0 |
| 2 | F | 10 | 0 | 0 | 1 | 0 |
| 2 | G | 15 | 0 | 0 | 0 | 0 |
| 2 | H | 15 | 0 | 0 | 0 | 0 |
| 2 | I | 10 | 0 | 0 | 0 | 0 |
| 2 | J | 20 | 0 | 0 | 0 | 0 |
| 2 | K | 10 | 0 | 0 | 0 | 0 |
| 2 | L | 10 | 0 | 0 | 0 | 0 |
| 2 | M | 15 | 0 | 0 | 0 | 0 |
| 2 | N | 10 | 0 | 0 | 1 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | E | 1 | 0 | 0 | 0 | 0 |
| 3 | F | 1 | 0 | 0 | 0 | 0 |
| 3 | G | 1 | 0 | 0 | 0 | 0 |
| 3 | H | 1 | 0 | 0 | 0 | 0 |
| 3 | I | 1 | 0 | 0 | 0 | 0 |
| 3 | J | 1 | 0 | 0 | 0 | 0 |
| 3 | K | 1 | 0 | 0 | 0 | 0 |
| 3 | L | 1 | 0 | 0 | 0 | 0 |
| 3 | M | 1 | 0 | 0 | 0 | 0 |
| 3 | N | 1 | 0 | 0 | 0 | 0 |
| 4 | A | 16 | 0 | 28 | 0 | 0 |
| 4 | B | 32 | 0 | 56 | 2 | 0 |
| 4 | C | 8 | 0 | 14 | 2 | 0 |
| 4 | D | 8 | 0 | 14 | 0 | 0 |
| 4 | E | 40 | 0 | 70 | 1 | 0 |
| 4 | F | 24 | 0 | 42 | 1 | 0 |
| 4 | G | 16 | 0 | 28 | 1 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | H | 16 | 0 | 28 | 2 | 0 |
| 4 | I | 24 | 0 | 42 | 0 | 0 |
| 4 | J | 8 | 0 | 14 | 0 | 0 |
| 4 | K | 16 | 0 | 28 | 2 | 0 |
| 4 | L | 8 | 0 | 14 | 0 | 0 |
| 4 | M | 8 | 0 | 14 | 3 | 0 |
| 4 | N | 24 | 0 | 42 | 9 | 0 |
| 5 | E | 7 | 0 | 10 | 0 | 0 |
| 6 | A | 60 | 0 | 0 | 1 | 0 |
| 6 | B | 76 | 0 | 0 | 3 | 0 |
| 6 | C | 55 | 0 | 0 | 2 | 0 |
| 6 | D | 79 | 0 | 0 | 5 | 0 |
| 6 | E | 64 | 0 | 0 | 1 | 0 |
| 6 | F | 65 | 0 | 0 | 1 | 0 |
| 6 | G | 84 | 0 | 0 | 2 | 0 |
| 6 | H | 61 | 0 | 0 | 2 | 0 |
| 6 | I | 63 | 0 | 0 | 2 | 0 |
| 6 | J | 45 | 0 | 0 | 5 | 0 |
| 6 | K | 52 | 0 | 0 | 3 | 0 |
| 6 | L | 32 | 0 | 0 | 1 | 0 |
| 6 | M | 49 | 0 | 0 | 3 | 0 |
| 6 | N | 62 | 0 | 0 | 1 | 0 |
| All | All | 55301 | 0 | 56108 | 1943 | 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 18.

All (1943) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:270:ILE:HG23 | 1:C:231:ARG:HH12 | 1.20 | 1.03 |
| 1:B:329:THR:HG22 | 6:B:3165:HOH:O | 1.60 | 1.01 |
| 1:D:242:LYS:HG2 | 1:E:231:ARG:NH2 | 1.78 | 0.97 |
| 1:B:326:ASN:HD22 | 1:B:329:THR:HB | 1.31 | 0.94 |
| 1:K:272:LYS:NZ | 1:L:229:ASN:HD21 | 1.65 | 0.94 |
| 1:E:270:ILE:HG23 | 1:F:231:ARG:HH12 | 1.33 | 0.93 |
| 1:M:235:PRO:HG3 | 1:M:310:GLU:HA | 1.51 | 0.92 |
| 1:C:176:THR:HG21 | 1:C:333:ILE:HD13 | 1.49 | 0.92 |
| 1:H:235:PRO:HG3 | 1:H:310:GLU:HA | 1.53 | 0.89 |
| 1:E:270:ILE:HG23 | 1:F:231:ARG:NH1 | 1.88 | 0.87 |
| 1:K:235:PRO:HG3 | 1:K:310:GLU:HA | 1.56 | 0.87 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:235:PRO:HG3 | 1:J:310:GLU:HA | 1.57 | 0.87 |
| 1:L:235:PRO:HG3 | 1:L:310:GLU:HA | 1.56 | 0.86 |
| 1:B:331:THR:HG22 | 6:B:3165:HOH:O | 1.77 | 0.84 |
| 1:I:183:LEU:O | 1:I:184:GLN:HB2 | 1.77 | 0.83 |
| 1:M:290:GLN:HG3 | 6:M:3113:HOH:O | 1.77 | 0.83 |
| 1:N:235:PRO:HG3 | 1:N:310:GLU:HA | 1.60 | 0.82 |
| 1:K:183:LEU:O | 1:K:184:GLN:HB2 | 1.77 | 0.82 |
| 1:M:85:ALA:HB1 | 1:M:499:VAL:HG12 | 1.61 | 0.82 |
| 1:J:183:LEU:O | 1:J:184:GLN:HB2 | 1.80 | 0.82 |
| 1:G:176:THR:HG21 | 1:G:333:ILE:HD13 | 1.60 | 0.81 |
| 1:M:34:LYS:HE2 | 1:N:118:ARG:HH22 | 1.45 | 0.81 |
| 1:H:176:THR:HG21 | 1:H:333:ILE:HD13 | 1.61 | 0.81 |
| 1:B:239:ALA:HB1 | 1:B:314:LEU:HG | 1.63 | 0.81 |
| 1:J:85:ALA:HB1 | 1:J:499:VAL:HG12 | 1.62 | 0.80 |
| 1:B:270:ILE:HG23 | 1:C:231:ARG:NH1 | 1.97 | 0.80 |
| 1:H:183:LEU:O | 1:H:184:GLN:HB2 | 1.82 | 0.80 |
| 1:C:239:ALA:HB1 | 1:C:314:LEU:HG | 1.63 | 0.79 |
| 1:F:235:PRO:HG3 | 1:F:310:GLU:HA | 1.64 | 0.79 |
| 1:G:235:PRO:HG3 | 1:G:310:GLU:HA | 1.62 | 0.78 |
| 1:M:183:LEU:O | 1:M:184:GLN:HB2 | 1.81 | 0.78 |
| 1:M:272:LYS:NZ | 1:N:229:ASN:ND2 | 2.30 | 0.78 |
| 1:N:183:LEU:O | 1:N:184:GLN:HB2 | 1.82 | 0.78 |
| 1:G:27:VAL:HG12 | 1:G:90:THR:HG23 | 1.66 | 0.78 |
| 1:L:85:ALA:HB1 | 1:L:499:VAL:HG12 | 1.63 | 0.78 |
| 1:H:85:ALA:HB1 | 1:H:499:VAL:HG12 | 1.64 | 0.78 |
| 1:L:183:LEU:O | 1:L:184:GLN:HB2 | 1.82 | 0.78 |
| 1:I:235:PRO:HG3 | 1:I:310:GLU:HA | 1.64 | 0.78 |
| 1:A:184:GLN:H | 1:A:382:GLY:HA3 | 1.49 | 0.78 |
| 1:I:85:ALA:HB1 | 1:I:499:VAL:HG12 | 1.63 | 0.78 |
| 1:N:85:ALA:HB1 | 1:N:499:VAL:HG12 | 1.66 | 0.77 |
| 1:C:235:PRO:HG3 | 1:C:310:GLU:HA | 1.65 | 0.77 |
| 1:L:272:LYS:NZ | 1:M:228:SER:HB3 | 2.00 | 0.77 |
| 1:K:200:LEU:HD21 | 1:K:277:LYS:HG3 | 1.65 | 0.77 |
| 1:J:218:PRO:HB3 | 1:J:246:PRO:HG2 | 1.67 | 0.77 |
| 1:E:200:LEU:HD21 | 1:E:277:LYS:HG3 | 1.67 | 0.76 |
| 1:L:228:SER:O | 1:L:257:GLU:HB3 | 1.84 | 0.76 |
| 1:E:27:VAL:HG12 | 1:E:90:THR:HG23 | 1.66 | 0.76 |
| 1:K:85:ALA:HB1 | 1:K:499:VAL:HG12 | 1.66 | 0.76 |
| 1:J:413:ALA:HB2 | 1:J:475:ASN:HD22 | 1.51 | 0.76 |
| 1:D:184:GLN:H | 1:D:382:GLY:HA3 | 1.51 | 0.75 |
| 1:E:184:GLN:H | 1:E:382:GLY:HA3 | 1.50 | 0.75 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:200:LEU:HD21 | 1:J:277:LYS:HG3 | 1.68 | 0.75 |
| 1:F:404:ARG:HG2 | 1:F:404:ARG:HH11 | 1.50 | 0.75 |
| 1:N:445:ARG:HH22 | 4:N:1515:MPD:H12 | 1.51 | 0.75 |
| 1:M:218:PRO:HB3 | 1:M:246:PRO:HG2 | 1.68 | 0.74 |
| 1:N:200:LEU:HD21 | 1:N:277:LYS:HG3 | 1.67 | 0.74 |
| 1:B:184:GLN:H | 1:B:382:GLY:HA3 | 1.52 | 0.74 |
| 1:C:404:ARG:HH11 | 1:C:404:ARG:HG2 | 1.52 | 0.74 |
| 1:J:183:LEU:HD13 | 1:J:184:GLN:HG3 | 1.69 | 0.74 |
| 1:B:272:LYS:HZ1 | 1:C:229:ASN:HD22 | 1.35 | 0.74 |
| 1:H:183:LEU:HD13 | 1:H:184:GLN:HG3 | 1.68 | 0.74 |
| 1:L:176:THR:HG21 | 1:L:333:ILE:HD13 | 1.69 | 0.74 |
| 1:F:176:THR:HG21 | 1:F:333:ILE:HD13 | 1.70 | 0.74 |
| 1:G:200:LEU:HD21 | 1:G:277:LYS:HG3 | 1.70 | 0.74 |
| 1:G:234:LEU:O | 1:G:238:GLU:HG3 | 1.88 | 0.74 |
| 1:I:183:LEU:HD13 | 1:I:184:GLN:HG3 | 1.70 | 0.74 |
| 1:G:359:ASP:O | 1:G:363:GLU:HG3 | 1.88 | 0.74 |
| 1:M:413:ALA:H | 1:M:475:ASN:ND2 | 1.86 | 0.74 |
| 1:H:404:ARG:HG2 | 1:H:404:ARG:HH11 | 1.51 | 0.73 |
| 1:C:326:ASN:HD22 | 1:C:329:THR:HB | 1.53 | 0.73 |
| 1:E:314:LEU:HD23 | 1:E:317:LEU:HD22 | 1.70 | 0.73 |
| 1:F:57:ALA:O | 1:F:75:LYS:HE3 | 1.87 | 0.73 |
| 1:D:359:ASP:O | 1:D:363:GLU:HG3 | 1.89 | 0.73 |
| 1:F:184:GLN:H | 1:F:382:GLY:HA3 | 1.53 | 0.73 |
| 1:A:230:ILE:HD13 | 1:A:261:THR:HG21 | 1.69 | 0.73 |
| 1:F:27:VAL:HG12 | 1:F:90:THR:HG23 | 1.69 | 0.73 |
| 1:G:183:LEU:O | 1:G:183:LEU:HD13 | 1.88 | 0.73 |
| 1:C:118:ARG:NH2 | 6:C:3133:HOH:O | 2.21 | 0.73 |
| 1:K:272:LYS:HZ2 | 1:L:229:ASN:HD21 | 1.34 | 0.73 |
| 1:L:413:ALA:HB2 | 1:L:475:ASN:HD22 | 1.54 | 0.73 |
| 1:F:326:ASN:HD22 | 1:F:329:THR:HB | 1.54 | 0.73 |
| 1:L:218:PRO:HB3 | 1:L:246:PRO:HG2 | 1.71 | 0.73 |
| 1:K:413:ALA:HB2 | 1:K:475:ASN:HD22 | 1.54 | 0.72 |
| 1:E:131:LEU:HD13 | 1:E:422:VAL:HG21 | 1.70 | 0.72 |
| 1:J:404:ARG:HH11 | 1:J:404:ARG:HG2 | 1.54 | 0.72 |
| 1:N:445:ARG:HH22 | 4:N:1515:MPD:C1 | 2.02 | 0.72 |
| 1:B:218:PRO:HB3 | 1:B:246:PRO:HG2 | 1.71 | 0.72 |
| 1:N:183:LEU:HD13 | 1:N:184:GLN:HG3 | 1.70 | 0.72 |
| 1:K:272:LYS:NZ | 1:L:229:ASN:ND2 | 2.37 | 0.72 |
| 1:C:27:VAL:HG12 | 1:C:90:THR:HG23 | 1.71 | 0.72 |
| 1:J:284:ARG:NH2 | 6:J:3072:HOH:O | 2.23 | 0.72 |
| 1:B:272:LYS:NZ | 1:C:229:ASN:HD22 | 1.88 | 0.71 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:219:PHE:HB3 | 1:L:317:LEU:HD23 | 1.71 | 0.71 |
| 1:N:176:THR:HG21 | 1:N:333:ILE:HD13 | 1.72 | 0.71 |
| 1:E:235:PRO:HG3 | 1:E:310:GLU:HA | 1.72 | 0.71 |
| 1:H:413:ALA:HB2 | 1:H:475:ASN:HD22 | 1.55 | 0.71 |
| 1:A:449:ALA:HB3 | 1:A:450:PRO:HD3 | 1.71 | 0.71 |
| 1:L:404:ARG:HG2 | 1:L:404:ARG:HH11 | 1.54 | 0.71 |
| 1:A:183:LEU:O | 1:A:183:LEU:HD13 | 1.89 | 0.71 |
| 1:H:247:LEU:HD21 | 1:H:249:ILE:HD11 | 1.71 | 0.71 |
| 1:J:224:ASP:O | 1:J:225:LYS:HB3 | 1.90 | 0.71 |
| 1:C:184:GLN:H | 1:C:382:GLY:HA3 | 1.56 | 0.71 |
| 1:E:239:ALA:HB1 | 1:E:314:LEU:HG | 1.72 | 0.71 |
| 1:F:105:LYS:HA | 4:F:1522:MPD:HM2 | 1.73 | 0.71 |
| 1:A:200:LEU:HD21 | 1:A:277:LYS:HG3 | 1.71 | 0.71 |
| 1:I:359:ASP:O | 1:I:363:GLU:HG2 | 1.89 | 0.71 |
| 1:I:131:LEU:HD13 | 1:I:422:VAL:HG21 | 1.72 | 0.71 |
| 1:M:228:SER:O | 1:M:257:GLU:HB3 | 1.91 | 0.71 |
| 1:G:184:GLN:H | 1:G:382:GLY:HA3 | 1.56 | 0.71 |
| 1:G:57:ALA:O | 1:G:75:LYS:HE3 | 1.91 | 0.71 |
| 1:J:160:LYS:O | 1:J:164:GLU:HG3 | 1.91 | 0.71 |
| 1:K:228:SER:O | 1:K:257:GLU:HB3 | 1.91 | 0.71 |
| 1:N:359:ASP:O | 1:N:363:GLU:HG2 | 1.91 | 0.70 |
| 1:A:235:PRO:HG3 | 1:A:310:GLU:HA | 1.71 | 0.70 |
| 1:H:200:LEU:HD21 | 1:H:277:LYS:HG3 | 1.71 | 0.70 |
| 1:B:27:VAL:HG12 | 1:B:90:THR:HG23 | 1.72 | 0.70 |
| 1:J:348:GLN:O | 1:J:352:GLN:HG2 | 1.92 | 0.70 |
| 1:K:420:ILE:HG13 | 1:K:448:GLU:HG2 | 1.72 | 0.70 |
| 1:G:420:ILE:HG13 | 1:G:448:GLU:HG2 | 1.74 | 0.70 |
| 1:H:449:ALA:HB3 | 1:H:450:PRO:HD3 | 1.74 | 0.70 |
| 1:G:291:ASP:OD2 | 1:G:368:ARG:HD2 | 1.91 | 0.70 |
| 1:F:242:LYS:HG2 | 1:G:231:ARG:NH2 | 2.07 | 0.70 |
| 1:G:239:ALA:HB1 | 1:G:314:LEU:HG | 1.73 | 0.70 |
| 1:I:404:ARG:HH11 | 1:I:404:ARG:HG2 | 1.55 | 0.70 |
| 1:D:27:VAL:HG12 | 1:D:90:THR:HG23 | 1.73 | 0.70 |
| 1:N:420:ILE:HG13 | 1:N:448:GLU:HG2 | 1.74 | 0.70 |
| 1:D:176:THR:HG21 | 1:D:333:ILE:HD13 | 1.73 | 0.69 |
| 1:B:362:ARG:HG2 | 1:B:366:GLN:NE2 | 2.07 | 0.69 |
| 1:B:291:ASP:OD2 | 1:B:368:ARG:HD2 | 1.92 | 0.69 |
| 1:K:219:PHE:HB3 | 1:K:317:LEU:HD23 | 1.72 | 0.69 |
| 1:M:131:LEU:HD13 | 1:M:422:VAL:HG21 | 1.74 | 0.69 |
| 1:A:27:VAL:HG12 | 1:A:90:THR:HG23 | 1.74 | 0.69 |
| 1:K:348:GLN:O | 1:K:352:GLN:HG2 | 1.92 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:420:ILE:HG13 | 1:A:448:GLU:HG2 | 1.72 | 0.69 |
| 1:N:131:LEU:HD13 | 1:N:422:VAL:HG21 | 1.75 | 0.69 |
| 1:N:193:MET:HG3 | 1:N:371:LYS:HB3 | 1.73 | 0.69 |
| 1:N:413:ALA:HB2 | 1:N:475:ASN:HD22 | 1.56 | 0.69 |
| 1:D:200:LEU:HD21 | 1:D:277:LYS:HG3 | 1.74 | 0.69 |
| 1:E:404:ARG:HG2 | 1:E:404:ARG:HH11 | 1.58 | 0.69 |
| 1:K:183:LEU:HD13 | 1:K:184:GLN:HG3 | 1.75 | 0.69 |
| 1:M:183:LEU:HD13 | 1:M:184:GLN:HG3 | 1.73 | 0.69 |
| 1:M:413:ALA:HB2 | 1:M:475:ASN:HD22 | 1.56 | 0.69 |
| 1:B:385:THR:H | 1:C:281:PHE:HE1 | 1.38 | 0.69 |
| 1:I:413:ALA:H | 1:I:475:ASN:ND2 | 1.89 | 0.69 |
| 1:C:183:LEU:HD13 | 1:C:183:LEU:O | 1.93 | 0.69 |
| 1:F:404:ARG:NH1 | 1:F:404:ARG:HG2 | 2.07 | 0.69 |
| 1:F:420:ILE:HG13 | 1:F:448:GLU:HG2 | 1.74 | 0.69 |
| 1:D:183:LEU:O | 1:D:183:LEU:HD13 | 1.92 | 0.69 |
| 1:L:27:VAL:HG12 | 1:L:90:THR:HG23 | 1.74 | 0.69 |
| 1:M:29:VAL:HG12 | 4:M:1518:MPD:H12 | 1.75 | 0.69 |
| 1:I:193:MET:HE2 | 1:I:292:ILE:HG12 | 1.75 | 0.68 |
| 1:K:404:ARG:HG2 | 1:K:404:ARG:HH11 | 1.59 | 0.68 |
| 1:M:270:ILE:HG23 | 1:N:231:ARG:NH1 | 2.07 | 0.68 |
| 1:M:272:LYS:NZ | 1:N:229:ASN:HD22 | 1.89 | 0.68 |
| 1:C:383:ALA:O | 1:C:384:ALA:HB3 | 1.93 | 0.68 |
| 1:F:384:ALA:O | 1:F:385:THR:HG23 | 1.93 | 0.68 |
| 1:I:176:THR:HG21 | 1:I:333:ILE:HD13 | 1.74 | 0.68 |
| 1:H:420:ILE:HG13 | 1:H:448:GLU:HG2 | 1.76 | 0.68 |
| 1:L:287:ALA:HB1 | 1:L:368:ARG:NH1 | 2.08 | 0.68 |
| 1:C:242:LYS:C | 1:C:244:GLY:H | 1.97 | 0.68 |
| 1:E:57:ALA:O | 1:E:75:LYS:HE3 | 1.93 | 0.68 |
| 1:I:218:PRO:HB3 | 1:I:246:PRO:HG2 | 1.75 | 0.68 |
| 1:B:272:LYS:NZ | 1:C:229:ASN:ND2 | 2.41 | 0.68 |
| 1:N:404:ARG:HH11 | 1:N:404:ARG:HG2 | 1.59 | 0.68 |
| 1:H:404:ARG:HG2 | 1:H:404:ARG:NH1 | 2.08 | 0.68 |
| 1:H:413:ALA:H | 1:H:475:ASN:ND2 | 1.91 | 0.68 |
| 1:I:413:ALA:HB2 | 1:I:475:ASN:HD22 | 1.59 | 0.68 |
| 1:J:176:THR:HG21 | 1:J:333:ILE:HD13 | 1.74 | 0.68 |
| 1:L:413:ALA:H | 1:L:475:ASN:ND2 | 1.92 | 0.68 |
| 1:E:269:GLY:HA2 | 1:E:272:LYS:HZ2 | 1.57 | 0.68 |
| 1:I:420:ILE:HG13 | 1:I:448:GLU:HG2 | 1.76 | 0.68 |
| 1:J:202:PRO:O | 1:J:203:TYR:HB2 | 1.93 | 0.68 |
| 1:J:359:ASP:O | 1:J:363:GLU:HG2 | 1.94 | 0.68 |
| 1:K:413:ALA:H | 1:K:475:ASN:ND2 | 1.91 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:83:ASP:OD2 | 1:N:327:LYS:HD2 | 1.93 | 0.68 |
| 1:B:420:ILE:HG13 | 1:B:448:GLU:HG2 | 1.75 | 0.68 |
| 1:M:200:LEU:HD21 | 1:M:277:LYS:HG3 | 1.76 | 0.68 |
| 1:B:359:ASP:HA | 1:B:362:ARG:NH1 | 2.09 | 0.68 |
| 1:K:455:VAL:HG13 | 1:K:460:GLU:HB2 | 1.76 | 0.68 |
| 1:D:57:ALA:O | 1:D:75:LYS:HE3 | 1.94 | 0.67 |
| 1:E:291:ASP:OD2 | 1:E:368:ARG:HD2 | 1.93 | 0.67 |
| 1:N:413:ALA:H | 1:N:475:ASN:ND2 | 1.92 | 0.67 |
| 1:D:326:ASN:HD22 | 1:D:329:THR:HB | 1.59 | 0.67 |
| 1:J:455:VAL:HG13 | 1:J:460:GLU:HB2 | 1.76 | 0.67 |
| 1:M:420:ILE:HG13 | 1:M:448:GLU:HG2 | 1.76 | 0.67 |
| 1:E:420:ILE:HG13 | 1:E:448:GLU:HG2 | 1.76 | 0.67 |
| 1:L:200:LEU:HD21 | 1:L:277:LYS:HG3 | 1.74 | 0.67 |
| 1:N:218:PRO:HB3 | 1:N:246:PRO:HG2 | 1.77 | 0.67 |
| 1:D:239:ALA:HB1 | 1:D:314:LEU:HG | 1.76 | 0.67 |
| 1:F:202:PRO:O | 1:F:203:TYR:HB2 | 1.93 | 0.67 |
| 1:J:352:GLN:HB2 | 1:J:365:LEU:HD13 | 1.77 | 0.67 |
| 1:M:142:LYS:O | 1:M:146:GLN:HG3 | 1.94 | 0.67 |
| 1:D:235:PRO:HG3 | 1:D:310:GLU:HA | 1.76 | 0.67 |
| 1:B:183:LEU:HD13 | 1:B:183:LEU:O | 1.94 | 0.67 |
| 1:I:202:PRO:O | 1:I:203:TYR:HB2 | 1.95 | 0.67 |
| 1:L:221:LEU:HD23 | 1:L:249:ILE:HD12 | 1.77 | 0.67 |
| 1:E:69:MET:O | 1:E:73:MET:HG3 | 1.95 | 0.67 |
| 1:J:420:ILE:HG13 | 1:J:448:GLU:HG2 | 1.76 | 0.67 |
| 1:N:224:ASP:O | 1:N:225:LYS:HB3 | 1.94 | 0.67 |
| 1:B:404:ARG:HH11 | 1:B:404:ARG:HG2 | 1.58 | 0.67 |
| 1:C:219:PHE:O | 1:C:247:LEU:HD12 | 1.95 | 0.67 |
| 1:K:272:LYS:HZ3 | 1:L:229:ASN:HD21 | 1.42 | 0.67 |
| 1:M:272:LYS:HZ2 | 1:N:229:ASN:ND2 | 1.92 | 0.66 |
| 1:N:455:VAL:HG13 | 1:N:460:GLU:HB2 | 1.76 | 0.66 |
| 1:A:326:ASN:HD22 | 1:A:329:THR:HB | 1.59 | 0.66 |
| 1:C:404:ARG:NH1 | 1:C:404:ARG:HG2 | 2.09 | 0.66 |
| 1:C:69:MET:O | 1:C:73:MET:HG3 | 1.94 | 0.66 |
| 1:J:131:LEU:HD13 | 1:J:422:VAL:HG21 | 1.77 | 0.66 |
| 1:K:224:ASP:O | 1:K:225:LYS:HB3 | 1.95 | 0.66 |
| 1:H:131:LEU:HD13 | 1:H:422:VAL:HG21 | 1.77 | 0.66 |
| 1:K:218:PRO:HB3 | 1:K:246:PRO:HG2 | 1.77 | 0.66 |
| 1:D:132:LYS:HE2 | 6:D:3055:HOH:O | 1.95 | 0.66 |
| 1:G:69:MET:O | 1:G:73:MET:HG3 | 1.96 | 0.66 |
| 1:D:234:LEU:O | 1:D:238:GLU:HG3 | 1.96 | 0.66 |
| 1:H:202:PRO:O | 1:H:203:TYR:HB2 | 1.94 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:247:LEU:HD21 | 1:A:249:ILE:HD11 | 1.77 | 0.66 |
| 1:B:202:PRO:O | 1:B:204:PHE:N | 2.28 | 0.66 |
| 1:E:142:LYS:O | 1:E:146:GLN:HG3 | 1.95 | 0.66 |
| 1:F:291:ASP:OD2 | 1:F:368:ARG:HD2 | 1.96 | 0.66 |
| 1:H:194:GLN:O | 1:H:371:LYS:HE3 | 1.95 | 0.66 |
| 1:H:348:GLN:O | 1:H:352:GLN:HG2 | 1.95 | 0.66 |
| 1:I:5:ASP:HB2 | 1:I:524:LEU:HD12 | 1.77 | 0.66 |
| 1:K:359:ASP:O | 1:K:363:GLU:HG2 | 1.96 | 0.66 |
| 1:L:224:ASP:O | 1:L:225:LYS:HB3 | 1.95 | 0.66 |
| 1:M:348:GLN:O | 1:M:352:GLN:HG2 | 1.96 | 0.66 |
| 1:D:420:ILE:HG13 | 1:D:448:GLU:HG2 | 1.77 | 0.66 |
| 1:G:404:ARG:HG2 | 1:G:404:ARG:HH11 | 1.60 | 0.66 |
| 1:K:284:ARG:NH2 | 6:K:3052:HOH:O | 2.27 | 0.66 |
| 1:D:414:GLY:O | 1:D:417:VAL:HG13 | 1.94 | 0.66 |
| 1:I:270:ILE:O | 1:I:271:VAL:HB | 1.95 | 0.66 |
| 1:L:230:ILE:HD13 | 1:L:261:THR:CG2 | 2.25 | 0.66 |
| 1:N:27:VAL:HG12 | 1:N:90:THR:HG23 | 1.78 | 0.66 |
| 1:D:247:LEU:HD21 | 1:D:249:ILE:HD11 | 1.77 | 0.66 |
| 1:E:183:LEU:O | 1:E:183:LEU:HD13 | 1.95 | 0.66 |
| 1:A:404:ARG:HH11 | 1:A:404:ARG:HG2 | 1.61 | 0.65 |
| 1:C:31:LEU:HD13 | 1:C:90:THR:HG21 | 1.78 | 0.65 |
| 1:F:130:GLU:HB3 | 1:F:422:VAL:HG22 | 1.78 | 0.65 |
| 1:B:314:LEU:HD23 | 1:B:317:LEU:HD22 | 1.77 | 0.65 |
| 1:D:291:ASP:OD2 | 1:D:368:ARG:HD2 | 1.96 | 0.65 |
| 1:F:183:LEU:O | 1:F:183:LEU:HD13 | 1.95 | 0.65 |
| 1:N:194:GLN:O | 1:N:371:LYS:HE3 | 1.96 | 0.65 |
| 1:C:420:ILE:HG13 | 1:C:448:GLU:HG2 | 1.79 | 0.65 |
| 1:C:27:VAL:CG1 | 1:C:90:THR:HG23 | 2.26 | 0.65 |
| 1:E:218:PRO:HB3 | 1:E:246:PRO:HG2 | 1.77 | 0.65 |
| 1:H:455:VAL:HG13 | 1:H:460:GLU:HB2 | 1.78 | 0.65 |
| 1:I:200:LEU:HD21 | 1:I:277:LYS:HG3 | 1.77 | 0.65 |
| 1:L:455:VAL:HG13 | 1:L:460:GLU:HB2 | 1.78 | 0.65 |
| 1:A:142:LYS:O | 1:A:146:GLN:HG3 | 1.97 | 0.65 |
| 1:N:142:LYS:O | 1:N:146:GLN:HG3 | 1.97 | 0.65 |
| 1:N:414:GLY:O | 1:N:417:VAL:HG13 | 1.96 | 0.65 |
| 1:F:234:LEU:O | 1:F:238:GLU:HG3 | 1.96 | 0.65 |
| 1:J:27:VAL:HG12 | 1:J:90:THR:HG23 | 1.78 | 0.65 |
| 1:L:131:LEU:HD13 | 1:L:422:VAL:HG21 | 1.78 | 0.65 |
| 1:I:455:VAL:HG13 | 1:I:460:GLU:HB2 | 1.78 | 0.65 |
| 1:A:131:LEU:HD13 | 1:A:422:VAL:HG21 | 1.78 | 0.65 |
| 1:E:247:LEU:HD21 | 1:E:249:ILE:HD11 | 1.77 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:326:ASN:HD22 | 1:E:329:THR:HB | 1.61 | 0.65 |
| 1:E:183:LEU:HB2 | 1:E:384:ALA:HB2 | 1.78 | 0.65 |
| 1:L:449:ALA:HB3 | 1:L:450:PRO:HD3 | 1.79 | 0.65 |
| 1:M:27:VAL:HG12 | 1:M:90:THR:HG23 | 1.79 | 0.65 |
| 1:D:142:LYS:O | 1:D:146:GLN:HG3 | 1.97 | 0.64 |
| 1:I:449:ALA:HB3 | 1:I:450:PRO:HD3 | 1.79 | 0.64 |
| 1:M:193:MET:HG2 | 1:M:194:GLN:N | 2.12 | 0.64 |
| 1:M:455:VAL:HG13 | 1:M:460:GLU:HB2 | 1.79 | 0.64 |
| 1:D:384:ALA:O | 1:D:385:THR:HG23 | 1.98 | 0.64 |
| 1:G:131:LEU:HD13 | 1:G:422:VAL:HG21 | 1.80 | 0.64 |
| 1:I:142:LYS:O | 1:I:146:GLN:HG3 | 1.97 | 0.64 |
| 1:K:414:GLY:O | 1:K:417:VAL:HG13 | 1.97 | 0.64 |
| 1:J:413:ALA:H | 1:J:475:ASN:ND2 | 1.94 | 0.64 |
| 1:L:404:ARG:HG2 | 1:L:404:ARG:NH1 | 2.11 | 0.64 |
| 1:L:420:ILE:HG13 | 1:L:448:GLU:HG2 | 1.78 | 0.64 |
| 1:B:384:ALA:O | 1:B:385:THR:HG23 | 1.98 | 0.64 |
| 1:C:384:ALA:O | 1:C:385:THR:HG23 | 1.97 | 0.64 |
| 1:G:242:LYS:C | 1:G:244:GLY:H | 2.01 | 0.64 |
| 1:I:414:GLY:O | 1:I:417:VAL:HG13 | 1.96 | 0.64 |
| 1:K:29:VAL:HG12 | 4:K:1506:MPD:H12 | 1.79 | 0.64 |
| 1:L:5:ASP:HB2 | 1:L:524:LEU:HD12 | 1.80 | 0.64 |
| 1:E:359:ASP:HA | 1:E:362:ARG:NH1 | 2.13 | 0.64 |
| 1:J:5:ASP:HB2 | 1:J:524:LEU:HD12 | 1.78 | 0.64 |
| 1:N:5:ASP:HB2 | 1:N:524:LEU:HD12 | 1.79 | 0.64 |
| 1:B:69:MET:O | 1:B:73:MET:HG3 | 1.98 | 0.64 |
| 1:H:218:PRO:HB3 | 1:H:246:PRO:HG2 | 1.80 | 0.64 |
| 1:H:284:ARG:NH2 | 6:H:3055:HOH:O | 2.30 | 0.64 |
| 1:B:449:ALA:HB3 | 1:B:450:PRO:HD3 | 1.79 | 0.64 |
| 1:C:57:ALA:O | 1:C:75:LYS:HE3 | 1.98 | 0.64 |
| 1:D:242:LYS:C | 1:D:244:GLY:H | 2.00 | 0.64 |
| 1:H:160:LYS:O | 1:H:164:GLU:HG3 | 1.98 | 0.64 |
| 1:H:414:GLY:O | 1:H:417:VAL:HG13 | 1.97 | 0.64 |
| 1:C:131:LEU:HD13 | 1:C:422:VAL:HG21 | 1.78 | 0.64 |
| 1:E:234:LEU:O | 1:E:238:GLU:HG3 | 1.97 | 0.64 |
| 1:G:449:ALA:HB3 | 1:G:450:PRO:HD3 | 1.80 | 0.64 |
| 1:J:414:GLY:O | 1:J:417:VAL:HG13 | 1.97 | 0.64 |
| 1:M:5:ASP:HB2 | 1:M:524:LEU:HD12 | 1.79 | 0.64 |
| 1:A:359:ASP:O | 1:A:363:GLU:HG3 | 1.98 | 0.63 |
| 1:E:193:MET:HG3 | 1:E:371:LYS:HB3 | 1.81 | 0.63 |
| 1:K:34:LYS:HE2 | 1:L:118:ARG:HH22 | 1.63 | 0.63 |
| 1:L:348:GLN:O | 1:L:352:GLN:HG2 | 1.98 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:5:ASP:HB2 | 1:H:524:LEU:HD12 | 1.80 | 0.63 |
| 1:A:239:ALA:HB1 | 1:A:314:LEU:HG | 1.81 | 0.63 |
| 1:A:13:ARG:NH2 | 1:A:518:GLU:OE2 | 2.30 | 0.63 |
| 1:B:142:LYS:O | 1:B:146:GLN:HG3 | 1.99 | 0.63 |
| 1:B:414:GLY:O | 1:B:417:VAL:HG13 | 1.97 | 0.63 |
| 1:D:173:GLY:O | 1:D:404:ARG:NH2 | 2.31 | 0.63 |
| 1:K:5:ASP:HB2 | 1:K:524:LEU:HD12 | 1.78 | 0.63 |
| 1:N:445:ARG:HH12 | 4:N:1515:MPD:H31 | 1.62 | 0.63 |
| 1:B:234:LEU:O | 1:B:238:GLU:HG3 | 1.99 | 0.63 |
| 1:J:449:ALA:HB3 | 1:J:450:PRO:HD3 | 1.81 | 0.63 |
| 1:L:142:LYS:O | 1:L:146:GLN:HG3 | 1.99 | 0.63 |
| 1:A:57:ALA:O | 1:A:75:LYS:HE3 | 1.99 | 0.63 |
| 1:D:28:LYS:HD2 | 1:D:453:GLN:OE1 | 1.99 | 0.63 |
| 1:A:513:LEU:HD13 | 1:G:49:ILE:HD12 | 1.80 | 0.63 |
| 1:L:181:THR:O | 1:M:282:GLY:HA3 | 1.98 | 0.63 |
| 1:M:414:GLY:O | 1:M:417:VAL:HG13 | 1.99 | 0.63 |
| 1:B:326:ASN:ND2 | 1:B:329:THR:HB | 2.11 | 0.63 |
| 1:B:404:ARG:NH1 | 1:B:404:ARG:HG2 | 2.13 | 0.63 |
| 1:B:57:ALA:O | 1:B:75:LYS:HE3 | 1.99 | 0.63 |
| 1:M:224:ASP:O | 1:M:225:LYS:HB3 | 1.99 | 0.63 |
| 1:M:270:ILE:HA | 1:N:231:ARG:NH1 | 2.14 | 0.63 |
| 1:N:228:SER:O | 1:N:257:GLU:HB3 | 1.99 | 0.63 |
| 1:E:242:LYS:C | 1:E:244:GLY:H | 2.03 | 0.63 |
| 1:F:239:ALA:HB1 | 1:F:314:LEU:HG | 1.79 | 0.63 |
| 1:F:383:ALA:O | 1:F:384:ALA:HB3 | 1.99 | 0.63 |
| 1:H:287:ALA:HB1 | 1:H:368:ARG:NH1 | 2.14 | 0.63 |
| 1:J:142:LYS:O | 1:J:146:GLN:HG3 | 1.98 | 0.62 |
| 1:B:295:LEU:HA | 1:B:342:ILE:HD11 | 1.81 | 0.62 |
| 1:H:242:LYS:O | 1:H:243:ALA:HB3 | 2.00 | 0.62 |
| 1:M:230:ILE:HD13 | 1:M:261:THR:CG2 | 2.29 | 0.62 |
| 1:D:131:LEU:HD13 | 1:D:422:VAL:HG21 | 1.81 | 0.62 |
| 1:D:404:ARG:HG2 | 1:D:404:ARG:HH11 | 1.63 | 0.62 |
| 1:M:269:GLY:HA3 | 1:N:229:ASN:CG | 2.20 | 0.62 |
| 1:N:449:ALA:HB3 | 1:N:450:PRO:HD3 | 1.81 | 0.62 |
| 1:H:359:ASP:O | 1:H:363:GLU:HG2 | 2.00 | 0.62 |
| 1:K:449:ALA:HB3 | 1:K:450:PRO:HD3 | 1.80 | 0.62 |
| 1:C:174:VAL:HG12 | 1:C:376:VAL:HG13 | 1.81 | 0.62 |
| 1:K:142:LYS:O | 1:K:146:GLN:HG3 | 1.99 | 0.62 |
| 1:F:200:LEU:HD21 | 1:F:277:LYS:HG3 | 1.82 | 0.62 |
| 1:H:27:VAL:HG12 | 1:H:90:THR:HG23 | 1.82 | 0.62 |
| 1:I:27:VAL:HG12 | 1:I:90:THR:HG23 | 1.81 | 0.62 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:194:GLN:O | 1:J:371:LYS:HE3 | 1.99 | 0.62 |
| 1:K:131:LEU:HD13 | 1:K:422:VAL:HG21 | 1.82 | 0.62 |
| 1:F:142:LYS:O | 1:F:146:GLN:HG3 | 1.98 | 0.62 |
| 1:I:193:MET:CE | 1:I:292:ILE:HG12 | 2.29 | 0.62 |
| 1:J:242:LYS:O | 1:J:243:ALA:HB3 | 2.00 | 0.62 |
| 1:A:242:LYS:C | 1:A:244:GLY:H | 2.01 | 0.62 |
| 1:E:384:ALA:O | 1:E:385:THR:HG23 | 2.00 | 0.62 |
| 1:L:183:LEU:HD13 | 1:L:184:GLN:HG3 | 1.81 | 0.62 |
| 1:N:404:ARG:HG2 | 1:N:404:ARG:NH1 | 2.14 | 0.62 |
| 1:H:230:ILE:HD13 | 1:H:261:THR:CG2 | 2.30 | 0.62 |
| 1:I:404:ARG:HG2 | 1:I:404:ARG:NH1 | 2.13 | 0.62 |
| 1:N:27:VAL:CG1 | 1:N:90:THR:HG23 | 2.30 | 0.62 |
| 1:K:404:ARG:HG2 | 1:K:404:ARG:NH1 | 2.15 | 0.61 |
| 1:L:230:ILE:HG21 | 1:L:261:THR:HG21 | 1.81 | 0.61 |
| 1:A:404:ARG:NH1 | 1:A:404:ARG:HG2 | 2.15 | 0.61 |
| 1:A:69:MET:O | 1:A:73:MET:HG3 | 2.01 | 0.61 |
| 1:D:383:ALA:O | 1:D:384:ALA:HB3 | 1.98 | 0.61 |
| 1:F:27:VAL:CG1 | 1:F:90:THR:HG23 | 2.30 | 0.61 |
| 1:G:414:GLY:O | 1:G:417:VAL:HG13 | 1.99 | 0.61 |
| 1:F:183:LEU:HB2 | 1:F:384:ALA:HB2 | 1.82 | 0.61 |
| 1:A:314:LEU:HD23 | 1:A:317:LEU:HD22 | 1.83 | 0.61 |
| 1:B:183:LEU:HB2 | 1:B:384:ALA:HB2 | 1.82 | 0.61 |
| 1:C:142:LYS:O | 1:C:146:GLN:HG3 | 2.00 | 0.61 |
| 1:C:193:MET:CE | 1:C:292:ILE:HG12 | 2.31 | 0.61 |
| 1:E:359:ASP:O | 1:E:363:GLU:HG3 | 2.00 | 0.61 |
| 1:J:27:VAL:CG1 | 1:J:90:THR:HG23 | 2.30 | 0.61 |
| 1:M:352:GLN:HB2 | 1:M:365:LEU:HD13 | 1.82 | 0.61 |
| 1:M:359:ASP:O | 1:M:363:GLU:HG2 | 2.00 | 0.61 |
| 1:G:221:LEU:HD23 | 1:G:249:ILE:HD12 | 1.82 | 0.61 |
| 1:M:160:LYS:O | 1:M:164:GLU:HG3 | 2.00 | 0.61 |
| 1:M:404:ARG:HG2 | 1:M:404:ARG:HH11 | 1.64 | 0.61 |
| 1:C:234:LEU:O | 1:C:238:GLU:HG3 | 1.99 | 0.61 |
| 1:E:13:ARG:NH2 | 1:E:518:GLU:OE2 | 2.34 | 0.61 |
| 1:G:359:ASP:HA | 1:G:362:ARG:NH1 | 2.16 | 0.61 |
| 1:A:130:GLU:HB3 | 1:A:422:VAL:HG22 | 1.83 | 0.61 |
| 1:A:27:VAL:CG1 | 1:A:90:THR:HG23 | 2.30 | 0.61 |
| 1:J:404:ARG:NH1 | 1:J:404:ARG:HG2 | 2.11 | 0.61 |
| 1:L:359:ASP:O | 1:L:363:GLU:HG2 | 2.01 | 0.61 |
| 1:C:414:GLY:O | 1:C:417:VAL:HG13 | 2.01 | 0.60 |
| 1:E:130:GLU:HB3 | 1:E:422:VAL:HG22 | 1.83 | 0.60 |
| 1:I:28:LYS:HD2 | 1:I:453:GLN:OE1 | 2.00 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:414:GLY:O | 1:A:417:VAL:HG13 | 2.02 | 0.60 |
| 1:F:359:ASP:O | 1:F:363:GLU:HG3 | 2.01 | 0.60 |
| 1:G:404:ARG:NH1 | 1:G:404:ARG:HG2 | 2.15 | 0.60 |
| 1:I:224:ASP:O | 1:I:225:LYS:HB3 | 2.01 | 0.60 |
| 1:B:235:PRO:HG3 | 1:B:310:GLU:HA | 1.84 | 0.60 |
| 1:C:359:ASP:O | 1:C:363:GLU:HG3 | 2.01 | 0.60 |
| 1:H:263:VAL:O | 1:H:267:MET:HB2 | 2.01 | 0.60 |
| 1:H:496:PRO:HB2 | 1:H:499:VAL:HG13 | 1.83 | 0.60 |
| 1:L:269:GLY:HA3 | 1:M:257:GLU:HB2 | 1.81 | 0.60 |
| 1:F:242:LYS:O | 1:F:243:ALA:HB3 | 2.00 | 0.60 |
| 1:D:449:ALA:HB3 | 1:D:450:PRO:HD3 | 1.83 | 0.60 |
| 1:C:291:ASP:OD2 | 1:C:368:ARG:HD2 | 2.01 | 0.60 |
| 1:E:27:VAL:CG1 | 1:E:90:THR:HG23 | 2.29 | 0.60 |
| 1:E:449:ALA:HB3 | 1:E:450:PRO:HD3 | 1.83 | 0.60 |
| 1:N:348:GLN:O | 1:N:352:GLN:HG2 | 2.01 | 0.60 |
| 1:F:414:GLY:O | 1:F:417:VAL:HG13 | 2.01 | 0.60 |
| 1:H:27:VAL:CG1 | 1:H:90:THR:HG23 | 2.31 | 0.60 |
| 1:D:404:ARG:HG2 | 1:D:404:ARG:NH1 | 2.16 | 0.60 |
| 1:G:384:ALA:O | 1:G:385:THR:HG23 | 2.01 | 0.60 |
| 1:L:225:LYS:HD2 | 1:L:226:LYS:O | 2.01 | 0.60 |
| 1:M:272:LYS:HZ2 | 1:N:229:ASN:HD22 | 1.49 | 0.60 |
| 1:C:449:ALA:HB3 | 1:C:450:PRO:HD3 | 1.84 | 0.60 |
| 1:C:413:ALA:HB2 | 1:C:475:ASN:HD22 | 1.67 | 0.60 |
| 1:E:220:ILE:HD12 | 1:E:296:THR:HG21 | 1.84 | 0.60 |
| 1:M:242:LYS:O | 1:M:243:ALA:HB3 | 2.02 | 0.60 |
| 1:A:173:GLY:O | 1:A:404:ARG:NH2 | 2.34 | 0.59 |
| 1:E:191:GLU:O | 1:E:334:ASP:HA | 2.02 | 0.59 |
| 1:E:202:PRO:O | 1:E:204:PHE:N | 2.30 | 0.59 |
| 1:F:131:LEU:HD13 | 1:F:422:VAL:HG21 | 1.84 | 0.59 |
| 1:F:359:ASP:HA | 1:F:362:ARG:NH1 | 2.17 | 0.59 |
| 1:F:362:ARG:HG2 | 1:F:366:GLN:NE2 | 2.17 | 0.59 |
| 1:G:314:LEU:HD23 | 1:G:317:LEU:HD22 | 1.84 | 0.59 |
| 1:C:173:GLY:O | 1:C:404:ARG:NH2 | 2.35 | 0.59 |
| 1:G:27:VAL:CG1 | 1:G:90:THR:HG23 | 2.32 | 0.59 |
| 1:J:181:THR:O | 1:K:282:GLY:HA3 | 2.03 | 0.59 |
| 1:B:359:ASP:O | 1:B:363:GLU:HG3 | 2.02 | 0.59 |
| 1:H:224:ASP:O | 1:H:225:LYS:HB3 | 2.02 | 0.59 |
| 1:L:414:GLY:O | 1:L:417:VAL:HG13 | 2.01 | 0.59 |
| 1:C:200:LEU:HD21 | 1:C:277:LYS:HG3 | 1.84 | 0.59 |
| 1:I:352:GLN:HB2 | 1:I:365:LEU:HD13 | 1.84 | 0.59 |
| 1:L:272:LYS:HZ3 | 1:M:228:SER:HB3 | 1.67 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:202:PRO:O | 1:C:203:TYR:HB2 | 2.02 | 0.59 |
| 1:E:218:PRO:HD2 | 1:E:320:ALA:O | 2.03 | 0.59 |
| 1:F:455:VAL:HG13 | 1:F:460:GLU:HB2 | 1.84 | 0.59 |
| 1:G:455:VAL:HG13 | 1:G:460:GLU:HB2 | 1.85 | 0.59 |
| 1:L:235:PRO:CG | 1:L:310:GLU:HA | 2.31 | 0.59 |
| 1:L:272:LYS:HZ1 | 1:M:228:SER:HB3 | 1.64 | 0.59 |
| 1:M:28:LYS:HD2 | 1:M:453:GLN:OE1 | 2.03 | 0.59 |
| 1:B:319:GLN:O | 1:B:336:VAL:HG23 | 2.02 | 0.59 |
| 1:E:221:LEU:HD23 | 1:E:249:ILE:HD12 | 1.84 | 0.59 |
| 1:J:228:SER:O | 1:J:257:GLU:HB3 | 2.02 | 0.59 |
| 1:D:130:GLU:HB3 | 1:D:422:VAL:HG22 | 1.84 | 0.59 |
| 1:J:191:GLU:O | 1:J:334:ASP:HA | 2.03 | 0.59 |
| 1:H:142:LYS:O | 1:H:146:GLN:HG3 | 2.03 | 0.58 |
| 1:J:472:GLY:HA3 | 1:J:476:TYR:CD2 | 2.38 | 0.58 |
| 1:K:242:LYS:O | 1:K:243:ALA:HB3 | 2.02 | 0.58 |
| 1:M:272:LYS:HZ1 | 1:N:229:ASN:ND2 | 1.99 | 0.58 |
| 1:H:228:SER:O | 1:H:257:GLU:HB3 | 2.02 | 0.58 |
| 1:I:193:MET:HG3 | 1:I:371:LYS:HB3 | 1.84 | 0.58 |
| 1:K:27:VAL:HG12 | 1:K:90:THR:HG23 | 1.84 | 0.58 |
| 1:L:27:VAL:CG1 | 1:L:90:THR:HG23 | 2.32 | 0.58 |
| 1:H:183:LEU:HD22 | 1:H:184:GLN:H | 1.68 | 0.58 |
| 1:J:413:ALA:CB | 1:J:475:ASN:HD22 | 2.16 | 0.58 |
| 1:M:270:ILE:HA | 1:N:231:ARG:HH11 | 1.67 | 0.58 |
| 1:A:451:LEU:HD23 | 1:A:451:LEU:C | 2.24 | 0.58 |
| 1:C:455:VAL:HG13 | 1:C:460:GLU:HB2 | 1.84 | 0.58 |
| 1:E:319:GLN:O | 1:E:336:VAL:HG23 | 2.03 | 0.58 |
| 1:E:404:ARG:HG2 | 1:E:404:ARG:NH1 | 2.15 | 0.58 |
| 1:G:183:LEU:HB2 | 1:G:384:ALA:HB2 | 1.85 | 0.58 |
| 1:H:270:ILE:O | 1:H:271:VAL:HB | 2.04 | 0.58 |
| 1:K:254:VAL:HG12 | 1:K:259:LEU:HB2 | 1.85 | 0.58 |
| 1:M:413:ALA:N | 1:M:475:ASN:ND2 | 2.51 | 0.58 |
| 1:A:218:PRO:HD2 | 1:A:320:ALA:O | 2.04 | 0.58 |
| 1:A:455:VAL:HG13 | 1:A:460:GLU:HB2 | 1.85 | 0.58 |
| 1:I:336:VAL:O | 1:I:336:VAL:HG12 | 2.02 | 0.58 |
| 1:I:38:VAL:HG13 | 1:J:519:CYS:HB3 | 1.86 | 0.58 |
| 1:J:34:LYS:HE2 | 1:K:118:ARG:HH22 | 1.68 | 0.58 |
| 1:A:291:ASP:OD2 | 1:A:368:ARG:HD2 | 2.04 | 0.58 |
| 1:D:230:ILE:HD13 | 1:D:261:THR:HG21 | 1.86 | 0.58 |
| 1:G:142:LYS:O | 1:G:146:GLN:HG3 | 2.02 | 0.58 |
| 1:L:200:LEU:HG | 1:L:276:VAL:HA | 1.86 | 0.58 |
| 1:M:193:MET:CE | 1:M:292:ILE:HG12 | 2.34 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:221:LEU:HD23 | 1:M:249:ILE:HD12 | 1.86 | 0.58 |
| 1:D:69:MET:O | 1:D:73:MET:HG3 | 2.04 | 0.58 |
| 1:F:270:ILE:O | 1:F:271:VAL:HB | 2.04 | 0.58 |
| 1:I:242:LYS:O | 1:I:243:ALA:HB3 | 2.01 | 0.58 |
| 1:J:221:LEU:HD23 | 1:J:249:ILE:HD12 | 1.85 | 0.58 |
| 1:K:140:ASP:OD2 | 1:K:142:LYS:HB3 | 2.03 | 0.58 |
| 1:M:449:ALA:HB3 | 1:M:450:PRO:HD3 | 1.86 | 0.58 |
| 1:A:230:ILE:HD13 | 1:A:261:THR:CG2 | 2.34 | 0.58 |
| 1:D:193:MET:CE | 1:D:292:ILE:HG12 | 2.34 | 0.58 |
| 1:K:193:MET:CE | 1:K:292:ILE:HG12 | 2.33 | 0.58 |
| 1:C:290:GLN:HB3 | 1:C:345:ARG:NH2 | 2.19 | 0.58 |
| 1:M:383:ALA:HB3 | 1:M:389:MET:HB2 | 1.84 | 0.58 |
| 1:N:352:GLN:HB2 | 1:N:365:LEU:HD13 | 1.86 | 0.58 |
| 1:C:202:PRO:O | 1:C:204:PHE:N | 2.33 | 0.57 |
| 1:E:455:VAL:HG13 | 1:E:460:GLU:HB2 | 1.84 | 0.57 |
| 1:K:218:PRO:HD2 | 1:K:320:ALA:O | 2.04 | 0.57 |
| 1:M:472:GLY:HA3 | 1:M:476:TYR:CD2 | 2.39 | 0.57 |
| 1:E:269:GLY:HA3 | 1:F:229:ASN:CG | 2.23 | 0.57 |
| 1:G:273:VAL:HG12 | 1:G:274:ALA:N | 2.19 | 0.57 |
| 1:J:140:ASP:OD2 | 1:J:142:LYS:HB3 | 2.03 | 0.57 |
| 1:K:221:LEU:HD23 | 1:K:249:ILE:HD12 | 1.87 | 0.57 |
| 1:M:259:LEU:O | 1:M:263:VAL:HG23 | 2.04 | 0.57 |
| 1:M:404:ARG:HG2 | 1:M:404:ARG:NH1 | 2.19 | 0.57 |
| 1:N:445:ARG:NH1 | 4:N:1515:MPD:H31 | 2.19 | 0.57 |
| 1:A:349:ILE:CG2 | 1:A:369:VAL:HG13 | 2.35 | 0.57 |
| 1:K:413:ALA:CB | 1:K:475:ASN:HD22 | 2.18 | 0.57 |
| 1:C:413:ALA:H | 1:C:475:ASN:ND2 | 2.02 | 0.57 |
| 1:F:69:MET:O | 1:F:73:MET:HG3 | 2.05 | 0.57 |
| 1:I:160:LYS:O | 1:I:164:GLU:HG3 | 2.04 | 0.57 |
| 1:L:242:LYS:O | 1:L:243:ALA:HB3 | 2.03 | 0.57 |
| 1:L:496:PRO:HB2 | 1:L:499:VAL:HG13 | 1.86 | 0.57 |
| 1:H:28:LYS:HD2 | 1:H:453:GLN:OE1 | 2.04 | 0.57 |
| 1:B:173:GLY:O | 1:B:404:ARG:NH2 | 2.37 | 0.57 |
| 1:D:202:PRO:O | 1:D:203:TYR:HB2 | 2.04 | 0.57 |
| 1:D:242:LYS:HG2 | 1:E:231:ARG:CZ | 2.33 | 0.57 |
| 1:M:193:MET:HE2 | 1:M:292:ILE:HG12 | 1.87 | 0.57 |
| 1:H:193:MET:HG3 | 1:H:371:LYS:HB3 | 1.87 | 0.57 |
| 1:I:348:GLN:O | 1:I:352:GLN:HG2 | 2.05 | 0.57 |
| 1:K:202:PRO:O | 1:K:204:PHE:N | 2.37 | 0.57 |
| 1:C:130:GLU:HB3 | 1:C:422:VAL:HG22 | 1.85 | 0.57 |
| 1:H:310:GLU:N | 1:H:310:GLU:OE1 | 2.38 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:270:ILE:O | 1:J:271:VAL:HB | 2.04 | 0.57 |
| 1:N:413:ALA:N | 1:N:475:ASN:ND2 | 2.53 | 0.57 |
| 1:A:384:ALA:O | 1:A:385:THR:HG23 | 2.05 | 0.57 |
| 1:B:455:VAL:HG13 | 1:B:460:GLU:HB2 | 1.87 | 0.57 |
| 1:G:359:ASP:HA | 1:G:362:ARG:HH12 | 1.70 | 0.57 |
| 1:G:383:ALA:O | 1:G:384:ALA:HB3 | 2.04 | 0.57 |
| 1:G:173:GLY:O | 1:G:404:ARG:NH2 | 2.38 | 0.57 |
| 1:D:455:VAL:HG13 | 1:D:460:GLU:HB2 | 1.86 | 0.57 |
| 1:G:326:ASN:HD22 | 1:G:329:THR:HB | 1.70 | 0.57 |
| 1:H:305:ILE:O | 1:H:305:ILE:HG22 | 2.04 | 0.57 |
| 1:J:287:ALA:HB1 | 1:J:368:ARG:NH1 | 2.20 | 0.57 |
| 1:N:383:ALA:HB3 | 1:N:389:MET:HB2 | 1.87 | 0.57 |
| 1:A:234:LEU:O | 1:A:238:GLU:HG3 | 2.04 | 0.56 |
| 1:A:383:ALA:O | 1:A:384:ALA:HB3 | 2.05 | 0.56 |
| 1:B:413:ALA:HB2 | 1:B:475:ASN:HD22 | 1.69 | 0.56 |
| 1:C:270:ILE:O | 1:C:271:VAL:HB | 2.04 | 0.56 |
| 1:C:359:ASP:HA | 1:C:362:ARG:NH1 | 2.20 | 0.56 |
| 1:H:140:ASP:OD2 | 1:H:142:LYS:HB3 | 2.05 | 0.56 |
| 1:A:413:ALA:HB2 | 1:A:475:ASN:HD22 | 1.70 | 0.56 |
| 1:C:183:LEU:HB2 | 1:C:384:ALA:HB2 | 1.86 | 0.56 |
| 1:H:266:THR:HG21 | 1:H:273:VAL:HB | 1.87 | 0.56 |
| 1:J:173:GLY:O | 1:J:404:ARG:NH2 | 2.38 | 0.56 |
| 1:K:28:LYS:HD2 | 1:K:453:GLN:OE1 | 2.05 | 0.56 |
| 1:N:140:ASP:OD2 | 1:N:142:LYS:HB3 | 2.05 | 0.56 |
| 1:B:220:ILE:HD12 | 1:B:296:THR:HG21 | 1.87 | 0.56 |
| 1:B:359:ASP:HA | 1:B:362:ARG:HH12 | 1.70 | 0.56 |
| 1:G:202:PRO:O | 1:G:203:TYR:HB2 | 2.05 | 0.56 |
| 1:J:225:LYS:HD2 | 1:J:226:LYS:O | 2.06 | 0.56 |
| 1:N:230:ILE:HD13 | 1:N:261:THR:CG2 | 2.35 | 0.56 |
| 1:N:472:GLY:HA3 | 1:N:476:TYR:CD2 | 2.40 | 0.56 |
| 1:F:449:ALA:HB3 | 1:F:450:PRO:HD3 | 1.86 | 0.56 |
| 1:H:413:ALA:N | 1:H:475:ASN:ND2 | 2.53 | 0.56 |
| 1:J:218:PRO:CB | 1:J:246:PRO:HG2 | 2.35 | 0.56 |
| 1:L:155:ASP:OD1 | 1:L:157:THR:HB | 2.05 | 0.56 |
| 1:L:72:GLN:OE1 | 1:L:75:LYS:HE3 | 2.05 | 0.56 |
| 1:M:202:PRO:O | 1:M:203:TYR:HB2 | 2.04 | 0.56 |
| 1:C:194:GLN:O | 1:C:371:LYS:HE3 | 2.05 | 0.56 |
| 1:H:231:ARG:NH1 | 1:N:241:ALA:CB | 2.69 | 0.56 |
| 1:I:171:LYS:HG2 | 6:I:3095:HOH:O | 2.04 | 0.56 |
| 1:I:27:VAL:CG1 | 1:I:90:THR:HG23 | 2.34 | 0.56 |
| 1:B:200:LEU:HD21 | 1:B:277:LYS:HG3 | 1.86 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:173:GLY:O | 1:I:404:ARG:NH2 | 2.39 | 0.56 |
| 1:M:413:ALA:CB | 1:M:475:ASN:HD22 | 2.19 | 0.56 |
| 1:H:191:GLU:O | 1:H:334:ASP:HA | 2.05 | 0.56 |
| 1:B:140:ASP:OD2 | 1:B:142:LYS:HB3 | 2.05 | 0.56 |
| 1:G:270:ILE:O | 1:G:271:VAL:HB | 2.05 | 0.56 |
| 1:A:359:ASP:HA | 1:A:362:ARG:NH1 | 2.20 | 0.56 |
| 1:D:27:VAL:CG1 | 1:D:90:THR:HG23 | 2.34 | 0.56 |
| 1:E:23:LEU:HD23 | 1:E:74:VAL:HG22 | 1.87 | 0.56 |
| 1:K:413:ALA:N | 1:K:475:ASN:ND2 | 2.53 | 0.56 |
| 1:L:28:LYS:HD2 | 1:L:453:GLN:OE1 | 2.06 | 0.56 |
| 1:A:194:GLN:O | 1:A:371:LYS:HE3 | 2.06 | 0.56 |
| 1:B:130:GLU:HB3 | 1:B:422:VAL:HG22 | 1.88 | 0.56 |
| 1:D:118:ARG:NH2 | 6:D:3039:HOH:O | 2.38 | 0.56 |
| 1:M:230:ILE:HD13 | 1:M:261:THR:HG21 | 1.86 | 0.56 |
| 1:A:140:ASP:OD2 | 1:A:142:LYS:HB3 | 2.06 | 0.56 |
| 1:B:242:LYS:C | 1:B:244:GLY:H | 2.08 | 0.56 |
| 1:B:27:VAL:CG1 | 1:B:90:THR:HG23 | 2.36 | 0.56 |
| 1:H:225:LYS:HD2 | 1:H:226:LYS:O | 2.06 | 0.56 |
| 1:I:383:ALA:HB3 | 1:I:389:MET:HB2 | 1.86 | 0.56 |
| 1:K:160:LYS:O | 1:K:164:GLU:HG3 | 2.06 | 0.56 |
| 1:B:218:PRO:HD2 | 1:B:320:ALA:O | 2.05 | 0.55 |
| 1:F:242:LYS:C | 1:F:244:GLY:H | 2.10 | 0.55 |
| 1:G:202:PRO:O | 1:G:204:PHE:N | 2.35 | 0.55 |
| 1:I:305:ILE:HG22 | 1:I:305:ILE:O | 2.05 | 0.55 |
| 1:J:319:GLN:HB3 | 1:J:336:VAL:HG21 | 1.88 | 0.55 |
| 1:L:413:ALA:CB | 1:L:475:ASN:HD22 | 2.19 | 0.55 |
| 1:C:140:ASP:OD2 | 1:C:142:LYS:HB3 | 2.06 | 0.55 |
| 1:E:109:ALA:HB2 | 1:I:109:ALA:HB2 | 1.89 | 0.55 |
| 1:G:23:LEU:HD23 | 1:G:74:VAL:HG22 | 1.87 | 0.55 |
| 1:A:259:LEU:O | 1:A:263:VAL:HG23 | 2.05 | 0.55 |
| 1:D:416:GLY:HA2 | 6:D:3097:HOH:O | 2.06 | 0.55 |
| 1:J:28:LYS:HD2 | 1:J:453:GLN:OE1 | 2.06 | 0.55 |
| 1:M:183:LEU:HD22 | 1:M:184:GLN:H | 1.71 | 0.55 |
| 1:A:183:LEU:HB2 | 1:A:384:ALA:HB2 | 1.87 | 0.55 |
| 1:B:131:LEU:HD13 | 1:B:422:VAL:HG21 | 1.87 | 0.55 |
| 1:I:140:ASP:OD2 | 1:I:142:LYS:HB3 | 2.06 | 0.55 |
| 1:J:383:ALA:HB3 | 1:J:389:MET:HB2 | 1.88 | 0.55 |
| 1:B:201:SER:O | 1:B:202:PRO:O | 2.24 | 0.55 |
| 1:G:200:LEU:HG | 1:G:276:VAL:HA | 1.89 | 0.55 |
| 1:K:220:ILE:HD12 | 1:K:296:THR:HG21 | 1.89 | 0.55 |
| 1:K:193:MET:HG3 | 1:K:371:LYS:HB3 | 1.89 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:472:GLY:HA3 | 1:K:476:TYR:CD2 | 2.41 | 0.55 |
| 1:M:270:ILE:HG23 | 1:N:231:ARG:CZ | 2.36 | 0.55 |
| 1:J:155:ASP:OD1 | 1:J:157:THR:HB | 2.07 | 0.55 |
| 1:K:234:LEU:O | 1:K:238:GLU:HG3 | 2.06 | 0.55 |
| 1:A:220:ILE:HD12 | 1:A:296:THR:HG21 | 1.88 | 0.55 |
| 1:B:451:LEU:HD23 | 1:B:451:LEU:C | 2.27 | 0.55 |
| 1:D:183:LEU:HB2 | 1:D:384:ALA:HB2 | 1.89 | 0.55 |
| 1:D:242:LYS:O | 1:D:244:GLY:N | 2.35 | 0.55 |
| 1:H:83:ASP:OD2 | 1:H:327:LYS:HD3 | 2.06 | 0.55 |
| 1:J:230:ILE:HD13 | 1:J:261:THR:CG2 | 2.37 | 0.55 |
| 1:J:263:VAL:O | 1:J:267:MET:HB2 | 2.07 | 0.55 |
| 1:N:242:LYS:O | 1:N:243:ALA:HB3 | 2.07 | 0.55 |
| 1:D:23:LEU:HD23 | 1:D:74:VAL:HG22 | 1.89 | 0.55 |
| 1:E:385:THR:H | 1:F:281:PHE:HE1 | 1.54 | 0.55 |
| 1:E:414:GLY:O | 1:E:417:VAL:HG13 | 2.06 | 0.55 |
| 1:H:259:LEU:O | 1:H:263:VAL:HG23 | 2.07 | 0.55 |
| 1:I:413:ALA:N | 1:I:475:ASN:ND2 | 2.54 | 0.55 |
| 1:L:345:ARG:HA | 1:L:348:GLN:HE21 | 1.72 | 0.55 |
| 1:L:352:GLN:HB2 | 1:L:365:LEU:HD13 | 1.89 | 0.55 |
| 1:M:27:VAL:CG1 | 1:M:90:THR:HG23 | 2.36 | 0.55 |
| 1:N:160:LYS:O | 1:N:164:GLU:HG3 | 2.07 | 0.55 |
| 1:H:228:SER:HB3 | 1:N:272:LYS:NZ | 2.22 | 0.55 |
| 1:A:200:LEU:HG | 1:A:276:VAL:HA | 1.89 | 0.55 |
| 1:A:178:GLU:HA | 1:A:393:LYS:HE2 | 1.89 | 0.55 |
| 1:A:413:ALA:H | 1:A:475:ASN:ND2 | 2.05 | 0.55 |
| 1:B:193:MET:HG3 | 1:B:371:LYS:HB3 | 1.89 | 0.55 |
| 1:G:451:LEU:C | 1:G:451:LEU:HD23 | 2.27 | 0.55 |
| 1:I:472:GLY:HA3 | 1:I:476:TYR:CD2 | 2.42 | 0.55 |
| 1:L:194:GLN:O | 1:L:371:LYS:HE3 | 2.07 | 0.55 |
| 1:L:472:GLY:HA3 | 1:L:476:TYR:CD2 | 2.41 | 0.55 |
| 1:B:242:LYS:O | 1:B:243:ALA:HB3 | 2.08 | 0.54 |
| 1:C:230:ILE:HD13 | 1:C:261:THR:HG21 | 1.89 | 0.54 |
| 1:K:349:ILE:HA | 1:K:352:GLN:HG3 | 1.88 | 0.54 |
| 1:K:27:VAL:CG1 | 1:K:90:THR:HG23 | 2.37 | 0.54 |
| 1:C:362:ARG:HG2 | 1:C:366:GLN:NE2 | 2.23 | 0.54 |
| 1:G:263:VAL:O | 1:G:267:MET:HB2 | 2.08 | 0.54 |
| 1:L:413:ALA:N | 1:L:475:ASN:ND2 | 2.54 | 0.54 |
| 1:A:23:LEU:HD23 | 1:A:74:VAL:HG22 | 1.88 | 0.54 |
| 1:C:242:LYS:O | 1:C:244:GLY:N | 2.38 | 0.54 |
| 1:D:259:LEU:O | 1:D:263:VAL:HG23 | 2.06 | 0.54 |
| 1:J:305:ILE:O | 1:J:305:ILE:HG22 | 2.08 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:239:ALA:HB1 | 1:M:314:LEU:HG | 1.89 | 0.54 |
| 1:M:235:PRO:CG | 1:M:310:GLU:HA | 2.32 | 0.54 |
| 1:D:359:ASP:HA | 1:D:362:ARG:NH1 | 2.23 | 0.54 |
| 1:E:194:GLN:O | 1:E:371:LYS:HE3 | 2.07 | 0.54 |
| 1:I:72:GLN:OE1 | 1:I:75:LYS:HE3 | 2.07 | 0.54 |
| 1:L:191:GLU:O | 1:L:334:ASP:HA | 2.08 | 0.54 |
| 1:G:140:ASP:OD2 | 1:G:142:LYS:HB3 | 2.07 | 0.54 |
| 1:K:221:LEU:HD11 | 1:K:301:ILE:HD12 | 1.90 | 0.54 |
| 1:L:77:VAL:HG21 | 1:L:510:VAL:HB | 1.89 | 0.54 |
| 1:D:362:ARG:HG2 | 1:D:366:GLN:NE2 | 2.22 | 0.54 |
| 1:E:140:ASP:OD2 | 1:E:142:LYS:HB3 | 2.06 | 0.54 |
| 1:F:28:LYS:HD2 | 1:F:453:GLN:OE1 | 2.07 | 0.54 |
| 1:H:413:ALA:CB | 1:H:475:ASN:HD22 | 2.19 | 0.54 |
| 1:H:472:GLY:HA3 | 1:H:476:TYR:CD2 | 2.42 | 0.54 |
| 1:J:262:LEU:O | 1:J:266:THR:HG23 | 2.07 | 0.54 |
| 1:L:236:VAL:HG22 | 1:L:312:ALA:O | 2.07 | 0.54 |
| 1:N:413:ALA:CB | 1:N:475:ASN:HD22 | 2.20 | 0.54 |
| 1:A:242:LYS:O | 1:A:243:ALA:HB3 | 2.07 | 0.54 |
| 1:D:314:LEU:HD23 | 1:D:317:LEU:HD22 | 1.89 | 0.54 |
| 1:J:413:ALA:N | 1:J:475:ASN:ND2 | 2.56 | 0.54 |
| 1:M:219:PHE:HB3 | 1:M:317:LEU:HD23 | 1.90 | 0.54 |
| 1:H:230:ILE:HD13 | 1:H:261:THR:HG21 | 1.89 | 0.54 |
| 1:H:252:GLU:O | 1:H:253:ASP:HB2 | 2.08 | 0.54 |
| 1:J:193:MET:HG3 | 1:J:371:LYS:HB3 | 1.90 | 0.54 |
| 1:B:383:ALA:O | 1:B:384:ALA:HB3 | 2.08 | 0.54 |
| 1:E:451:LEU:HD23 | 1:E:451:LEU:C | 2.28 | 0.54 |
| 1:G:130:GLU:HB3 | 1:G:422:VAL:HG22 | 1.89 | 0.54 |
| 1:I:31:LEU:HD13 | 1:I:90:THR:CG2 | 2.38 | 0.54 |
| 1:N:349:ILE:HA | 1:N:352:GLN:HG3 | 1.90 | 0.54 |
| 1:E:247:LEU:CD2 | 1:E:249:ILE:HD11 | 2.38 | 0.54 |
| 1:H:383:ALA:HB3 | 1:H:389:MET:HB2 | 1.88 | 0.54 |
| 1:F:218:PRO:HB3 | 1:F:246:PRO:HG2 | 1.90 | 0.53 |
| 1:F:314:LEU:HD23 | 1:F:317:LEU:HD22 | 1.90 | 0.53 |
| 1:H:57:ALA:O | 1:H:75:LYS:HD2 | 2.08 | 0.53 |
| 1:L:342:ILE:O | 1:L:346:VAL:HG23 | 2.08 | 0.53 |
| 1:L:349:ILE:O | 1:L:353:ILE:HG13 | 2.08 | 0.53 |
| 1:D:32:GLY:HA3 | 1:D:454:ILE:HG23 | 1.89 | 0.53 |
| 1:H:72:GLN:OE1 | 1:H:75:LYS:HE3 | 2.08 | 0.53 |
| 1:J:217:SER:N | 1:J:218:PRO:CD | 2.72 | 0.53 |
| 1:K:130:GLU:HB3 | 1:K:422:VAL:HG22 | 1.90 | 0.53 |
| 1:L:266:THR:HG21 | 1:L:273:VAL:HB | 1.89 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:57:ALA:O | 1:M:75:LYS:HD2 | 2.08 | 0.53 |
| 1:N:202:PRO:O | 1:N:203:TYR:HB2 | 2.09 | 0.53 |
| 1:K:230:ILE:HD13 | 1:K:261:THR:CG2 | 2.38 | 0.53 |
| 1:K:72:GLN:OE1 | 1:K:75:LYS:HE3 | 2.08 | 0.53 |
| 1:N:349:ILE:O | 1:N:353:ILE:HG13 | 2.09 | 0.53 |
| 1:D:270:ILE:O | 1:D:271:VAL:HB | 2.08 | 0.53 |
| 1:F:140:ASP:OD2 | 1:F:142:LYS:HB3 | 2.08 | 0.53 |
| 1:G:425:LYS:NZ | 6:G:3204:HOH:O | 2.38 | 0.53 |
| 1:H:349:ILE:HA | 1:H:352:GLN:HG3 | 1.90 | 0.53 |
| 1:J:193:MET:CE | 1:J:292:ILE:HG12 | 2.38 | 0.53 |
| 1:K:201:SER:O | 1:K:202:PRO:O | 2.27 | 0.53 |
| 1:M:194:GLN:O | 1:M:371:LYS:HE3 | 2.08 | 0.53 |
| 1:M:349:ILE:HA | 1:M:352:GLN:HG3 | 1.91 | 0.53 |
| 1:M:287:ALA:HB1 | 1:M:368:ARG:NH1 | 2.23 | 0.53 |
| 1:D:349:ILE:CG2 | 1:D:369:VAL:HG13 | 2.38 | 0.53 |
| 1:E:173:GLY:O | 1:E:404:ARG:NH2 | 2.41 | 0.53 |
| 1:H:339:GLU:O | 1:H:343:GLN:HB2 | 2.08 | 0.53 |
| 1:I:218:PRO:HD2 | 1:I:320:ALA:O | 2.09 | 0.53 |
| 1:B:178:GLU:HA | 1:B:393:LYS:HE2 | 1.91 | 0.53 |
| 1:C:284:ARG:NH1 | 1:C:364:LYS:HD2 | 2.24 | 0.53 |
| 1:E:199:TYR:CZ | 1:E:327:LYS:HA | 2.44 | 0.53 |
| 1:L:217:SER:N | 1:L:218:PRO:CD | 2.72 | 0.53 |
| 1:N:270:ILE:O | 1:N:271:VAL:HB | 2.09 | 0.53 |
| 1:A:202:PRO:O | 1:A:203:TYR:HB2 | 2.08 | 0.53 |
| 1:C:31:LEU:HD13 | 1:C:90:THR:CG2 | 2.38 | 0.53 |
| 1:D:202:PRO:O | 1:D:204:PHE:N | 2.37 | 0.53 |
| 1:E:383:ALA:O | 1:E:384:ALA:HB3 | 2.08 | 0.53 |
| 1:J:218:PRO:HD2 | 1:J:320:ALA:O | 2.09 | 0.53 |
| 1:C:451:LEU:HD23 | 1:C:451:LEU:C | 2.28 | 0.53 |
| 1:G:201:SER:O | 1:G:202:PRO:O | 2.26 | 0.53 |
| 1:H:183:LEU:HD22 | 1:H:184:GLN:N | 2.24 | 0.53 |
| 1:H:235:PRO:CG | 1:H:310:GLU:HA | 2.33 | 0.53 |
| 1:K:200:LEU:HG | 1:K:276:VAL:HA | 1.91 | 0.53 |
| 1:E:413:ALA:H | 1:E:475:ASN:ND2 | 2.07 | 0.53 |
| 1:C:200:LEU:HG | 1:C:276:VAL:HA | 1.90 | 0.53 |
| 1:G:201:SER:C | 1:G:202:PRO:O | 2.46 | 0.53 |
| 1:L:319:GLN:HB3 | 1:L:336:VAL:HG21 | 1.91 | 0.53 |
| 1:L:349:ILE:HA | 1:L:352:GLN:HG3 | 1.90 | 0.53 |
| 1:N:496:PRO:HB2 | 1:N:499:VAL:HG13 | 1.91 | 0.53 |
| 1:B:10:ASN:ND2 | 4:B:1510:MPD:H51 | 2.24 | 0.52 |
| 1:D:183:LEU:O | 1:D:184:GLN:HG3 | 2.10 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:23:LEU:HD23 | 1:F:74:VAL:HG22 | 1.91 | 0.52 |
| 1:G:71:ALA:O | 1:G:75:LYS:HB2 | 2.10 | 0.52 |
| 1:L:258:ALA:O | 1:L:262:LEU:HG | 2.09 | 0.52 |
| 1:M:37:ASN:ND2 | 1:M:51:LYS:HG3 | 2.23 | 0.52 |
| 1:M:496:PRO:HB2 | 1:M:499:VAL:HG13 | 1.91 | 0.52 |
| 1:M:155:ASP:OD1 | 1:M:157:THR:HB | 2.09 | 0.52 |
| 1:M:173:GLY:O | 1:M:404:ARG:NH2 | 2.42 | 0.52 |
| 1:N:336:VAL:HG12 | 1:N:336:VAL:O | 2.10 | 0.52 |
| 1:C:18:ARG:HG2 | 1:C:67:GLU:CD | 2.29 | 0.52 |
| 1:E:359:ASP:HA | 1:E:362:ARG:HH12 | 1.73 | 0.52 |
| 1:G:191:GLU:O | 1:G:334:ASP:HA | 2.10 | 0.52 |
| 4:H:1516:MPD:HM1 | 1:I:518:GLU:HG3 | 1.90 | 0.52 |
| 1:H:155:ASP:OD1 | 1:H:157:THR:HB | 2.09 | 0.52 |
| 1:H:173:GLY:O | 1:H:404:ARG:NH2 | 2.42 | 0.52 |
| 1:I:349:ILE:HA | 1:I:352:GLN:HG3 | 1.90 | 0.52 |
| 1:J:114:MET:HB3 | 6:J:3085:HOH:O | 2.09 | 0.52 |
| 1:K:352:GLN:HB2 | 1:K:365:LEU:HD13 | 1.91 | 0.52 |
| 1:A:242:LYS:O | 1:A:244:GLY:N | 2.41 | 0.52 |
| 1:G:28:LYS:HD2 | 1:G:453:GLN:OE1 | 2.10 | 0.52 |
| 1:B:305:ILE:HB | 1:B:307:MET:HE3 | 1.91 | 0.52 |
| 1:J:336:VAL:HG12 | 1:J:336:VAL:O | 2.09 | 0.52 |
| 1:L:49:ILE:HD12 | 1:M:513:LEU:HD13 | 1.90 | 0.52 |
| 1:B:71:ALA:O | 1:B:75:LYS:HB2 | 2.10 | 0.52 |
| 1:C:109:ALA:HB2 | 1:K:109:ALA:HB2 | 1.92 | 0.52 |
| 1:C:71:ALA:O | 1:C:75:LYS:HB2 | 2.09 | 0.52 |
| 1:D:242:LYS:O | 1:D:243:ALA:HB3 | 2.09 | 0.52 |
| 1:J:72:GLN:OE1 | 1:J:75:LYS:HE3 | 2.10 | 0.52 |
| 1:C:273:VAL:HG12 | 1:C:274:ALA:N | 2.25 | 0.52 |
| 1:C:23:LEU:HD23 | 1:C:74:VAL:HG22 | 1.92 | 0.52 |
| 1:K:239:ALA:HB1 | 1:K:314:LEU:HG | 1.90 | 0.52 |
| 1:K:77:VAL:HG21 | 1:K:510:VAL:HB | 1.92 | 0.52 |
| 1:E:201:SER:O | 1:E:202:PRO:O | 2.28 | 0.52 |
| 1:G:242:LYS:O | 1:G:243:ALA:HB3 | 2.09 | 0.52 |
| 1:J:230:ILE:HD13 | 1:J:261:THR:HG21 | 1.92 | 0.52 |
| 1:A:71:ALA:O | 1:A:75:LYS:HB2 | 2.10 | 0.52 |
| 1:K:305:ILE:O | 1:K:305:ILE:HG22 | 2.10 | 0.52 |
| 1:K:336:VAL:HG12 | 1:K:336:VAL:O | 2.10 | 0.52 |
| 1:J:49:ILE:HD12 | 1:K:513:LEU:HD13 | 1.91 | 0.52 |
| 1:L:230:ILE:HD13 | 1:L:261:THR:HG21 | 1.91 | 0.52 |
| 1:N:130:GLU:HB3 | 1:N:422:VAL:HG22 | 1.92 | 0.52 |
| 1:A:230:ILE:HG22 | 1:A:257:GLU:OE2 | 2.10 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:460:GLU:O | 1:G:462:PRO:HD3 | 2.10 | 0.52 |
| 1:M:7:LYS:HG3 | 1:M:66:PHE:CZ | 2.43 | 0.52 |
| 1:B:85:ALA:HB1 | 1:B:499:VAL:HG12 | 1.92 | 0.51 |
| 1:D:194:GLN:O | 1:D:371:LYS:HE3 | 2.10 | 0.51 |
| 1:D:193:MET:HG3 | 1:D:371:LYS:HB3 | 1.92 | 0.51 |
| 1:F:174:VAL:HG12 | 1:F:376:VAL:HG13 | 1.91 | 0.51 |
| 1:H:38:VAL:HG13 | 1:I:519:CYS:HB3 | 1.91 | 0.51 |
| 1:I:230:ILE:HD13 | 1:I:261:THR:CG2 | 2.40 | 0.51 |
| 1:L:140:ASP:OD2 | 1:L:142:LYS:HB3 | 2.10 | 0.51 |
| 1:H:513:LEU:HD13 | 1:N:49:ILE:HD12 | 1.92 | 0.51 |
| 1:D:218:PRO:HD2 | 1:D:320:ALA:O | 2.10 | 0.51 |
| 1:F:413:ALA:H | 1:F:475:ASN:ND2 | 2.08 | 0.51 |
| 1:J:496:PRO:HB2 | 1:J:499:VAL:HG13 | 1.92 | 0.51 |
| 1:C:319:GLN:O | 1:C:336:VAL:HG23 | 2.11 | 0.51 |
| 1:J:70:GLY:HA2 | 1:J:73:MET:HE3 | 1.91 | 0.51 |
| 1:L:102:GLU:HB2 | 1:L:442:VAL:HG13 | 1.92 | 0.51 |
| 1:L:310:GLU:OE1 | 1:L:310:GLU:N | 2.43 | 0.51 |
| 1:L:7:LYS:HG3 | 1:L:66:PHE:CZ | 2.45 | 0.51 |
| 1:N:155:ASP:OD1 | 1:N:157:THR:HB | 2.10 | 0.51 |
| 1:N:191:GLU:O | 1:N:334:ASP:HA | 2.10 | 0.51 |
| 1:F:183:LEU:HA | 1:F:383:ALA:N | 2.26 | 0.51 |
| 1:H:191:GLU:OE1 | 1:H:342:ILE:HD13 | 2.11 | 0.51 |
| 1:K:194:GLN:O | 1:K:371:LYS:HE3 | 2.10 | 0.51 |
| 1:L:130:GLU:HB3 | 1:L:422:VAL:HG22 | 1.92 | 0.51 |
| 1:M:270:ILE:O | 1:M:271:VAL:HB | 2.09 | 0.51 |
| 1:M:413:ALA:H | 1:M:475:ASN:HD22 | 1.58 | 0.51 |
| 1:A:176:THR:HG21 | 1:A:333:ILE:HD13 | 1.93 | 0.51 |
| 1:B:219:PHE:HB3 | 1:B:317:LEU:HD23 | 1.91 | 0.51 |
| 1:B:199:TYR:CZ | 1:B:327:LYS:HA | 2.46 | 0.51 |
| 1:E:362:ARG:HG2 | 1:E:366:GLN:NE2 | 2.26 | 0.51 |
| 1:I:102:GLU:HB2 | 1:I:442:VAL:HG13 | 1.92 | 0.51 |
| 1:C:220:ILE:HD12 | 1:C:296:THR:HG21 | 1.92 | 0.51 |
| 1:D:201:SER:O | 1:D:202:PRO:O | 2.28 | 0.51 |
| 1:D:242:LYS:C | 1:D:244:GLY:N | 2.64 | 0.51 |
| 1:F:263:VAL:O | 1:F:267:MET:HB2 | 2.11 | 0.51 |
| 1:H:193:MET:HG2 | 1:H:194:GLN:N | 2.25 | 0.51 |
| 1:L:219:PHE:O | 1:L:247:LEU:HD12 | 2.10 | 0.51 |
| 1:C:85:ALA:HB1 | 1:C:499:VAL:HG12 | 1.92 | 0.51 |
| 1:E:201:SER:C | 1:E:202:PRO:O | 2.49 | 0.51 |
| 1:F:193:MET:HG3 | 1:F:371:LYS:HB3 | 1.93 | 0.51 |
| 1:G:146:GLN:NE2 | 4:G:1509:MPD:H4 | 2.26 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:102:GLU:HB2 | 1:K:442:VAL:HG13 | 1.91 | 0.51 |
| 1:B:191:GLU:O | 1:B:334:ASP:HA | 2.11 | 0.51 |
| 1:I:155:ASP:OD1 | 1:I:157:THR:HB | 2.11 | 0.51 |
| 1:I:413:ALA:CB | 1:I:475:ASN:HD22 | 2.23 | 0.51 |
| 1:J:349:ILE:HA | 1:J:352:GLN:HG3 | 1.93 | 0.51 |
| 1:L:193:MET:CE | 1:L:292:ILE:HG12 | 2.41 | 0.51 |
| 1:M:230:ILE:HG21 | 1:M:261:THR:HG21 | 1.93 | 0.51 |
| 1:A:201:SER:O | 1:A:202:PRO:O | 2.29 | 0.51 |
| 1:H:221:LEU:HD23 | 1:H:249:ILE:HD12 | 1.92 | 0.51 |
| 1:J:102:GLU:HB2 | 1:J:442:VAL:HG13 | 1.93 | 0.51 |
| 1:E:247:LEU:HB3 | 1:E:273:VAL:HG22 | 1.92 | 0.50 |
| 1:J:118:ARG:NH2 | 6:J:3085:HOH:O | 2.41 | 0.50 |
| 1:F:305:ILE:HG22 | 1:F:305:ILE:O | 2.11 | 0.50 |
| 1:K:230:ILE:HD13 | 1:K:261:THR:HG21 | 1.92 | 0.50 |
| 1:K:463:SER:O | 1:K:467:ASN:HB2 | 2.11 | 0.50 |
| 1:L:31:LEU:HD13 | 1:L:90:THR:CG2 | 2.41 | 0.50 |
| 1:B:166:MET:CE | 1:B:171:LYS:HA | 2.41 | 0.50 |
| 1:C:314:LEU:HD23 | 1:C:317:LEU:HD22 | 1.92 | 0.50 |
| 1:D:451:LEU:C | 1:D:451:LEU:HD23 | 2.32 | 0.50 |
| 1:I:191:GLU:O | 1:I:334:ASP:HA | 2.11 | 0.50 |
| 1:I:460:GLU:O | 1:I:462:PRO:HD3 | 2.11 | 0.50 |
| 1:N:223:ALA:O | 1:N:251:ALA:HA | 2.12 | 0.50 |
| 1:B:230:ILE:HD13 | 1:B:261:THR:HG21 | 1.94 | 0.50 |
| 1:B:270:ILE:HA | 1:C:231:ARG:NH1 | 2.26 | 0.50 |
| 1:H:247:LEU:CD2 | 1:H:249:ILE:HD11 | 2.41 | 0.50 |
| 1:J:259:LEU:O | 1:J:263:VAL:HG23 | 2.12 | 0.50 |
| 1:N:248:LEU:HD13 | 1:N:325:ILE:HD11 | 1.94 | 0.50 |
| 1:D:263:VAL:O | 1:D:267:MET:HB2 | 2.12 | 0.50 |
| 1:E:264:VAL:HG12 | 1:E:265:ASN:N | 2.27 | 0.50 |
| 1:F:259:LEU:O | 1:F:263:VAL:HG23 | 2.11 | 0.50 |
| 1:F:18:ARG:HG2 | 1:F:67:GLU:CD | 2.32 | 0.50 |
| 1:J:7:LYS:HG3 | 1:J:66:PHE:CZ | 2.47 | 0.50 |
| 1:K:155:ASP:OD1 | 1:K:157:THR:HB | 2.11 | 0.50 |
| 1:L:193:MET:HG3 | 1:L:371:LYS:HB3 | 1.94 | 0.50 |
| 1:M:193:MET:HG3 | 1:M:371:LYS:HB3 | 1.92 | 0.50 |
| 1:N:230:ILE:HG21 | 1:N:261:THR:HG21 | 1.94 | 0.50 |
| 1:C:230:ILE:HG22 | 1:C:257:GLU:OE2 | 2.11 | 0.50 |
| 1:I:218:PRO:CB | 1:I:246:PRO:HG2 | 2.41 | 0.50 |
| 1:M:191:GLU:O | 1:M:334:ASP:HA | 2.12 | 0.50 |
| 1:M:37:ASN:HD21 | 1:M:51:LYS:HE3 | 1.75 | 0.50 |
| 1:E:270:ILE:O | 1:E:271:VAL:HB | 2.12 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:183:LEU:O | 1:G:184:GLN:HG3 | 2.12 | 0.50 |
| 1:G:242:LYS:O | 1:G:244:GLY:N | 2.44 | 0.50 |
| 1:G:461:GLU:HB3 | 6:G:3186:HOH:O | 2.10 | 0.50 |
| 1:H:39:VAL:HG12 | 1:I:69:MET:HE2 | 1.92 | 0.50 |
| 1:H:83:ASP:OD2 | 1:H:327:LYS:CD | 2.60 | 0.50 |
| 1:I:228:SER:O | 1:I:257:GLU:HB3 | 2.11 | 0.50 |
| 1:K:173:GLY:O | 1:K:404:ARG:NH2 | 2.44 | 0.50 |
| 1:M:269:GLY:CA | 1:N:229:ASN:CG | 2.79 | 0.50 |
| 1:N:201:SER:O | 1:N:202:PRO:O | 2.30 | 0.50 |
| 1:N:173:GLY:O | 1:N:404:ARG:NH2 | 2.45 | 0.50 |
| 1:N:72:GLN:OE1 | 1:N:75:LYS:HE3 | 2.10 | 0.50 |
| 1:A:183:LEU:O | 1:A:184:GLN:HG3 | 2.12 | 0.50 |
| 1:A:201:SER:C | 1:A:202:PRO:O | 2.50 | 0.50 |
| 1:J:77:VAL:HG21 | 1:J:510:VAL:HB | 1.93 | 0.50 |
| 1:A:202:PRO:O | 1:A:204:PHE:N | 2.38 | 0.50 |
| 1:B:104:LEU:HB3 | 4:B:1510:MPD:H31 | 1.94 | 0.50 |
| 1:D:413:ALA:H | 1:D:475:ASN:ND2 | 2.10 | 0.50 |
| 1:G:413:ALA:CB | 1:G:417:VAL:HG22 | 2.42 | 0.50 |
| 1:G:23:LEU:CD2 | 1:G:74:VAL:HG22 | 2.41 | 0.50 |
| 1:I:130:GLU:HB3 | 1:I:422:VAL:HG22 | 1.94 | 0.50 |
| 1:L:229:ASN:HA | 1:L:257:GLU:OE1 | 2.12 | 0.50 |
| 1:M:153:ASN:O | 1:M:154:SER:HB2 | 2.12 | 0.50 |
| 1:M:381:VAL:HG21 | 1:M:393:LYS:HA | 1.93 | 0.50 |
| 1:M:413:ALA:N | 1:M:475:ASN:HD22 | 2.10 | 0.50 |
| 1:B:183:LEU:HA | 1:B:383:ALA:N | 2.27 | 0.49 |
| 1:G:346:VAL:O | 1:G:350:ARG:HB2 | 2.12 | 0.49 |
| 1:H:349:ILE:O | 1:H:353:ILE:HG13 | 2.11 | 0.49 |
| 1:I:77:VAL:HG21 | 1:I:510:VAL:HB | 1.94 | 0.49 |
| 1:K:310:GLU:OE1 | 1:K:310:GLU:N | 2.44 | 0.49 |
| 1:K:287:ALA:HB1 | 1:K:368:ARG:NH1 | 2.27 | 0.49 |
| 1:L:239:ALA:HB1 | 1:L:314:LEU:HG | 1.93 | 0.49 |
| 1:M:140:ASP:OD2 | 1:M:142:LYS:HB3 | 2.12 | 0.49 |
| 1:N:263:VAL:O | 1:N:267:MET:HB2 | 2.12 | 0.49 |
| 1:C:225:LYS:NZ | 1:C:232:GLU:OE2 | 2.46 | 0.49 |
| 1:G:413:ALA:H | 1:G:475:ASN:ND2 | 2.08 | 0.49 |
| 1:L:202:PRO:O | 1:L:204:PHE:N | 2.43 | 0.49 |
| 1:L:202:PRO:O | 1:L:203:TYR:HB2 | 2.12 | 0.49 |
| 1:L:230:ILE:HB | 1:L:258:ALA:HA | 1.94 | 0.49 |
| 1:N:28:LYS:HD2 | 1:N:453:GLN:OE1 | 2.13 | 0.49 |
| 1:D:178:GLU:HA | 1:D:393:LYS:HE2 | 1.94 | 0.49 |
| 1:F:178:GLU:HA | 1:F:393:LYS:HE2 | 1.93 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:49:ILE:HD12 | 1:F:513:LEU:HD13 | 1.94 | 0.49 |
| 1:I:26:ALA:HA | 1:J:8:PHE:HE1 | 1.77 | 0.49 |
| 1:J:37:ASN:ND2 | 1:J:51:LYS:HG3 | 2.27 | 0.49 |
| 1:K:247:LEU:HD21 | 1:K:249:ILE:HD11 | 1.95 | 0.49 |
| 1:M:336:VAL:O | 1:M:336:VAL:HG12 | 2.11 | 0.49 |
| 1:M:72:GLN:OE1 | 1:M:75:LYS:HE3 | 2.12 | 0.49 |
| 1:D:273:VAL:HG12 | 1:D:274:ALA:N | 2.27 | 0.49 |
| 1:D:40:LEU:HD13 | 1:D:59:GLU:HG3 | 1.93 | 0.49 |
| 1:H:352:GLN:HB2 | 1:H:365:LEU:HD13 | 1.94 | 0.49 |
| 1:H:37:ASN:ND2 | 1:H:51:LYS:HG3 | 2.27 | 0.49 |
| 1:K:383:ALA:HB3 | 1:K:389:MET:HB2 | 1.94 | 0.49 |
| 1:L:216:GLU:C | 1:L:218:PRO:HD3 | 2.31 | 0.49 |
| 1:L:305:ILE:HD12 | 1:L:307:MET:HE2 | 1.93 | 0.49 |
| 1:M:102:GLU:HB2 | 1:M:442:VAL:HG13 | 1.94 | 0.49 |
| 1:N:218:PRO:CB | 1:N:246:PRO:HG2 | 2.42 | 0.49 |
| 1:B:413:ALA:H | 1:B:475:ASN:ND2 | 2.11 | 0.49 |
| 1:C:413:ALA:CB | 1:C:475:ASN:HD22 | 2.25 | 0.49 |
| 1:D:193:MET:HE1 | 1:D:292:ILE:HG12 | 1.94 | 0.49 |
| 1:D:200:LEU:HG | 1:D:276:VAL:HA | 1.95 | 0.49 |
| 1:E:284:ARG:NH1 | 1:E:364:LYS:HD2 | 2.27 | 0.49 |
| 1:G:178:GLU:HA | 1:G:393:LYS:HE2 | 1.94 | 0.49 |
| 1:G:18:ARG:HG2 | 1:G:67:GLU:CD | 2.33 | 0.49 |
| 1:K:270:ILE:O | 1:K:271:VAL:HB | 2.12 | 0.49 |
| 1:K:496:PRO:HB2 | 1:K:499:VAL:HG13 | 1.94 | 0.49 |
| 1:L:218:PRO:CB | 1:L:246:PRO:HG2 | 2.43 | 0.49 |
| 1:L:313:THR:O | 1:L:317:LEU:HD13 | 2.13 | 0.49 |
| 1:N:200:LEU:HG | 1:N:276:VAL:HA | 1.94 | 0.49 |
| 1:D:183:LEU:HA | 1:D:383:ALA:N | 2.28 | 0.49 |
| 1:D:18:ARG:HG2 | 1:D:67:GLU:CD | 2.33 | 0.49 |
| 1:E:178:GLU:HA | 1:E:393:LYS:HE2 | 1.95 | 0.49 |
| 1:I:217:SER:N | 1:I:218:PRO:CD | 2.75 | 0.49 |
| 1:L:16:MET:O | 1:L:20:VAL:HG13 | 2.12 | 0.49 |
| 1:M:221:LEU:HD11 | 1:M:301:ILE:HD12 | 1.94 | 0.49 |
| 1:M:77:VAL:HG21 | 1:M:510:VAL:HB | 1.95 | 0.49 |
| 1:C:166:MET:CE | 1:C:171:LYS:HA | 2.42 | 0.49 |
| 1:E:183:LEU:HA | 1:E:383:ALA:N | 2.27 | 0.49 |
| 1:F:183:LEU:O | 1:F:184:GLN:HG3 | 2.12 | 0.49 |
| 1:G:247:LEU:HD21 | 1:G:249:ILE:HD11 | 1.93 | 0.49 |
| 1:I:263:VAL:O | 1:I:267:MET:HB2 | 2.13 | 0.49 |
| 1:K:248:LEU:HD13 | 1:K:325:ILE:HD11 | 1.95 | 0.49 |
| 1:M:248:LEU:HD13 | 1:M:325:ILE:HD11 | 1.94 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:263:VAL:O | 1:M:267:MET:HB2 | 2.12 | 0.49 |
| 1:N:219:PHE:HB3 | 1:N:317:LEU:HD23 | 1.95 | 0.49 |
| 1:F:284:ARG:NH1 | 1:F:364:LYS:HD2 | 2.28 | 0.49 |
| 1:H:314:LEU:HA | 1:H:317:LEU:HD22 | 1.95 | 0.49 |
| 1:L:160:LYS:O | 1:L:164:GLU:HG3 | 2.12 | 0.49 |
| 1:L:34:LYS:HE2 | 1:M:118:ARG:HH22 | 1.77 | 0.49 |
| 1:N:259:LEU:O | 1:N:263:VAL:HG23 | 2.12 | 0.49 |
| 1:N:460:GLU:O | 1:N:462:PRO:HD3 | 2.13 | 0.49 |
| 1:A:430:ARG:NH2 | 6:A:3018:HOH:O | 2.45 | 0.49 |
| 1:B:23:LEU:HD23 | 1:B:74:VAL:HG22 | 1.94 | 0.49 |
| 1:C:183:LEU:O | 1:C:184:GLN:HG3 | 2.13 | 0.49 |
| 1:H:77:VAL:HG21 | 1:H:510:VAL:HB | 1.95 | 0.49 |
| 1:K:272:LYS:HZ3 | 1:L:229:ASN:ND2 | 2.04 | 0.49 |
| 1:K:68:ASN:O | 1:K:72:GLN:HG2 | 2.13 | 0.49 |
| 1:L:221:LEU:HB3 | 1:L:249:ILE:HD13 | 1.94 | 0.49 |
| 1:L:336:VAL:HG12 | 1:L:336:VAL:O | 2.13 | 0.49 |
| 1:L:383:ALA:HB3 | 1:L:389:MET:HB2 | 1.93 | 0.49 |
| 1:M:305:ILE:O | 1:M:305:ILE:HG22 | 2.12 | 0.49 |
| 1:D:496:PRO:HB2 | 1:D:499:VAL:HG13 | 1.95 | 0.49 |
| 1:E:413:ALA:HB2 | 1:E:475:ASN:HD22 | 1.78 | 0.49 |
| 1:H:102:GLU:HB2 | 1:H:442:VAL:HG13 | 1.94 | 0.49 |
| 1:H:68:ASN:O | 1:H:72:GLN:HG2 | 2.13 | 0.49 |
| 1:K:259:LEU:O | 1:K:263:VAL:HG23 | 2.13 | 0.49 |
| 1:L:302:SER:H | 1:L:307:MET:CE | 2.26 | 0.49 |
| 1:N:102:GLU:HB2 | 1:N:442:VAL:HG13 | 1.95 | 0.49 |
| 1:N:193:MET:CE | 1:N:292:ILE:HG12 | 2.43 | 0.49 |
| 1:C:49:ILE:HD12 | 1:D:513:LEU:HD13 | 1.95 | 0.48 |
| 1:D:413:ALA:CB | 1:D:417:VAL:HG22 | 2.43 | 0.48 |
| 1:E:242:LYS:O | 1:E:243:ALA:HB3 | 2.12 | 0.48 |
| 1:F:273:VAL:HG12 | 1:F:274:ALA:N | 2.28 | 0.48 |
| 1:F:413:ALA:HB2 | 1:F:475:ASN:HD22 | 1.78 | 0.48 |
| 1:F:83:ASP:OD2 | 1:F:327:LYS:HD3 | 2.12 | 0.48 |
| 1:G:413:ALA:HB2 | 1:G:475:ASN:HD22 | 1.77 | 0.48 |
| 1:H:463:SER:O | 1:H:467:ASN:HB2 | 2.12 | 0.48 |
| 1:I:230:ILE:HD13 | 1:I:261:THR:HG21 | 1.93 | 0.48 |
| 1:J:310:GLU:N | 1:J:310:GLU:OE1 | 2.43 | 0.48 |
| 1:L:132:LYS:O | 1:L:135:SER:HB3 | 2.13 | 0.48 |
| 1:N:202:PRO:C | 1:N:204:PHE:H | 2.16 | 0.48 |
| 1:A:383:ALA:HB3 | 1:A:389:MET:HB2 | 1.95 | 0.48 |
| 1:A:40:LEU:HD13 | 1:A:59:GLU:HG3 | 1.95 | 0.48 |
| 1:B:183:LEU:O | 1:B:184:GLN:HG3 | 2.13 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:266:THR:CG2 | 1:C:273:VAL:H | 2.26 | 0.48 |
| 1:E:18:ARG:HG2 | 1:E:67:GLU:CD | 2.32 | 0.48 |
| 1:F:266:THR:CG2 | 1:F:273:VAL:HB | 2.43 | 0.48 |
| 1:H:457:ASN:OD1 | 4:H:1516:MPD:H13 | 2.13 | 0.48 |
| 1:J:319:GLN:HB3 | 1:J:336:VAL:CG2 | 2.43 | 0.48 |
| 1:L:463:SER:O | 1:L:467:ASN:HB2 | 2.13 | 0.48 |
| 1:E:182:GLY:O | 1:E:183:LEU:C | 2.52 | 0.48 |
| 1:F:85:ALA:HB1 | 1:F:499:VAL:HG12 | 1.95 | 0.48 |
| 1:I:70:GLY:HA2 | 1:I:73:MET:HE3 | 1.95 | 0.48 |
| 1:J:57:ALA:O | 1:J:75:LYS:HD2 | 2.13 | 0.48 |
| 1:L:221:LEU:HD11 | 1:L:301:ILE:HD12 | 1.96 | 0.48 |
| 1:M:479:ASN:ND2 | 1:M:493:ILE:HD11 | 2.28 | 0.48 |
| 1:A:381:VAL:HG21 | 1:A:393:LYS:HA | 1.95 | 0.48 |
| 1:D:247:LEU:CD2 | 1:D:249:ILE:HD11 | 2.43 | 0.48 |
| 1:H:217:SER:N | 1:H:218:PRO:CD | 2.76 | 0.48 |
| 1:I:153:ASN:O | 1:I:154:SER:HB2 | 2.14 | 0.48 |
| 1:J:130:GLU:HB3 | 1:J:422:VAL:HG22 | 1.96 | 0.48 |
| 1:I:272:LYS:NZ | 1:J:228:SER:HB3 | 2.29 | 0.48 |
| 1:A:303:GLU:O | 1:A:306:GLY:N | 2.41 | 0.48 |
| 1:B:303:GLU:O | 1:B:306:GLY:N | 2.40 | 0.48 |
| 1:D:191:GLU:O | 1:D:334:ASP:HA | 2.13 | 0.48 |
| 1:E:183:LEU:O | 1:E:184:GLN:HG3 | 2.14 | 0.48 |
| 1:F:173:GLY:O | 1:F:404:ARG:NH2 | 2.46 | 0.48 |
| 1:I:314:LEU:HA | 1:I:317:LEU:HD22 | 1.94 | 0.48 |
| 1:I:496:PRO:HB2 | 1:I:499:VAL:HG13 | 1.94 | 0.48 |
| 1:L:305:ILE:HG22 | 1:L:305:ILE:O | 2.12 | 0.48 |
| 1:L:344:GLY:O | 1:L:347:ALA:HB3 | 2.14 | 0.48 |
| 1:N:222:LEU:HD11 | 1:N:293:ALA:HA | 1.96 | 0.48 |
| 1:N:57:ALA:O | 1:N:75:LYS:HD2 | 2.13 | 0.48 |
| 1:B:18:ARG:HG2 | 1:B:67:GLU:CD | 2.34 | 0.48 |
| 1:C:217:SER:N | 1:C:218:PRO:CD | 2.77 | 0.48 |
| 1:C:242:LYS:C | 1:C:244:GLY:N | 2.64 | 0.48 |
| 1:D:16:MET:HB3 | 1:D:514:MET:HE1 | 1.96 | 0.48 |
| 1:F:71:ALA:O | 1:F:75:LYS:HB2 | 2.14 | 0.48 |
| 1:J:430:ARG:HD2 | 6:J:3082:HOH:O | 2.13 | 0.48 |
| 1:L:153:ASN:O | 1:L:154:SER:HB2 | 2.13 | 0.48 |
| 1:L:381:VAL:HG21 | 1:L:393:LYS:HA | 1.95 | 0.48 |
| 1:M:269:GLY:HA2 | 1:N:229:ASN:ND2 | 2.28 | 0.48 |
| 1:A:166:MET:CE | 1:A:171:LYS:HA | 2.44 | 0.48 |
| 1:C:178:GLU:HA | 1:C:393:LYS:HE2 | 1.95 | 0.48 |
| 1:D:23:LEU:CD2 | 1:D:74:VAL:HG22 | 2.44 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:202:PRO:O | 1:E:203:TYR:HB2 | 2.12 | 0.48 |
| 1:E:269:GLY:CA | 1:F:229:ASN:ND2 | 2.76 | 0.48 |
| 1:E:215:LEU:HB2 | 1:E:323:VAL:HG22 | 1.96 | 0.48 |
| 1:G:266:THR:CG2 | 1:G:273:VAL:HB | 2.44 | 0.48 |
| 1:I:193:MET:HG2 | 1:I:194:GLN:N | 2.28 | 0.48 |
| 1:J:193:MET:HG2 | 1:J:194:GLN:N | 2.28 | 0.48 |
| 1:K:349:ILE:O | 1:K:353:ILE:HG13 | 2.13 | 0.48 |
| 1:L:144:ILE:HG23 | 1:L:403:THR:CG2 | 2.44 | 0.48 |
| 1:N:221:LEU:HD23 | 1:N:249:ILE:HD12 | 1.95 | 0.48 |
| 1:B:305:ILE:O | 1:B:305:ILE:HG22 | 2.12 | 0.48 |
| 1:F:383:ALA:HB3 | 1:F:389:MET:HB2 | 1.95 | 0.48 |
| 1:F:478:TYR:CE2 | 1:F:480:ALA:HA | 2.49 | 0.48 |
| 1:H:193:MET:CE | 1:H:292:ILE:HG12 | 2.44 | 0.48 |
| 1:H:336:VAL:O | 1:H:336:VAL:HG12 | 2.13 | 0.48 |
| 1:H:70:GLY:HA2 | 1:H:73:MET:HE3 | 1.96 | 0.48 |
| 1:I:287:ALA:HB1 | 1:I:368:ARG:NH1 | 2.28 | 0.48 |
| 1:L:220:ILE:HD12 | 1:L:296:THR:HG21 | 1.95 | 0.48 |
| 1:L:270:ILE:O | 1:L:271:VAL:HB | 2.14 | 0.48 |
| 1:N:217:SER:N | 1:N:218:PRO:CD | 2.76 | 0.48 |
| 1:D:201:SER:C | 1:D:202:PRO:O | 2.50 | 0.48 |
| 1:F:197:ARG:HD2 | 1:F:277:LYS:HB2 | 1.96 | 0.48 |
| 1:G:242:LYS:C | 1:G:244:GLY:N | 2.67 | 0.48 |
| 1:H:134:LEU:HD11 | 1:H:475:ASN:ND2 | 2.28 | 0.48 |
| 1:I:118:ARG:HG3 | 6:I:3052:HOH:O | 2.14 | 0.48 |
| 1:I:5:ASP:HB2 | 1:I:524:LEU:CD1 | 2.44 | 0.48 |
| 1:J:478:TYR:CE2 | 1:J:480:ALA:HA | 2.49 | 0.48 |
| 1:K:217:SER:N | 1:K:218:PRO:CD | 2.76 | 0.48 |
| 1:M:451:LEU:HD23 | 1:M:455:VAL:HG23 | 1.96 | 0.48 |
| 1:A:496:PRO:HB2 | 1:A:499:VAL:HG13 | 1.96 | 0.48 |
| 1:D:288:MET:HG2 | 1:D:368:ARG:HD3 | 1.94 | 0.48 |
| 1:D:359:ASP:HA | 1:D:362:ARG:HH12 | 1.78 | 0.48 |
| 1:E:28:LYS:HD2 | 1:E:453:GLN:OE1 | 2.13 | 0.48 |
| 1:H:146:GLN:O | 1:H:150:ILE:HG13 | 2.14 | 0.48 |
| 1:H:231:ARG:NH1 | 1:N:241:ALA:HB3 | 2.29 | 0.48 |
| 1:H:460:GLU:O | 1:H:462:PRO:HD3 | 2.13 | 0.48 |
| 1:N:463:SER:O | 1:N:467:ASN:HB2 | 2.14 | 0.48 |
| 1:B:217:SER:N | 1:B:218:PRO:CD | 2.77 | 0.47 |
| 1:C:455:VAL:CG1 | 1:C:460:GLU:HB2 | 2.44 | 0.47 |
| 1:G:266:THR:HG21 | 1:G:273:VAL:HB | 1.96 | 0.47 |
| 1:H:200:LEU:HG | 1:H:276:VAL:HA | 1.96 | 0.47 |
| 1:I:37:ASN:ND2 | 1:I:51:LYS:HG3 | 2.28 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:272:LYS:NZ | 1:K:228:SER:HB3 | 2.29 | 0.47 |
| 1:J:342:ILE:O | 1:J:346:VAL:HG23 | 2.14 | 0.47 |
| 1:J:438:VAL:O | 1:J:442:VAL:HG23 | 2.14 | 0.47 |
| 4:K:1506:MPD:H53 | 6:K:3099:HOH:O | 2.14 | 0.47 |
| 1:M:345:ARG:HD3 | 6:M:3113:HOH:O | 2.14 | 0.47 |
| 1:N:5:ASP:HB2 | 1:N:524:LEU:CD1 | 2.44 | 0.47 |
| 1:A:18:ARG:HG2 | 1:A:67:GLU:CD | 2.35 | 0.47 |
| 1:D:413:ALA:HB2 | 1:D:475:ASN:HD22 | 1.79 | 0.47 |
| 1:F:182:GLY:O | 1:F:183:LEU:C | 2.52 | 0.47 |
| 1:H:31:LEU:HD13 | 1:H:90:THR:HG22 | 1.96 | 0.47 |
| 1:K:37:ASN:ND2 | 1:K:51:LYS:HG3 | 2.29 | 0.47 |
| 1:M:199:TYR:C | 1:M:201:SER:H | 2.18 | 0.47 |
| 1:M:217:SER:N | 1:M:218:PRO:CD | 2.77 | 0.47 |
| 1:N:7:LYS:HG3 | 1:N:66:PHE:CZ | 2.49 | 0.47 |
| 1:F:215:LEU:HB2 | 1:F:323:VAL:HG22 | 1.96 | 0.47 |
| 1:F:266:THR:HG21 | 1:F:273:VAL:HB | 1.95 | 0.47 |
| 1:G:259:LEU:O | 1:G:263:VAL:HG23 | 2.14 | 0.47 |
| 1:H:228:SER:HB3 | 1:N:272:LYS:HZ1 | 1.78 | 0.47 |
| 1:N:222:LEU:CD1 | 1:N:293:ALA:HA | 2.44 | 0.47 |
| 1:A:242:LYS:C | 1:A:244:GLY:N | 2.66 | 0.47 |
| 1:A:268:ARG:O | 1:A:270:ILE:HG13 | 2.14 | 0.47 |
| 1:C:305:ILE:O | 1:C:305:ILE:HG22 | 2.12 | 0.47 |
| 1:C:83:ASP:OD2 | 1:C:327:LYS:HD3 | 2.14 | 0.47 |
| 1:D:220:ILE:HD12 | 1:D:296:THR:HG21 | 1.96 | 0.47 |
| 1:E:217:SER:N | 1:E:218:PRO:HD3 | 2.30 | 0.47 |
| 1:A:513:LEU:HD13 | 1:G:49:ILE:CD1 | 2.45 | 0.47 |
| 1:H:130:GLU:HB3 | 1:H:422:VAL:HG22 | 1.96 | 0.47 |
| 1:M:218:PRO:CB | 1:M:246:PRO:HG2 | 2.41 | 0.47 |
| 1:A:28:LYS:HD2 | 1:A:453:GLN:OE1 | 2.15 | 0.47 |
| 1:B:182:GLY:O | 1:B:183:LEU:C | 2.53 | 0.47 |
| 1:B:353:ILE:HD13 | 1:B:366:GLN:HG3 | 1.97 | 0.47 |
| 1:B:28:LYS:HD2 | 1:B:453:GLN:OE1 | 2.15 | 0.47 |
| 1:C:349:ILE:O | 1:C:353:ILE:HG13 | 2.15 | 0.47 |
| 1:E:369:VAL:HG23 | 1:E:370:ALA:N | 2.29 | 0.47 |
| 1:I:7:LYS:HG3 | 1:I:66:PHE:CZ | 2.49 | 0.47 |
| 1:I:272:LYS:HZ1 | 1:J:228:SER:HB3 | 1.80 | 0.47 |
| 1:B:230:ILE:HG22 | 1:B:257:GLU:OE2 | 2.14 | 0.47 |
| 1:C:259:LEU:O | 1:C:263:VAL:HG23 | 2.14 | 0.47 |
| 1:H:39:VAL:CG1 | 1:I:69:MET:HE2 | 2.45 | 0.47 |
| 1:I:57:ALA:O | 1:I:75:LYS:HD2 | 2.15 | 0.47 |
| 1:J:153:ASN:O | 1:J:154:SER:HB2 | 2.13 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:68:ASN:O | 1:J:72:GLN:HG2 | 2.14 | 0.47 |
| 1:K:186:GLU:HB2 | 1:K:380:LYS:HB2 | 1.97 | 0.47 |
| 1:K:202:PRO:C | 1:K:204:PHE:H | 2.17 | 0.47 |
| 1:M:349:ILE:O | 1:M:353:ILE:HG13 | 2.14 | 0.47 |
| 1:N:220:ILE:HD12 | 1:N:296:THR:HG21 | 1.96 | 0.47 |
| 1:A:359:ASP:HA | 1:A:362:ARG:HH12 | 1.79 | 0.47 |
| 1:D:472:GLY:HA3 | 1:D:476:TYR:CD2 | 2.49 | 0.47 |
| 1:E:40:LEU:HD13 | 1:E:59:GLU:HG3 | 1.96 | 0.47 |
| 1:G:305:ILE:O | 1:G:305:ILE:HG22 | 2.15 | 0.47 |
| 1:I:247:LEU:HD21 | 1:I:249:ILE:HD11 | 1.97 | 0.47 |
| 1:M:183:LEU:HD22 | 1:M:184:GLN:N | 2.30 | 0.47 |
| 1:F:191:GLU:O | 1:F:334:ASP:HA | 2.15 | 0.47 |
| 1:F:217:SER:N | 1:F:218:PRO:CD | 2.77 | 0.47 |
| 1:I:354:GLU:C | 1:I:356:ALA:H | 2.17 | 0.47 |
| 1:J:152:ALA:O | 1:J:153:ASN:HB3 | 2.15 | 0.47 |
| 1:A:413:ALA:CB | 1:A:475:ASN:HD22 | 2.27 | 0.47 |
| 1:E:200:LEU:HG | 1:E:276:VAL:HA | 1.95 | 0.47 |
| 1:E:217:SER:N | 1:E:218:PRO:CD | 2.77 | 0.47 |
| 1:E:263:VAL:O | 1:E:267:MET:HB2 | 2.15 | 0.47 |
| 1:L:460:GLU:O | 1:L:462:PRO:HD3 | 2.15 | 0.47 |
| 1:L:478:TYR:CE2 | 1:L:480:ALA:HA | 2.50 | 0.47 |
| 1:M:247:LEU:HD21 | 1:M:249:ILE:HD11 | 1.97 | 0.47 |
| 1:N:183:LEU:HD22 | 1:N:184:GLN:H | 1.80 | 0.47 |
| 1:B:263:VAL:O | 1:B:267:MET:HB2 | 2.15 | 0.47 |
| 1:C:383:ALA:O | 1:C:384:ALA:CB | 2.59 | 0.47 |
| 1:C:472:GLY:HA3 | 1:C:476:TYR:CD2 | 2.50 | 0.47 |
| 1:E:524:LEU:HD12 | 1:E:524:LEU:HA | 1.75 | 0.47 |
| 1:K:144:ILE:HG23 | 1:K:403:THR:CG2 | 2.44 | 0.47 |
| 1:K:220:ILE:CD1 | 1:K:296:THR:HG21 | 2.44 | 0.47 |
| 1:K:429:LEU:HG | 1:K:440:ILE:HD13 | 1.96 | 0.47 |
| 1:L:358:SER:HB3 | 1:L:361:ASP:OD1 | 2.15 | 0.47 |
| 1:C:28:LYS:HD2 | 1:C:453:GLN:OE1 | 2.14 | 0.47 |
| 1:E:23:LEU:CD2 | 1:E:74:VAL:HG22 | 2.45 | 0.47 |
| 1:E:386:GLU:HB2 | 1:F:281:PHE:HB3 | 1.97 | 0.47 |
| 1:G:202:PRO:C | 1:G:204:PHE:H | 2.16 | 0.47 |
| 1:H:385:THR:OG1 | 1:H:388:GLU:HG3 | 2.15 | 0.47 |
| 1:I:217:SER:N | 1:I:218:PRO:HD3 | 2.30 | 0.47 |
| 1:K:38:VAL:HG13 | 1:L:519:CYS:HB3 | 1.95 | 0.47 |
| 1:N:266:THR:HG21 | 1:N:273:VAL:HB | 1.97 | 0.47 |
| 1:A:326:ASN:HB3 | 1:A:327:LYS:H | 1.61 | 0.46 |
| 1:D:217:SER:N | 1:D:218:PRO:CD | 2.77 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:166:MET:CE | 1:E:171:LYS:HA | 2.44 | 0.46 |
| 1:E:269:GLY:HA3 | 1:F:229:ASN:ND2 | 2.30 | 0.46 |
| 1:E:472:GLY:HA3 | 1:E:476:TYR:CD2 | 2.49 | 0.46 |
| 1:G:344:GLY:O | 1:G:347:ALA:HB3 | 2.14 | 0.46 |
| 1:K:193:MET:HE1 | 1:K:292:ILE:HG12 | 1.97 | 0.46 |
| 1:K:193:MET:HG2 | 1:K:194:GLN:N | 2.29 | 0.46 |
| 1:A:183:LEU:HA | 1:A:383:ALA:N | 2.30 | 0.46 |
| 1:A:362:ARG:HG2 | 1:A:366:GLN:NE2 | 2.31 | 0.46 |
| 1:C:193:MET:HE1 | 1:C:292:ILE:HG12 | 1.96 | 0.46 |
| 1:F:202:PRO:C | 1:F:204:PHE:H | 2.18 | 0.46 |
| 1:L:319:GLN:O | 1:L:336:VAL:HG23 | 2.16 | 0.46 |
| 1:M:130:GLU:HB3 | 1:M:422:VAL:HG22 | 1.96 | 0.46 |
| 1:M:453:GLN:HE22 | 4:M:1518:MPD:H11 | 1.80 | 0.46 |
| 1:N:152:ALA:O | 1:N:153:ASN:HB3 | 2.14 | 0.46 |
| 1:N:77:VAL:HG21 | 1:N:510:VAL:HB | 1.96 | 0.46 |
| 1:B:201:SER:C | 1:B:202:PRO:O | 2.51 | 0.46 |
| 1:B:496:PRO:HB2 | 1:B:499:VAL:HG13 | 1.97 | 0.46 |
| 1:H:26:ALA:HA | 1:I:8:PHE:HE1 | 1.79 | 0.46 |
| 1:H:478:TYR:CE2 | 1:H:480:ALA:HA | 2.50 | 0.46 |
| 1:K:16:MET:HB3 | 1:K:514:MET:CE | 2.45 | 0.46 |
| 1:L:259:LEU:O | 1:L:263:VAL:HG23 | 2.16 | 0.46 |
| 1:L:349:ILE:CG2 | 1:L:369:VAL:HG13 | 2.45 | 0.46 |
| 1:N:413:ALA:N | 1:N:475:ASN:HD22 | 2.13 | 0.46 |
| 1:A:273:VAL:HG12 | 1:A:274:ALA:N | 2.30 | 0.46 |
| 1:D:478:TYR:CE2 | 1:D:480:ALA:HA | 2.50 | 0.46 |
| 1:G:455:VAL:CG1 | 1:G:460:GLU:HB2 | 2.44 | 0.46 |
| 1:I:201:SER:C | 1:I:202:PRO:O | 2.51 | 0.46 |
| 1:B:131:LEU:HD21 | 1:B:500:THR:HG22 | 1.98 | 0.46 |
| 1:C:201:SER:C | 1:C:202:PRO:O | 2.52 | 0.46 |
| 1:C:248:LEU:HD13 | 1:C:325:ILE:HD11 | 1.98 | 0.46 |
| 1:F:200:LEU:HG | 1:F:276:VAL:HA | 1.96 | 0.46 |
| 1:H:152:ALA:O | 1:H:153:ASN:HB3 | 2.16 | 0.46 |
| 1:H:266:THR:CG2 | 1:H:273:VAL:HB | 2.45 | 0.46 |
| 1:H:413:ALA:N | 1:H:475:ASN:HD22 | 2.14 | 0.46 |
| 1:K:230:ILE:HG21 | 1:K:261:THR:HG21 | 1.97 | 0.46 |
| 1:K:266:THR:HG21 | 1:K:273:VAL:HB | 1.97 | 0.46 |
| 1:K:16:MET:HB3 | 1:K:514:MET:HE1 | 1.98 | 0.46 |
| 1:N:413:ALA:HB3 | 1:N:417:VAL:HG22 | 1.98 | 0.46 |
| 1:D:429:LEU:HD12 | 6:D:3081:HOH:O | 2.15 | 0.46 |
| 1:H:381:VAL:HG21 | 1:H:393:LYS:HA | 1.97 | 0.46 |
| 1:I:152:ALA:O | 1:I:153:ASN:HB3 | 2.15 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:16:MET:HB3 | 1:I:514:MET:CE | 2.46 | 0.46 |
| 1:I:314:LEU:HD23 | 1:I:317:LEU:HD22 | 1.97 | 0.46 |
| 1:L:25:ASP:OD1 | 1:L:28:LYS:HE2 | 2.15 | 0.46 |
| 1:L:173:GLY:O | 1:L:404:ARG:NH2 | 2.48 | 0.46 |
| 1:M:455:VAL:CG1 | 1:M:460:GLU:HB2 | 2.44 | 0.46 |
| 1:N:305:ILE:HG22 | 1:N:305:ILE:O | 2.16 | 0.46 |
| 1:N:441:LYS:O | 1:N:445:ARG:HB2 | 2.15 | 0.46 |
| 1:A:217:SER:N | 1:A:218:PRO:CD | 2.78 | 0.46 |
| 1:B:346:VAL:O | 1:B:350:ARG:HB2 | 2.16 | 0.46 |
| 1:C:353:ILE:HD13 | 1:C:366:GLN:HG3 | 1.97 | 0.46 |
| 1:D:349:ILE:O | 1:D:353:ILE:HG13 | 2.16 | 0.46 |
| 1:E:169:VAL:CG1 | 1:E:377:ALA:HB2 | 2.46 | 0.46 |
| 1:E:383:ALA:HB3 | 1:E:389:MET:HB2 | 1.98 | 0.46 |
| 1:I:429:LEU:HG | 1:I:440:ILE:HD13 | 1.97 | 0.46 |
| 1:I:455:VAL:CG1 | 1:I:460:GLU:HB2 | 2.46 | 0.46 |
| 1:K:13:ARG:NH1 | 1:K:518:GLU:OE2 | 2.48 | 0.46 |
| 1:K:381:VAL:HG21 | 1:K:393:LYS:HA | 1.98 | 0.46 |
| 1:L:16:MET:HB3 | 1:L:514:MET:CE | 2.45 | 0.46 |
| 1:L:193:MET:HG2 | 1:L:194:GLN:N | 2.31 | 0.46 |
| 1:L:57:ALA:O | 1:L:75:LYS:HD2 | 2.15 | 0.46 |
| 1:M:349:ILE:HA | 1:M:352:GLN:CG | 2.45 | 0.46 |
| 1:A:247:LEU:CD2 | 1:A:249:ILE:HD11 | 2.46 | 0.46 |
| 1:B:134:LEU:HD12 | 1:B:422:VAL:HG23 | 1.98 | 0.46 |
| 1:J:186:GLU:HB2 | 1:J:380:LYS:HB2 | 1.98 | 0.46 |
| 1:J:349:ILE:O | 1:J:353:ILE:HG13 | 2.14 | 0.46 |
| 1:M:183:LEU:O | 1:M:184:GLN:CB | 2.58 | 0.46 |
| 1:N:193:MET:HG2 | 1:N:194:GLN:N | 2.31 | 0.46 |
| 1:C:191:GLU:O | 1:C:334:ASP:HA | 2.15 | 0.46 |
| 1:C:202:PRO:C | 1:C:204:PHE:H | 2.18 | 0.46 |
| 1:C:16:MET:HB3 | 1:C:514:MET:CE | 2.46 | 0.46 |
| 1:E:349:ILE:O | 1:E:353:ILE:HG13 | 2.15 | 0.46 |
| 1:G:77:VAL:HG12 | 1:G:506:TYR:HB3 | 1.98 | 0.46 |
| 1:I:200:LEU:HG | 1:I:276:VAL:HA | 1.98 | 0.46 |
| 1:I:204:PHE:O | 1:I:213:VAL:HG22 | 2.15 | 0.46 |
| 1:I:381:VAL:HG21 | 1:I:393:LYS:HA | 1.96 | 0.46 |
| 1:I:144:ILE:HG23 | 1:I:403:THR:CG2 | 2.45 | 0.46 |
| 1:K:413:ALA:N | 1:K:475:ASN:HD22 | 2.14 | 0.46 |
| 1:K:57:ALA:O | 1:K:75:LYS:HD2 | 2.15 | 0.46 |
| 1:L:183:LEU:HD22 | 1:L:184:GLN:H | 1.81 | 0.46 |
| 1:L:247:LEU:HD21 | 1:L:249:ILE:HD11 | 1.98 | 0.46 |
| 1:N:134:LEU:HD11 | 1:N:475:ASN:ND2 | 2.30 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:264:VAL:HG12 | 1:A:265:ASN:N | 2.31 | 0.46 |
| 1:B:364:LYS:O | 1:B:367:GLU:HB2 | 2.16 | 0.46 |
| 1:D:71:ALA:O | 1:D:75:LYS:HB2 | 2.16 | 0.46 |
| 1:E:289:LEU:HD23 | 1:E:289:LEU:HA | 1.77 | 0.46 |
| 1:E:413:ALA:CB | 1:E:417:VAL:HG22 | 2.46 | 0.46 |
| 1:H:257:GLU:HB2 | 1:N:269:GLY:HA3 | 1.97 | 0.46 |
| 1:H:31:LEU:HD13 | 1:H:90:THR:CG2 | 2.46 | 0.46 |
| 1:I:13:ARG:NH1 | 1:I:518:GLU:OE2 | 2.49 | 0.46 |
| 1:M:16:MET:HB3 | 1:M:514:MET:CE | 2.46 | 0.46 |
| 1:N:153:ASN:O | 1:N:154:SER:HB2 | 2.16 | 0.46 |
| 1:N:342:ILE:O | 1:N:346:VAL:HG23 | 2.16 | 0.46 |
| 1:N:349:ILE:CG2 | 1:N:369:VAL:HG13 | 2.46 | 0.46 |
| 1:N:131:LEU:HD21 | 1:N:500:THR:HG22 | 1.99 | 0.46 |
| 1:B:217:SER:N | 1:B:218:PRO:HD3 | 2.32 | 0.45 |
| 1:C:385:THR:OG1 | 1:C:388:GLU:HG3 | 2.16 | 0.45 |
| 1:E:290:GLN:O | 1:E:293:ALA:HB3 | 2.16 | 0.45 |
| 1:G:194:GLN:O | 1:G:371:LYS:HE3 | 2.16 | 0.45 |
| 1:H:114:MET:HB3 | 6:H:3064:HOH:O | 2.16 | 0.45 |
| 1:I:266:THR:HG21 | 1:I:273:VAL:HB | 1.98 | 0.45 |
| 1:I:18:ARG:HG3 | 1:I:67:GLU:CD | 2.36 | 0.45 |
| 1:J:25:ASP:OD1 | 1:J:28:LYS:HE2 | 2.17 | 0.45 |
| 1:K:202:PRO:O | 1:K:203:TYR:HB2 | 2.15 | 0.45 |
| 1:A:305:ILE:HG22 | 1:A:305:ILE:O | 2.16 | 0.45 |
| 1:A:349:ILE:HG21 | 1:A:369:VAL:HG13 | 1.98 | 0.45 |
| 1:B:144:ILE:HG23 | 1:B:403:THR:CG2 | 2.46 | 0.45 |
| 1:H:231:ARG:HH12 | 1:N:241:ALA:HB3 | 1.82 | 0.45 |
| 1:I:183:LEU:O | 1:I:184:GLN:CB | 2.54 | 0.45 |
| 1:J:217:SER:N | 1:J:218:PRO:HD3 | 2.32 | 0.45 |
| 1:A:120:ILE:O | 1:A:124:VAL:HG23 | 2.16 | 0.45 |
| 1:A:451:LEU:HD23 | 1:A:451:LEU:O | 2.17 | 0.45 |
| 1:D:305:ILE:O | 1:D:305:ILE:HG22 | 2.16 | 0.45 |
| 1:F:202:PRO:O | 1:F:203:TYR:CB | 2.61 | 0.45 |
| 1:F:194:GLN:O | 1:F:371:LYS:HE3 | 2.16 | 0.45 |
| 1:I:291:ASP:OD2 | 1:I:368:ARG:HD2 | 2.16 | 0.45 |
| 1:L:49:ILE:CD1 | 1:M:513:LEU:HD13 | 2.46 | 0.45 |
| 1:N:18:ARG:HH12 | 4:N:1526:MPD:H31 | 1.80 | 0.45 |
| 1:A:221:LEU:HD23 | 1:A:249:ILE:HD12 | 1.99 | 0.45 |
| 1:B:225:LYS:NZ | 1:B:232:GLU:OE2 | 2.50 | 0.45 |
| 1:E:77:VAL:HG21 | 1:E:510:VAL:HB | 1.99 | 0.45 |
| 1:I:16:MET:O | 1:I:20:VAL:HG13 | 2.16 | 0.45 |
| 1:I:270:ILE:O | 1:I:271:VAL:CB | 2.61 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:463:SER:O | 1:I:467:ASN:HB2 | 2.16 | 0.45 |
| 1:H:39:VAL:HG12 | 1:I:69:MET:CE | 2.47 | 0.45 |
| 1:K:49:ILE:HD12 | 1:L:513:LEU:HD13 | 1.98 | 0.45 |
| 1:L:413:ALA:N | 1:L:475:ASN:HD22 | 2.15 | 0.45 |
| 1:N:235:PRO:CG | 1:N:310:GLU:HA | 2.41 | 0.45 |
| 1:A:351:GLN:O | 1:A:354:GLU:HG2 | 2.17 | 0.45 |
| 1:A:472:GLY:HA3 | 1:A:476:TYR:CD2 | 2.51 | 0.45 |
| 1:D:326:ASN:HB3 | 1:D:327:LYS:H | 1.64 | 0.45 |
| 1:F:217:SER:O | 1:F:245:LYS:HD3 | 2.17 | 0.45 |
| 1:F:230:ILE:HD13 | 1:F:261:THR:HG21 | 1.98 | 0.45 |
| 1:G:176:THR:HG21 | 1:G:333:ILE:CD1 | 2.38 | 0.45 |
| 1:G:303:GLU:O | 1:G:306:GLY:N | 2.46 | 0.45 |
| 1:H:254:VAL:HG12 | 1:H:259:LEU:HB2 | 1.98 | 0.45 |
| 1:K:181:THR:O | 1:L:282:GLY:HA3 | 2.16 | 0.45 |
| 1:K:478:TYR:CE2 | 1:K:480:ALA:HA | 2.51 | 0.45 |
| 1:M:221:LEU:HB3 | 1:M:249:ILE:HD13 | 1.98 | 0.45 |
| 1:N:349:ILE:HA | 1:N:352:GLN:CG | 2.46 | 0.45 |
| 1:N:478:TYR:CE2 | 1:N:480:ALA:HA | 2.52 | 0.45 |
| 1:B:24:ALA:O | 1:B:28:LYS:HG2 | 2.17 | 0.45 |
| 1:B:301:ILE:HD13 | 1:B:312:ALA:HB2 | 1.98 | 0.45 |
| 1:B:90:THR:O | 1:B:94:VAL:HG13 | 2.17 | 0.45 |
| 1:C:23:LEU:CD2 | 1:C:74:VAL:HG22 | 2.46 | 0.45 |
| 1:E:270:ILE:HG12 | 1:F:231:ARG:HH11 | 1.82 | 0.45 |
| 1:H:349:ILE:CG2 | 1:H:369:VAL:HG13 | 2.47 | 0.45 |
| 1:H:413:ALA:HB1 | 1:H:488:MET:HG3 | 1.98 | 0.45 |
| 1:I:221:LEU:HD23 | 1:I:249:ILE:HD12 | 1.97 | 0.45 |
| 1:K:413:ALA:HB3 | 1:K:417:VAL:HG22 | 1.99 | 0.45 |
| 1:N:176:THR:HG22 | 1:N:177:VAL:N | 2.32 | 0.45 |
| 1:N:16:MET:O | 1:N:20:VAL:HG13 | 2.17 | 0.45 |
| 1:N:169:VAL:CG1 | 1:N:377:ALA:HB2 | 2.47 | 0.45 |
| 1:B:202:PRO:C | 1:B:204:PHE:H | 2.15 | 0.45 |
| 1:B:270:ILE:O | 1:B:271:VAL:HB | 2.16 | 0.45 |
| 1:B:295:LEU:HA | 1:B:342:ILE:CD1 | 2.47 | 0.45 |
| 1:B:16:MET:HB3 | 1:B:514:MET:CE | 2.47 | 0.45 |
| 1:C:183:LEU:HA | 1:C:383:ALA:N | 2.31 | 0.45 |
| 1:C:70:GLY:HA2 | 1:C:73:MET:HE2 | 1.99 | 0.45 |
| 1:D:383:ALA:HB3 | 1:D:389:MET:HB2 | 1.97 | 0.45 |
| 1:G:40:LEU:HD13 | 1:G:59:GLU:HG3 | 1.98 | 0.45 |
| 1:K:183:LEU:HD22 | 1:K:184:GLN:H | 1.81 | 0.45 |
| 1:K:191:GLU:O | 1:K:334:ASP:HA | 2.17 | 0.45 |
| 1:L:138:CYS:SG | 1:L:147:VAL:HG21 | 2.57 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:413:ALA:HB1 | 1:N:488:MET:HG3 | 1.99 | 0.45 |
| 1:B:23:LEU:CD2 | 1:B:74:VAL:HG22 | 2.47 | 0.45 |
| 1:E:7:LYS:HE3 | 1:E:15:LYS:HE3 | 1.99 | 0.45 |
| 1:F:201:SER:C | 1:F:202:PRO:O | 2.52 | 0.45 |
| 1:F:23:LEU:CD2 | 1:F:74:VAL:HG22 | 2.46 | 0.45 |
| 1:F:472:GLY:HA3 | 1:F:476:TYR:CD2 | 2.51 | 0.45 |
| 1:H:413:ALA:HB3 | 1:H:417:VAL:HG22 | 1.99 | 0.45 |
| 1:H:451:LEU:HD23 | 1:H:451:LEU:O | 2.16 | 0.45 |
| 1:I:25:ASP:OD1 | 1:I:28:LYS:HE2 | 2.16 | 0.45 |
| 1:K:201:SER:C | 1:K:202:PRO:O | 2.55 | 0.45 |
| 1:L:339:GLU:O | 1:L:343:GLN:HB2 | 2.17 | 0.45 |
| 1:N:524:LEU:HA | 1:N:524:LEU:HD12 | 1.81 | 0.45 |
| 1:A:193:MET:CE | 1:A:292:ILE:HG12 | 2.46 | 0.45 |
| 1:A:429:LEU:HG | 1:A:440:ILE:HD13 | 1.99 | 0.45 |
| 1:B:524:LEU:HA | 1:B:524:LEU:HD12 | 1.77 | 0.45 |
| 1:C:478:TYR:CE2 | 1:C:480:ALA:HA | 2.52 | 0.45 |
| 1:G:383:ALA:HB3 | 1:G:389:MET:HB2 | 1.99 | 0.45 |
| 1:J:200:LEU:HG | 1:J:276:VAL:HA | 1.99 | 0.45 |
| 1:L:198:GLY:O | 1:L:276:VAL:HG12 | 2.17 | 0.45 |
| 1:L:451:LEU:O | 1:L:451:LEU:HD23 | 2.17 | 0.45 |
| 1:M:478:TYR:CE2 | 1:M:480:ALA:HA | 2.52 | 0.45 |
| 1:N:230:ILE:HB | 1:N:258:ALA:HA | 1.99 | 0.45 |
| 1:N:413:ALA:CB | 1:N:417:VAL:HG22 | 2.47 | 0.45 |
| 1:A:223:ALA:O | 1:A:251:ALA:HA | 2.17 | 0.45 |
| 1:D:202:PRO:C | 1:D:204:PHE:H | 2.19 | 0.45 |
| 1:D:413:ALA:HB3 | 1:D:417:VAL:HG22 | 1.99 | 0.45 |
| 1:F:353:ILE:HD13 | 1:F:366:GLN:HG3 | 1.99 | 0.45 |
| 1:F:451:LEU:HD23 | 1:F:451:LEU:C | 2.37 | 0.45 |
| 1:F:455:VAL:CG1 | 1:F:460:GLU:HB2 | 2.46 | 0.45 |
| 1:G:270:ILE:O | 1:G:271:VAL:CB | 2.64 | 0.45 |
| 1:I:413:ALA:N | 1:I:475:ASN:HD22 | 2.14 | 0.45 |
| 1:J:13:ARG:NH1 | 1:J:518:GLU:OE2 | 2.50 | 0.45 |
| 1:J:18:ARG:HG3 | 1:J:67:GLU:CD | 2.37 | 0.45 |
| 1:J:463:SER:O | 1:J:467:ASN:HB2 | 2.16 | 0.45 |
| 1:K:152:ALA:O | 1:K:153:ASN:HB3 | 2.17 | 0.45 |
| 1:K:252:GLU:O | 1:K:253:ASP:HB2 | 2.16 | 0.45 |
| 1:N:230:ILE:HD13 | 1:N:261:THR:HG21 | 1.99 | 0.45 |
| 1:N:247:LEU:HD21 | 1:N:249:ILE:HD11 | 1.98 | 0.45 |
| 1:N:310:GLU:OE1 | 1:N:310:GLU:N | 2.47 | 0.45 |
| 1:C:247:LEU:HB3 | 1:C:273:VAL:HG22 | 1.98 | 0.44 |
| 1:C:460:GLU:O | 1:C:462:PRO:HD3 | 2.17 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:460:GLU:O | 1:E:462:PRO:HD3 | 2.17 | 0.44 |
| 1:H:231:ARG:NH1 | 1:N:241:ALA:C | 2.70 | 0.44 |
| 1:I:176:THR:HG22 | 1:I:177:VAL:N | 2.31 | 0.44 |
| 1:J:219:PHE:HB3 | 1:J:317:LEU:HD23 | 1.97 | 0.44 |
| 1:K:112:ASN:HA | 1:K:113:PRO:HD3 | 1.90 | 0.44 |
| 1:K:153:ASN:O | 1:K:154:SER:HB2 | 2.17 | 0.44 |
| 1:L:202:PRO:C | 1:L:204:PHE:H | 2.19 | 0.44 |
| 1:L:37:ASN:ND2 | 1:L:51:LYS:HG3 | 2.32 | 0.44 |
| 1:M:326:ASN:HB3 | 1:M:327:LYS:H | 1.57 | 0.44 |
| 1:M:392:LYS:O | 1:M:396:VAL:HG23 | 2.17 | 0.44 |
| 1:A:524:LEU:HD21 | 1:G:63:GLU:HB2 | 1.99 | 0.44 |
| 1:B:82:ASN:HB2 | 1:B:89:THR:OG1 | 2.17 | 0.44 |
| 1:E:413:ALA:HB3 | 1:E:417:VAL:HG22 | 1.99 | 0.44 |
| 1:L:5:ASP:HB2 | 1:L:524:LEU:CD1 | 2.46 | 0.44 |
| 1:M:252:GLU:O | 1:M:253:ASP:HB2 | 2.17 | 0.44 |
| 1:M:254:VAL:HG12 | 1:M:259:LEU:HB2 | 1.99 | 0.44 |
| 1:M:349:ILE:CG2 | 1:M:369:VAL:HG13 | 2.48 | 0.44 |
| 1:M:429:LEU:HG | 1:M:440:ILE:HD13 | 1.98 | 0.44 |
| 1:N:201:SER:C | 1:N:202:PRO:O | 2.55 | 0.44 |
| 1:C:496:PRO:HB2 | 1:C:499:VAL:HG13 | 1.98 | 0.44 |
| 1:F:193:MET:CE | 1:F:292:ILE:HG12 | 2.48 | 0.44 |
| 1:G:273:VAL:CG1 | 1:G:274:ALA:N | 2.80 | 0.44 |
| 1:H:273:VAL:HG12 | 1:H:274:ALA:N | 2.32 | 0.44 |
| 1:J:451:LEU:HD23 | 1:J:451:LEU:O | 2.17 | 0.44 |
| 1:K:100:ILE:O | 1:K:104:LEU:HG | 2.17 | 0.44 |
| 1:M:144:ILE:HG23 | 1:M:403:THR:CG2 | 2.48 | 0.44 |
| 1:N:144:ILE:HG23 | 1:N:403:THR:CG2 | 2.48 | 0.44 |
| 1:H:231:ARG:HH11 | 1:N:241:ALA:C | 2.21 | 0.44 |
| 1:N:83:ASP:OD2 | 1:N:327:LYS:CD | 2.63 | 0.44 |
| 1:A:23:LEU:CD2 | 1:A:74:VAL:HG22 | 2.46 | 0.44 |
| 1:B:290:GLN:HB3 | 1:B:345:ARG:NH2 | 2.33 | 0.44 |
| 1:D:109:ALA:HB2 | 1:J:109:ALA:HB2 | 2.00 | 0.44 |
| 1:E:314:LEU:HD23 | 1:E:317:LEU:CD2 | 2.45 | 0.44 |
| 1:F:385:THR:OG1 | 1:F:388:GLU:HG3 | 2.18 | 0.44 |
| 1:G:413:ALA:HB3 | 1:G:417:VAL:HG22 | 1.99 | 0.44 |
| 1:G:70:GLY:HA2 | 1:G:73:MET:HE2 | 1.99 | 0.44 |
| 1:H:270:ILE:O | 1:H:271:VAL:CB | 2.66 | 0.44 |
| 1:I:230:ILE:HG21 | 1:I:261:THR:HG21 | 1.99 | 0.44 |
| 1:J:266:THR:HG21 | 1:J:273:VAL:HB | 1.98 | 0.44 |
| 1:J:344:GLY:O | 1:J:347:ALA:HB3 | 2.17 | 0.44 |
| 1:J:38:VAL:HG13 | 1:K:519:CYS:HB3 | 2.00 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:455:VAL:CG1 | 1:K:460:GLU:HB2 | 2.45 | 0.44 |
| 1:L:152:ALA:O | 1:L:153:ASN:HB3 | 2.17 | 0.44 |
| 1:M:217:SER:N | 1:M:218:PRO:HD3 | 2.33 | 0.44 |
| 1:H:282:GLY:HA3 | 1:N:181:THR:O | 2.17 | 0.44 |
| 1:N:37:ASN:ND2 | 1:N:51:LYS:HG3 | 2.32 | 0.44 |
| 1:A:191:GLU:O | 1:A:334:ASP:HA | 2.17 | 0.44 |
| 1:E:310:GLU:OE1 | 1:E:310:GLU:N | 2.51 | 0.44 |
| 1:F:359:ASP:HA | 1:F:362:ARG:HH12 | 1.82 | 0.44 |
| 1:F:413:ALA:HB3 | 1:F:417:VAL:HG22 | 2.00 | 0.44 |
| 1:F:496:PRO:HB2 | 1:F:499:VAL:HG13 | 2.00 | 0.44 |
| 1:H:5:ASP:HB2 | 1:H:524:LEU:CD1 | 2.47 | 0.44 |
| 1:I:202:PRO:O | 1:I:203:TYR:CB | 2.62 | 0.44 |
| 1:I:31:LEU:HD13 | 1:I:90:THR:HG22 | 1.99 | 0.44 |
| 1:N:445:ARG:HH22 | 4:N:1515:MPD:H11 | 1.81 | 0.44 |
| 1:B:289:LEU:HD23 | 1:B:289:LEU:HA | 1.86 | 0.44 |
| 1:F:218:PRO:HD2 | 1:F:320:ALA:O | 2.17 | 0.44 |
| 1:G:183:LEU:HA | 1:G:383:ALA:N | 2.33 | 0.44 |
| 1:G:269:GLY:HA2 | 1:G:272:LYS:HZ2 | 1.83 | 0.44 |
| 1:H:262:LEU:O | 1:H:266:THR:HG23 | 2.17 | 0.44 |
| 1:H:272:LYS:NZ | 1:I:228:SER:HB3 | 2.33 | 0.44 |
| 1:H:455:VAL:CG1 | 1:H:460:GLU:HB2 | 2.48 | 0.44 |
| 1:I:112:ASN:HA | 1:I:113:PRO:HD3 | 1.91 | 0.44 |
| 1:I:236:VAL:HG22 | 1:I:312:ALA:O | 2.18 | 0.44 |
| 1:I:194:GLN:O | 1:I:371:LYS:HE3 | 2.18 | 0.44 |
| 1:J:366:GLN:O | 1:J:369:VAL:HG22 | 2.18 | 0.44 |
| 1:L:207:LYS:O | 1:L:211:GLY:N | 2.50 | 0.44 |
| 1:L:25:ASP:HA | 1:L:28:LYS:HE2 | 2.00 | 0.44 |
| 1:M:216:GLU:C | 1:M:218:PRO:HD3 | 2.38 | 0.44 |
| 1:M:451:LEU:HD23 | 1:M:451:LEU:O | 2.18 | 0.44 |
| 1:N:13:ARG:NH1 | 1:N:518:GLU:OE2 | 2.49 | 0.44 |
| 1:A:85:ALA:HB1 | 1:A:499:VAL:HG12 | 1.99 | 0.44 |
| 1:B:202:PRO:O | 1:B:203:TYR:HB2 | 2.18 | 0.44 |
| 1:C:364:LYS:O | 1:C:367:GLU:HB2 | 2.18 | 0.44 |
| 1:C:369:VAL:HG23 | 1:C:370:ALA:N | 2.32 | 0.44 |
| 1:D:460:GLU:O | 1:D:462:PRO:HD3 | 2.18 | 0.44 |
| 1:F:144:ILE:HG23 | 1:F:403:THR:CG2 | 2.48 | 0.44 |
| 1:H:219:PHE:HB3 | 1:H:317:LEU:HD23 | 2.00 | 0.44 |
| 1:I:242:LYS:O | 1:I:243:ALA:CB | 2.66 | 0.44 |
| 1:I:329:THR:O | 1:I:329:THR:HG22 | 2.18 | 0.44 |
| 1:J:202:PRO:O | 1:J:203:TYR:CB | 2.61 | 0.44 |
| 1:M:303:GLU:HG3 | 6:M:3108:HOH:O | 2.17 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:118:ARG:HH22 | 1:N:34:LYS:HE2 | 1.82 | 0.44 |
| 1:B:77:VAL:HG21 | 1:B:510:VAL:HB | 2.00 | 0.44 |
| 1:C:114:MET:HE2 | 6:C:3133:HOH:O | 2.18 | 0.44 |
| 1:C:263:VAL:O | 1:C:267:MET:HB2 | 2.18 | 0.44 |
| 1:D:16:MET:HB3 | 1:D:514:MET:CE | 2.48 | 0.44 |
| 1:E:429:LEU:HG | 1:E:440:ILE:HD13 | 1.99 | 0.44 |
| 1:F:220:ILE:HD12 | 1:F:296:THR:HG21 | 2.00 | 0.44 |
| 1:G:472:GLY:HA3 | 1:G:476:TYR:CD2 | 2.53 | 0.44 |
| 1:I:201:SER:O | 1:I:202:PRO:O | 2.36 | 0.44 |
| 1:I:23:LEU:CD2 | 1:I:74:VAL:HG22 | 2.48 | 0.44 |
| 1:I:349:ILE:O | 1:I:353:ILE:HG13 | 2.17 | 0.44 |
| 1:J:85:ALA:CB | 1:J:499:VAL:HG12 | 2.42 | 0.44 |
| 1:K:501:ARG:O | 1:K:505:GLN:HG3 | 2.17 | 0.44 |
| 1:L:224:ASP:O | 1:L:225:LYS:CB | 2.65 | 0.44 |
| 1:L:248:LEU:HD13 | 1:L:325:ILE:HD11 | 2.00 | 0.44 |
| 1:B:215:LEU:HB2 | 1:B:323:VAL:HG22 | 2.00 | 0.44 |
| 1:C:7:LYS:HG3 | 1:C:66:PHE:CZ | 2.53 | 0.44 |
| 1:E:191:GLU:OE2 | 4:E:1502:MPD:H53 | 2.17 | 0.44 |
| 1:E:217:SER:O | 1:E:245:LYS:HD3 | 2.18 | 0.44 |
| 1:E:77:VAL:HG12 | 1:E:506:TYR:HB3 | 2.00 | 0.44 |
| 1:G:82:ASN:HB2 | 1:G:89:THR:OG1 | 2.18 | 0.44 |
| 1:H:201:SER:C | 1:H:202:PRO:O | 2.55 | 0.44 |
| 1:I:195:PHE:HB2 | 1:I:279:PRO:HB3 | 2.00 | 0.44 |
| 1:I:305:ILE:HD12 | 1:I:307:MET:HE2 | 2.00 | 0.44 |
| 1:J:305:ILE:HD12 | 1:J:307:MET:HE2 | 2.00 | 0.44 |
| 1:J:71:ALA:O | 1:J:75:LYS:HB2 | 2.18 | 0.44 |
| 1:K:217:SER:N | 1:K:218:PRO:HD3 | 2.32 | 0.44 |
| 1:L:455:VAL:CG1 | 1:L:460:GLU:HB2 | 2.48 | 0.44 |
| 1:N:146:GLN:O | 1:N:150:ILE:HG13 | 2.18 | 0.44 |
| 1:N:381:VAL:HG21 | 1:N:393:LYS:HA | 2.00 | 0.44 |
| 1:N:445:ARG:HG2 | 2:N:1146:SO4:O2 | 2.18 | 0.44 |
| 1:N:70:GLY:HA2 | 1:N:73:MET:HE3 | 2.00 | 0.44 |
| 1:A:353:ILE:HG23 | 1:A:362:ARG:HG3 | 2.00 | 0.43 |
| 1:A:118:ARG:HD2 | 1:A:436:GLN:HE22 | 1.83 | 0.43 |
| 1:A:77:VAL:HG12 | 1:A:506:TYR:HB3 | 2.00 | 0.43 |
| 1:C:182:GLY:O | 1:C:183:LEU:C | 2.55 | 0.43 |
| 1:C:38:VAL:HG22 | 1:D:519:CYS:HB3 | 2.00 | 0.43 |
| 1:D:132:LYS:O | 1:D:135:SER:HB3 | 2.18 | 0.43 |
| 1:D:85:ALA:HB1 | 1:D:499:VAL:HG12 | 1.99 | 0.43 |
| 1:H:49:ILE:HD12 | 1:I:513:LEU:HD13 | 1.99 | 0.43 |
| 1:K:219:PHE:CB | 1:K:317:LEU:HD23 | 2.44 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:460:GLU:O | 1:K:462:PRO:HD3 | 2.18 | 0.43 |
| 1:M:201:SER:C | 1:M:202:PRO:O | 2.56 | 0.43 |
| 1:M:234:LEU:O | 1:M:238:GLU:HG3 | 2.18 | 0.43 |
| 1:M:339:GLU:O | 1:M:343:GLN:HB2 | 2.18 | 0.43 |
| 1:M:456:LEU:HG | 4:M:1518:MPD:HM2 | 2.00 | 0.43 |
| 1:A:263:VAL:O | 1:A:267:MET:HB2 | 2.18 | 0.43 |
| 1:B:494:LEU:C | 1:B:494:LEU:HD12 | 2.38 | 0.43 |
| 1:C:230:ILE:HD11 | 1:C:237:LEU:HD11 | 2.00 | 0.43 |
| 1:E:169:VAL:HG11 | 1:E:377:ALA:HB2 | 2.00 | 0.43 |
| 1:E:416:GLY:HA2 | 6:E:3146:HOH:O | 2.18 | 0.43 |
| 1:H:25:ASP:HA | 1:H:28:LYS:HE2 | 2.01 | 0.43 |
| 1:M:34:LYS:HE2 | 1:N:118:ARG:NH2 | 2.25 | 0.43 |
| 1:N:18:ARG:NH1 | 4:N:1526:MPD:H31 | 2.33 | 0.43 |
| 1:N:202:PRO:O | 1:N:204:PHE:N | 2.43 | 0.43 |
| 1:B:284:ARG:O | 1:B:288:MET:HG3 | 2.18 | 0.43 |
| 1:D:266:THR:CG2 | 1:D:273:VAL:H | 2.31 | 0.43 |
| 1:D:301:ILE:HD13 | 1:D:312:ALA:HB2 | 2.00 | 0.43 |
| 1:E:16:MET:HB3 | 1:E:514:MET:CE | 2.48 | 0.43 |
| 1:F:460:GLU:O | 1:F:462:PRO:HD3 | 2.18 | 0.43 |
| 1:G:372:LEU:HA | 1:G:372:LEU:HD12 | 1.76 | 0.43 |
| 1:H:518:GLU:HG3 | 4:N:1517:MPD:H12 | 2.00 | 0.43 |
| 1:I:451:LEU:HD23 | 1:I:455:VAL:HG23 | 1.99 | 0.43 |
| 1:J:247:LEU:HD21 | 1:J:249:ILE:HD11 | 2.00 | 0.43 |
| 1:J:353:ILE:HD13 | 1:J:366:GLN:OE1 | 2.18 | 0.43 |
| 1:L:417:VAL:O | 1:L:420:ILE:HG22 | 2.18 | 0.43 |
| 1:A:102:GLU:HB2 | 1:A:442:VAL:HG13 | 2.00 | 0.43 |
| 1:C:201:SER:O | 1:C:202:PRO:O | 2.36 | 0.43 |
| 1:B:272:LYS:HZ2 | 1:C:229:ASN:ND2 | 2.16 | 0.43 |
| 1:E:259:LEU:O | 1:E:263:VAL:HG23 | 2.18 | 0.43 |
| 1:E:122:LYS:HE2 | 1:E:429:LEU:HD11 | 2.00 | 0.43 |
| 1:E:478:TYR:CE2 | 1:E:480:ALA:HA | 2.53 | 0.43 |
| 1:H:144:ILE:HG23 | 1:H:403:THR:CG2 | 2.48 | 0.43 |
| 1:H:314:LEU:HD23 | 1:H:317:LEU:HD22 | 1.99 | 0.43 |
| 1:H:429:LEU:HG | 1:H:440:ILE:HD13 | 2.00 | 0.43 |
| 1:I:34:LYS:HE2 | 1:J:118:ARG:HH22 | 1.83 | 0.43 |
| 1:J:183:LEU:HD22 | 1:J:184:GLN:H | 1.82 | 0.43 |
| 1:J:417:VAL:O | 1:J:420:ILE:HG22 | 2.18 | 0.43 |
| 1:M:463:SER:O | 1:M:467:ASN:HB2 | 2.18 | 0.43 |
| 1:M:70:GLY:HA2 | 1:M:73:MET:HE3 | 2.00 | 0.43 |
| 1:C:236:VAL:CG2 | 1:C:312:ALA:HB3 | 2.48 | 0.43 |
| 1:D:218:PRO:HB3 | 1:D:246:PRO:HG2 | 2.00 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:24:ALA:O | 1:F:28:LYS:HG2 | 2.18 | 0.43 |
| 1:G:369:VAL:HG23 | 1:G:370:ALA:N | 2.33 | 0.43 |
| 1:I:266:THR:CG2 | 1:I:273:VAL:HB | 2.48 | 0.43 |
| 1:J:451:LEU:HD23 | 1:J:451:LEU:C | 2.39 | 0.43 |
| 1:K:372:LEU:HD12 | 1:K:372:LEU:HA | 1.86 | 0.43 |
| 1:A:266:THR:CG2 | 1:A:273:VAL:HB | 2.48 | 0.43 |
| 1:A:369:VAL:HG23 | 1:A:370:ALA:N | 2.33 | 0.43 |
| 1:A:90:THR:O | 1:A:94:VAL:HG13 | 2.18 | 0.43 |
| 1:B:200:LEU:CD1 | 1:B:254:VAL:HB | 2.49 | 0.43 |
| 1:C:296:THR:HB | 1:C:319:GLN:H | 1.83 | 0.43 |
| 1:D:166:MET:CE | 1:D:171:LYS:HA | 2.48 | 0.43 |
| 1:D:200:LEU:CD1 | 1:D:254:VAL:HB | 2.48 | 0.43 |
| 1:D:222:LEU:CD1 | 1:D:293:ALA:HA | 2.49 | 0.43 |
| 1:E:183:LEU:O | 1:E:184:GLN:CB | 2.66 | 0.43 |
| 1:E:242:LYS:C | 1:E:244:GLY:N | 2.70 | 0.43 |
| 1:F:349:ILE:CG2 | 1:F:369:VAL:HG13 | 2.48 | 0.43 |
| 1:H:16:MET:HB3 | 1:H:514:MET:CE | 2.49 | 0.43 |
| 1:J:18:ARG:HB2 | 6:J:3074:HOH:O | 2.18 | 0.43 |
| 1:J:193:MET:HE2 | 1:J:292:ILE:HG12 | 2.00 | 0.43 |
| 1:K:266:THR:CG2 | 1:K:273:VAL:HB | 2.48 | 0.43 |
| 1:M:258:ALA:O | 1:M:262:LEU:HG | 2.18 | 0.43 |
| 1:N:16:MET:HB3 | 1:N:514:MET:CE | 2.49 | 0.43 |
| 1:C:213:VAL:HB | 1:C:325:ILE:HB | 2.00 | 0.43 |
| 1:C:501:ARG:HH11 | 1:C:501:ARG:HG2 | 1.84 | 0.43 |
| 1:D:264:VAL:HG12 | 1:D:265:ASN:N | 2.34 | 0.43 |
| 1:D:319:GLN:O | 1:D:336:VAL:HG23 | 2.18 | 0.43 |
| 1:H:218:PRO:HD2 | 1:H:320:ALA:O | 2.18 | 0.43 |
| 1:J:131:LEU:HD21 | 1:J:500:THR:HG22 | 2.01 | 0.43 |
| 1:M:16:MET:O | 1:M:20:VAL:HG13 | 2.19 | 0.43 |
| 1:A:16:MET:O | 1:A:20:VAL:HG13 | 2.18 | 0.43 |
| 1:A:284:ARG:NH1 | 1:A:364:LYS:HD2 | 2.33 | 0.43 |
| 1:A:349:ILE:O | 1:A:353:ILE:HG13 | 2.19 | 0.43 |
| 1:B:183:LEU:O | 1:B:184:GLN:CB | 2.65 | 0.43 |
| 1:B:77:VAL:HG12 | 1:B:506:TYR:HB3 | 2.01 | 0.43 |
| 1:B:49:ILE:HD12 | 1:C:513:LEU:HD13 | 2.00 | 0.43 |
| 1:D:10:ASN:HB2 | 6:D:3029:HOH:O | 2.19 | 0.43 |
| 1:E:213:VAL:HB | 1:E:325:ILE:HB | 2.01 | 0.43 |
| 1:E:326:ASN:HB2 | 1:E:329:THR:HB | 2.01 | 0.43 |
| 1:I:180:GLY:HA3 | 1:I:381:VAL:O | 2.19 | 0.43 |
| 1:J:201:SER:C | 1:J:202:PRO:O | 2.56 | 0.43 |
| 1:L:217:SER:N | 1:L:218:PRO:HD3 | 2.34 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:112:ASN:HA | 1:M:113:PRO:HD3 | 1.90 | 0.43 |
| 1:N:305:ILE:HD12 | 1:N:307:MET:HE2 | 2.01 | 0.43 |
| 1:B:472:GLY:HA3 | 1:B:476:TYR:CD2 | 2.54 | 0.43 |
| 1:C:270:ILE:O | 1:C:271:VAL:CB | 2.66 | 0.43 |
| 1:F:40:LEU:HD13 | 1:F:59:GLU:HG3 | 1.99 | 0.43 |
| 1:G:182:GLY:O | 1:G:183:LEU:C | 2.57 | 0.43 |
| 1:I:123:ALA:HB2 | 1:I:440:ILE:HG23 | 2.01 | 0.43 |
| 1:I:413:ALA:CB | 1:I:417:VAL:HG22 | 2.49 | 0.43 |
| 1:L:176:THR:HG22 | 1:L:177:VAL:N | 2.33 | 0.43 |
| 1:M:198:GLY:O | 1:M:276:VAL:HG12 | 2.19 | 0.43 |
| 1:M:353:ILE:HG23 | 1:M:362:ARG:HG3 | 2.01 | 0.43 |
| 1:M:68:ASN:O | 1:M:72:GLN:HG2 | 2.18 | 0.43 |
| 1:C:16:MET:O | 1:C:20:VAL:HG13 | 2.18 | 0.43 |
| 1:H:451:LEU:HD23 | 1:H:455:VAL:HG23 | 2.00 | 0.43 |
| 1:I:413:ALA:HB3 | 1:I:417:VAL:HG22 | 1.99 | 0.43 |
| 1:J:413:ALA:HB3 | 1:J:417:VAL:HG22 | 2.00 | 0.43 |
| 1:K:349:ILE:HA | 1:K:352:GLN:CG | 2.48 | 0.43 |
| 1:M:176:THR:HG22 | 1:M:177:VAL:N | 2.34 | 0.43 |
| 1:M:18:ARG:HG3 | 1:M:67:GLU:CD | 2.38 | 0.43 |
| 1:M:201:SER:O | 1:M:202:PRO:O | 2.37 | 0.43 |
| 1:M:460:GLU:O | 1:M:462:PRO:HD3 | 2.18 | 0.43 |
| 1:N:144:ILE:HD11 | 1:N:171:LYS:HE2 | 2.00 | 0.43 |
| 1:B:183:LEU:HG | 1:B:384:ALA:HB2 | 2.01 | 0.42 |
| 1:B:462:PRO:HB2 | 2:B:1136:SO4:O1 | 2.19 | 0.42 |
| 1:C:326:ASN:ND2 | 1:C:329:THR:HB | 2.28 | 0.42 |
| 1:H:25:ASP:OD1 | 1:H:28:LYS:HE2 | 2.19 | 0.42 |
| 1:J:381:VAL:HG21 | 1:J:393:LYS:HA | 2.01 | 0.42 |
| 1:K:37:ASN:HD21 | 1:K:51:LYS:HE3 | 1.83 | 0.42 |
| 1:N:112:ASN:HA | 1:N:113:PRO:HD3 | 1.92 | 0.42 |
| 1:N:195:PHE:HB2 | 1:N:279:PRO:HB3 | 2.00 | 0.42 |
| 1:N:290:GLN:HB3 | 1:N:345:ARG:NH2 | 2.33 | 0.42 |
| 1:N:18:ARG:HG3 | 1:N:67:GLU:CD | 2.39 | 0.42 |
| 1:A:225:LYS:NZ | 1:A:232:GLU:OE2 | 2.52 | 0.42 |
| 1:B:386:GLU:HB2 | 1:C:281:PHE:HB3 | 2.00 | 0.42 |
| 1:C:364:LYS:HD3 | 1:C:364:LYS:HA | 1.88 | 0.42 |
| 1:F:112:ASN:HA | 1:F:113:PRO:HD3 | 1.93 | 0.42 |
| 1:I:190:VAL:HB | 1:I:334:ASP:OD1 | 2.19 | 0.42 |
| 1:I:372:LEU:HA | 1:I:372:LEU:HD12 | 1.88 | 0.42 |
| 1:I:49:ILE:HD12 | 1:J:513:LEU:HD13 | 2.01 | 0.42 |
| 1:L:158:VAL:HG13 | 1:L:396:VAL:HG22 | 2.01 | 0.42 |
| 1:L:242:LYS:O | 1:L:243:ALA:CB | 2.67 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:345:ARG:HA | 1:L:348:GLN:NE2 | 2.32 | 0.42 |
| 1:A:16:MET:HB3 | 1:A:514:MET:CE | 2.49 | 0.42 |
| 1:C:193:MET:HE2 | 1:C:292:ILE:HG12 | 2.00 | 0.42 |
| 1:C:169:VAL:CG1 | 1:C:377:ALA:HB2 | 2.49 | 0.42 |
| 1:E:455:VAL:CG1 | 1:E:460:GLU:HB2 | 2.49 | 0.42 |
| 1:F:242:LYS:O | 1:F:243:ALA:CB | 2.65 | 0.42 |
| 1:F:383:ALA:O | 1:F:384:ALA:CB | 2.64 | 0.42 |
| 1:F:82:ASN:HB2 | 1:F:89:THR:OG1 | 2.20 | 0.42 |
| 1:H:186:GLU:HB2 | 1:H:380:LYS:HB2 | 2.01 | 0.42 |
| 1:H:413:ALA:H | 1:H:475:ASN:HD21 | 1.67 | 0.42 |
| 1:I:501:ARG:O | 1:I:505:GLN:HG3 | 2.18 | 0.42 |
| 1:J:326:ASN:HB3 | 1:J:327:LYS:H | 1.67 | 0.42 |
| 1:J:472:GLY:HA3 | 1:J:476:TYR:HD2 | 1.84 | 0.42 |
| 1:K:16:MET:O | 1:K:20:VAL:HG13 | 2.18 | 0.42 |
| 1:M:230:ILE:HB | 1:M:258:ALA:HA | 2.00 | 0.42 |
| 1:M:501:ARG:O | 1:M:505:GLN:HG3 | 2.18 | 0.42 |
| 1:C:273:VAL:CG1 | 1:C:274:ALA:N | 2.82 | 0.42 |
| 1:D:252:GLU:O | 1:D:253:ASP:HB2 | 2.20 | 0.42 |
| 1:D:336:VAL:O | 1:D:336:VAL:HG12 | 2.18 | 0.42 |
| 1:E:296:THR:HB | 1:E:319:GLN:H | 1.84 | 0.42 |
| 1:E:131:LEU:HD21 | 1:E:500:THR:HG22 | 2.01 | 0.42 |
| 1:F:16:MET:HB3 | 1:F:514:MET:CE | 2.49 | 0.42 |
| 1:K:218:PRO:CB | 1:K:246:PRO:HG2 | 2.47 | 0.42 |
| 1:K:451:LEU:O | 1:K:451:LEU:HD23 | 2.18 | 0.42 |
| 1:L:223:ALA:O | 1:L:251:ALA:HA | 2.19 | 0.42 |
| 1:L:524:LEU:HA | 1:L:524:LEU:HD12 | 1.86 | 0.42 |
| 1:M:193:MET:HG2 | 1:M:194:GLN:H | 1.84 | 0.42 |
| 1:M:220:ILE:HD12 | 1:M:296:THR:HG21 | 2.00 | 0.42 |
| 1:M:293:ALA:O | 1:M:297:GLY:N | 2.52 | 0.42 |
| 1:M:499:VAL:CG2 | 1:M:500:THR:N | 2.83 | 0.42 |
| 1:A:118:ARG:HD2 | 1:A:436:GLN:NE2 | 2.34 | 0.42 |
| 1:C:359:ASP:HA | 1:C:362:ARG:HH12 | 1.84 | 0.42 |
| 1:D:182:GLY:O | 1:D:183:LEU:C | 2.58 | 0.42 |
| 1:D:41:ASP:HB2 | 1:E:69:MET:SD | 2.59 | 0.42 |
| 1:E:305:ILE:O | 1:E:305:ILE:HG22 | 2.18 | 0.42 |
| 1:F:326:ASN:HB3 | 1:F:327:LYS:H | 1.66 | 0.42 |
| 1:G:218:PRO:HB3 | 1:G:246:PRO:HG2 | 2.01 | 0.42 |
| 1:I:262:LEU:O | 1:I:266:THR:HG23 | 2.19 | 0.42 |
| 1:I:353:ILE:HG23 | 1:I:362:ARG:HG3 | 2.01 | 0.42 |
| 1:J:441:LYS:HA | 1:J:441:LYS:HD3 | 1.88 | 0.42 |
| 1:J:413:ALA:N | 1:J:475:ASN:HD22 | 2.18 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:166:MET:CE | 1:K:171:LYS:HA | 2.49 | 0.42 |
| 1:K:321:LYS:HD2 | 1:K:334:ASP:OD2 | 2.20 | 0.42 |
| 1:L:31:LEU:HD13 | 1:L:90:THR:HG22 | 2.00 | 0.42 |
| 1:M:372:LEU:HD12 | 1:M:372:LEU:HA | 1.88 | 0.42 |
| 1:B:248:LEU:HD13 | 1:B:325:ILE:HD11 | 2.01 | 0.42 |
| 1:F:364:LYS:O | 1:F:367:GLU:HB2 | 2.20 | 0.42 |
| 1:G:329:THR:HG22 | 1:G:329:THR:O | 2.19 | 0.42 |
| 1:H:16:MET:O | 1:H:20:VAL:HG13 | 2.19 | 0.42 |
| 1:H:441:LYS:O | 1:H:445:ARG:HB2 | 2.20 | 0.42 |
| 1:K:199:TYR:C | 1:K:201:SER:H | 2.21 | 0.42 |
| 1:K:7:LYS:HG3 | 1:K:66:PHE:CZ | 2.54 | 0.42 |
| 1:M:319:GLN:O | 1:M:336:VAL:HG23 | 2.19 | 0.42 |
| 1:M:37:ASN:ND2 | 1:M:51:LYS:HE3 | 2.33 | 0.42 |
| 1:N:123:ALA:HB2 | 1:N:440:ILE:HG23 | 2.02 | 0.42 |
| 1:N:451:LEU:C | 1:N:451:LEU:HD23 | 2.40 | 0.42 |
| 1:B:353:ILE:HG23 | 1:B:362:ARG:HG3 | 2.02 | 0.42 |
| 1:B:413:ALA:CB | 1:B:475:ASN:HD22 | 2.31 | 0.42 |
| 1:E:252:GLU:O | 1:E:253:ASP:HB2 | 2.19 | 0.42 |
| 1:E:436:GLN:O | 1:E:440:ILE:HG13 | 2.20 | 0.42 |
| 1:G:176:THR:HG22 | 1:G:177:VAL:N | 2.34 | 0.42 |
| 1:G:202:PRO:C | 1:G:204:PHE:N | 2.73 | 0.42 |
| 1:I:310:GLU:N | 1:I:310:GLU:OE1 | 2.49 | 0.42 |
| 1:J:203:TYR:C | 1:J:205:ILE:N | 2.73 | 0.42 |
| 1:J:363:GLU:H | 1:J:363:GLU:HG2 | 1.70 | 0.42 |
| 1:A:200:LEU:CD1 | 1:A:254:VAL:HB | 2.50 | 0.42 |
| 1:A:236:VAL:CG2 | 1:A:312:ALA:HB3 | 2.50 | 0.42 |
| 1:A:82:ASN:HB2 | 1:A:89:THR:OG1 | 2.19 | 0.42 |
| 1:C:166:MET:HE2 | 1:C:171:LYS:HA | 2.02 | 0.42 |
| 1:D:303:GLU:O | 1:D:306:GLY:N | 2.45 | 0.42 |
| 1:E:290:GLN:HB3 | 1:E:345:ARG:NH2 | 2.35 | 0.42 |
| 1:E:85:ALA:HB1 | 1:E:499:VAL:HG12 | 2.01 | 0.42 |
| 1:G:199:TYR:CD2 | 1:G:326:ASN:O | 2.73 | 0.42 |
| 1:H:358:SER:HB3 | 1:H:361:ASP:OD1 | 2.20 | 0.42 |
| 1:I:234:LEU:O | 1:I:238:GLU:HG3 | 2.20 | 0.42 |
| 1:I:221:LEU:HD11 | 1:I:301:ILE:HD12 | 2.02 | 0.42 |
| 1:I:68:ASN:O | 1:I:72:GLN:HG2 | 2.19 | 0.42 |
| 1:J:16:MET:HB3 | 1:J:514:MET:CE | 2.50 | 0.42 |
| 1:M:236:VAL:HG22 | 1:M:312:ALA:O | 2.19 | 0.42 |
| 1:N:186:GLU:HB2 | 1:N:380:LYS:HB2 | 2.02 | 0.42 |
| 1:B:194:GLN:O | 1:B:371:LYS:HE3 | 2.19 | 0.42 |
| 1:B:247:LEU:HD21 | 1:B:249:ILE:HD11 | 2.01 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:239:ALA:O | 1:C:314:LEU:HD11 | 2.19 | 0.42 |
| 1:D:429:LEU:HG | 1:D:440:ILE:HD13 | 2.01 | 0.42 |
| 1:D:118:ARG:HD2 | 1:D:436:GLN:HE22 | 1.84 | 0.42 |
| 1:E:266:THR:CG2 | 1:E:273:VAL:HB | 2.50 | 0.42 |
| 1:F:183:LEU:O | 1:F:184:GLN:CB | 2.68 | 0.42 |
| 1:F:319:GLN:O | 1:F:336:VAL:HG23 | 2.20 | 0.42 |
| 1:H:118:ARG:HD2 | 1:H:436:GLN:NE2 | 2.34 | 0.42 |
| 1:I:71:ALA:O | 1:I:75:LYS:HB2 | 2.20 | 0.42 |
| 1:J:270:ILE:O | 1:J:271:VAL:CB | 2.66 | 0.42 |
| 1:J:353:ILE:HG23 | 1:J:362:ARG:HG3 | 2.00 | 0.42 |
| 1:K:220:ILE:HD12 | 1:K:296:THR:CG2 | 2.50 | 0.42 |
| 1:M:132:LYS:O | 1:M:135:SER:HB3 | 2.20 | 0.42 |
| 1:M:186:GLU:HB2 | 1:M:380:LYS:HB2 | 2.01 | 0.42 |
| 1:N:234:LEU:O | 1:N:238:GLU:HG3 | 2.19 | 0.42 |
| 1:N:449:ALA:HA | 6:N:3091:HOH:O | 2.19 | 0.42 |
| 1:A:413:ALA:HB3 | 1:A:417:VAL:HG22 | 2.02 | 0.42 |
| 1:B:102:GLU:HB2 | 1:B:442:VAL:HG13 | 2.00 | 0.42 |
| 1:C:385:THR:H | 1:D:281:PHE:HE1 | 1.68 | 0.42 |
| 1:B:59:GLU:O | 1:C:4:LYS:HG3 | 2.20 | 0.42 |
| 1:E:16:MET:O | 1:E:20:VAL:HG13 | 2.20 | 0.42 |
| 1:E:218:PRO:CB | 1:E:246:PRO:HG2 | 2.46 | 0.42 |
| 1:F:413:ALA:CB | 1:F:417:VAL:HG22 | 2.49 | 0.42 |
| 1:G:7:LYS:HE3 | 1:G:15:LYS:HE3 | 2.01 | 0.42 |
| 1:H:304:GLU:C | 1:H:306:GLY:H | 2.23 | 0.42 |
| 1:I:349:ILE:HA | 1:I:352:GLN:CG | 2.49 | 0.42 |
| 1:J:118:ARG:HD2 | 1:J:436:GLN:NE2 | 2.34 | 0.42 |
| 1:L:349:ILE:HA | 1:L:352:GLN:CG | 2.48 | 0.42 |
| 1:L:441:LYS:O | 1:L:445:ARG:HB2 | 2.20 | 0.42 |
| 1:M:198:GLY:HA3 | 1:M:327:LYS:O | 2.20 | 0.42 |
| 1:M:413:ALA:HB1 | 1:M:488:MET:HG3 | 2.01 | 0.42 |
| 1:N:242:LYS:C | 1:N:244:GLY:H | 2.22 | 0.42 |
| 1:A:270:ILE:O | 1:A:271:VAL:HB | 2.19 | 0.41 |
| 1:B:169:VAL:CG1 | 1:B:377:ALA:HB2 | 2.50 | 0.41 |
| 1:B:239:ALA:O | 1:B:314:LEU:HD11 | 2.20 | 0.41 |
| 1:B:436:GLN:O | 1:B:440:ILE:HG13 | 2.19 | 0.41 |
| 1:B:460:GLU:O | 1:B:462:PRO:HD3 | 2.20 | 0.41 |
| 1:B:478:TYR:CE2 | 1:B:480:ALA:HA | 2.55 | 0.41 |
| 1:C:269:GLY:O | 1:D:229:ASN:OD1 | 2.38 | 0.41 |
| 1:D:118:ARG:HD2 | 1:D:436:GLN:NE2 | 2.35 | 0.41 |
| 1:G:501:ARG:HG2 | 1:G:501:ARG:HH11 | 1.84 | 0.41 |
| 1:J:455:VAL:CG1 | 1:J:460:GLU:HB2 | 2.47 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:242:LYS:O | 1:K:243:ALA:CB | 2.67 | 0.41 |
| 1:L:273:VAL:HG12 | 1:L:274:ALA:N | 2.35 | 0.41 |
| 1:L:451:LEU:C | 1:L:451:LEU:HD23 | 2.40 | 0.41 |
| 1:M:13:ARG:NH1 | 1:M:518:GLU:OE2 | 2.50 | 0.41 |
| 1:F:463:SER:HB3 | 1:N:461:GLU:OE2 | 2.20 | 0.41 |
| 1:A:478:TYR:CE2 | 1:A:480:ALA:HA | 2.55 | 0.41 |
| 1:C:457:ASN:OD1 | 4:C:1514:MPD:H13 | 2.20 | 0.41 |
| 1:C:40:LEU:HD13 | 1:C:59:GLU:HG3 | 2.01 | 0.41 |
| 1:D:254:VAL:HG21 | 1:D:275:ALA:HB1 | 2.01 | 0.41 |
| 1:F:217:SER:N | 1:F:218:PRO:HD3 | 2.35 | 0.41 |
| 1:H:202:PRO:C | 1:H:204:PHE:H | 2.23 | 0.41 |
| 1:I:236:VAL:O | 1:I:240:VAL:HG23 | 2.20 | 0.41 |
| 1:I:144:ILE:HG23 | 1:I:403:THR:HG21 | 2.02 | 0.41 |
| 1:I:83:ASP:OD2 | 1:I:327:LYS:HE2 | 2.19 | 0.41 |
| 1:J:30:THR:HG22 | 1:J:36:ARG:O | 2.19 | 0.41 |
| 1:K:207:LYS:O | 1:K:211:GLY:N | 2.53 | 0.41 |
| 1:K:451:LEU:C | 1:K:451:LEU:HD23 | 2.40 | 0.41 |
| 1:L:266:THR:CG2 | 1:L:273:VAL:HB | 2.50 | 0.41 |
| 1:M:218:PRO:HD2 | 1:M:320:ALA:O | 2.20 | 0.41 |
| 1:A:122:LYS:HE2 | 1:A:429:LEU:HD11 | 2.02 | 0.41 |
| 1:A:289:LEU:HA | 1:A:289:LEU:HD23 | 1.86 | 0.41 |
| 1:B:112:ASN:HA | 1:B:113:PRO:HD3 | 1.93 | 0.41 |
| 1:C:118:ARG:HD2 | 1:C:436:GLN:HE22 | 1.85 | 0.41 |
| 1:C:202:PRO:C | 1:C:204:PHE:N | 2.73 | 0.41 |
| 1:E:220:ILE:CD1 | 1:E:296:THR:HG21 | 2.48 | 0.41 |
| 1:G:217:SER:N | 1:G:218:PRO:CD | 2.84 | 0.41 |
| 1:I:349:ILE:CG2 | 1:I:369:VAL:HG13 | 2.50 | 0.41 |
| 1:J:413:ALA:CB | 1:J:417:VAL:HG22 | 2.50 | 0.41 |
| 1:K:132:LYS:O | 1:K:135:SER:HB3 | 2.20 | 0.41 |
| 1:L:326:ASN:HB3 | 1:L:327:LYS:H | 1.75 | 0.41 |
| 1:M:304:GLU:C | 1:M:306:GLY:H | 2.23 | 0.41 |
| 1:N:183:LEU:O | 1:N:184:GLN:CB | 2.58 | 0.41 |
| 1:N:262:LEU:O | 1:N:266:THR:HG23 | 2.19 | 0.41 |
| 1:C:218:PRO:HB3 | 1:C:246:PRO:HG2 | 2.02 | 0.41 |
| 1:F:130:GLU:HG3 | 6:F:3137:HOH:O | 2.19 | 0.41 |
| 1:F:158:VAL:HG13 | 1:F:396:VAL:HG22 | 2.03 | 0.41 |
| 1:G:353:ILE:HD13 | 1:G:366:GLN:HG3 | 2.01 | 0.41 |
| 1:H:438:VAL:O | 1:H:442:VAL:HG23 | 2.19 | 0.41 |
| 1:I:188:ASP:OD1 | 1:I:188:ASP:N | 2.54 | 0.41 |
| 1:J:123:ALA:HB2 | 1:J:440:ILE:HG23 | 2.01 | 0.41 |
| 1:J:134:LEU:HD13 | 1:J:134:LEU:O | 2.20 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:242:LYS:O | 1:J:243:ALA:CB | 2.64 | 0.41 |
| 1:J:369:VAL:HG23 | 1:J:370:ALA:N | 2.35 | 0.41 |
| 1:J:460:GLU:O | 1:J:462:PRO:HD3 | 2.20 | 0.41 |
| 1:K:144:ILE:HG23 | 1:K:403:THR:HG21 | 2.02 | 0.41 |
| 1:K:413:ALA:CB | 1:K:417:VAL:HG22 | 2.50 | 0.41 |
| 1:M:413:ALA:H | 1:M:475:ASN:HD21 | 1.65 | 0.41 |
| 1:A:269:GLY:O | 1:B:229:ASN:OD1 | 2.39 | 0.41 |
| 1:B:141:SER:HB3 | 6:B:3163:HOH:O | 2.19 | 0.41 |
| 1:C:24:ALA:O | 1:C:28:LYS:HG2 | 2.21 | 0.41 |
| 1:C:193:MET:HG3 | 1:C:371:LYS:HB3 | 2.03 | 0.41 |
| 1:B:63:GLU:HB2 | 1:C:524:LEU:HD21 | 2.03 | 0.41 |
| 1:D:299:THR:N | 1:D:316:ASP:O | 2.50 | 0.41 |
| 1:F:225:LYS:HB2 | 1:F:225:LYS:HE3 | 1.82 | 0.41 |
| 1:G:193:MET:CE | 1:G:292:ILE:HG12 | 2.51 | 0.41 |
| 1:G:342:ILE:O | 1:G:346:VAL:HG23 | 2.21 | 0.41 |
| 1:H:118:ARG:HD2 | 1:H:436:GLN:HE22 | 1.86 | 0.41 |
| 1:H:513:LEU:HD13 | 1:N:49:ILE:CD1 | 2.51 | 0.41 |
| 1:K:70:GLY:HA2 | 1:K:73:MET:HE3 | 2.02 | 0.41 |
| 1:L:319:GLN:HB3 | 1:L:336:VAL:CG2 | 2.49 | 0.41 |
| 1:M:272:LYS:NZ | 1:N:229:ASN:HD21 | 2.16 | 0.41 |
| 1:M:354:GLU:C | 1:M:356:ALA:H | 2.24 | 0.41 |
| 1:M:413:ALA:HB3 | 1:M:417:VAL:HG22 | 2.03 | 0.41 |
| 1:M:472:GLY:HA3 | 1:M:476:TYR:HD2 | 1.85 | 0.41 |
| 1:N:224:ASP:O | 1:N:225:LYS:CB | 2.65 | 0.41 |
| 1:B:452:ARG:HD3 | 2:B:1136:SO4:O2 | 2.20 | 0.41 |
| 1:B:193:MET:CE | 1:B:292:ILE:HG12 | 2.51 | 0.41 |
| 1:B:213:VAL:HB | 1:B:325:ILE:HB | 2.03 | 0.41 |
| 1:B:218:PRO:CB | 1:B:246:PRO:HG2 | 2.44 | 0.41 |
| 1:C:122:LYS:HE2 | 1:C:429:LEU:HD11 | 2.02 | 0.41 |
| 1:C:176:THR:HG22 | 1:C:177:VAL:N | 2.35 | 0.41 |
| 1:C:224:ASP:O | 1:C:225:LYS:HB3 | 2.21 | 0.41 |
| 1:E:203:TYR:C | 1:E:205:ILE:N | 2.74 | 0.41 |
| 1:E:342:ILE:O | 1:E:346:VAL:HG23 | 2.21 | 0.41 |
| 1:D:49:ILE:HD12 | 1:E:513:LEU:HD13 | 2.01 | 0.41 |
| 1:F:270:ILE:O | 1:F:271:VAL:CB | 2.68 | 0.41 |
| 1:G:364:LYS:O | 1:G:367:GLU:HB2 | 2.20 | 0.41 |
| 1:G:478:TYR:CE2 | 1:G:480:ALA:HA | 2.56 | 0.41 |
| 1:G:524:LEU:HA | 1:G:524:LEU:HD12 | 1.77 | 0.41 |
| 1:I:259:LEU:O | 1:I:263:VAL:HG23 | 2.20 | 0.41 |
| 1:J:429:LEU:HG | 1:J:440:ILE:HD13 | 2.03 | 0.41 |
| 1:K:300:VAL:O | 1:K:307:MET:HE1 | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:369:VAL:HG23 | 1:K:370:ALA:N | 2.35 | 0.41 |
| 1:M:25:ASP:OD1 | 1:M:28:LYS:HE2 | 2.21 | 0.41 |
| 1:N:205:ILE:HG23 | 1:N:212:ALA:O | 2.20 | 0.41 |
| 1:A:217:SER:N | 1:A:218:PRO:HD3 | 2.35 | 0.41 |
| 1:B:216:GLU:C | 1:B:218:PRO:HD3 | 2.41 | 0.41 |
| 1:B:305:ILE:HB | 1:B:307:MET:CE | 2.50 | 0.41 |
| 1:B:404:ARG:HH11 | 1:B:404:ARG:CG | 2.30 | 0.41 |
| 1:F:445:ARG:HG2 | 2:F:1141:SO4:O3 | 2.20 | 0.41 |
| 1:F:262:LEU:O | 1:F:266:THR:HG23 | 2.20 | 0.41 |
| 1:F:271:VAL:HG12 | 1:F:273:VAL:HG23 | 2.02 | 0.41 |
| 1:G:24:ALA:O | 1:G:28:LYS:HG2 | 2.21 | 0.41 |
| 1:G:420:ILE:CG1 | 1:G:448:GLU:HG2 | 2.46 | 0.41 |
| 1:I:183:LEU:HD22 | 1:I:184:GLN:H | 1.85 | 0.41 |
| 1:I:478:TYR:CE2 | 1:I:480:ALA:HA | 2.54 | 0.41 |
| 1:J:16:MET:O | 1:J:20:VAL:HG13 | 2.21 | 0.41 |
| 1:K:183:LEU:HD22 | 1:K:184:GLN:N | 2.36 | 0.41 |
| 1:L:230:ILE:HD13 | 1:L:261:THR:HG22 | 2.01 | 0.41 |
| 1:L:180:GLY:HA3 | 1:L:381:VAL:O | 2.21 | 0.41 |
| 1:N:183:LEU:HD22 | 1:N:184:GLN:N | 2.35 | 0.41 |
| 1:B:385:THR:OG1 | 1:B:388:GLU:HG3 | 2.20 | 0.41 |
| 1:B:38:VAL:HG22 | 1:C:519:CYS:HB3 | 2.03 | 0.41 |
| 1:C:242:LYS:O | 1:C:243:ALA:HB3 | 2.20 | 0.41 |
| 1:C:353:ILE:HG23 | 1:C:362:ARG:HG3 | 2.03 | 0.41 |
| 1:E:13:ARG:HD3 | 1:E:104:LEU:HD22 | 2.02 | 0.41 |
| 1:E:71:ALA:O | 1:E:75:LYS:HB2 | 2.21 | 0.41 |
| 1:G:166:MET:CE | 1:G:171:LYS:HA | 2.51 | 0.41 |
| 1:H:217:SER:N | 1:H:218:PRO:HD3 | 2.34 | 0.41 |
| 1:J:392:LYS:O | 1:J:396:VAL:HG23 | 2.20 | 0.41 |
| 1:K:224:ASP:O | 1:K:225:LYS:CB | 2.65 | 0.41 |
| 1:K:353:ILE:HG23 | 1:K:362:ARG:HG3 | 2.02 | 0.41 |
| 1:L:354:GLU:C | 1:L:356:ALA:H | 2.24 | 0.41 |
| 1:L:413:ALA:HB3 | 1:L:417:VAL:HG22 | 2.02 | 0.41 |
| 1:M:152:ALA:O | 1:M:153:ASN:HB3 | 2.21 | 0.41 |
| 1:M:193:MET:CG | 1:M:194:GLN:N | 2.82 | 0.41 |
| 1:M:85:ALA:CB | 1:M:499:VAL:HG12 | 2.41 | 0.41 |
| 1:N:218:PRO:CA | 1:N:246:PRO:HG2 | 2.50 | 0.41 |
| 1:N:314:LEU:HA | 1:N:317:LEU:HD22 | 2.03 | 0.41 |
| 1:N:352:GLN:H | 1:N:352:GLN:HG2 | 1.68 | 0.41 |
| 1:A:372:LEU:HD12 | 1:A:372:LEU:HA | 1.85 | 0.41 |
| 1:B:202:PRO:C | 1:B:204:PHE:N | 2.73 | 0.41 |
| 1:B:349:ILE:CG2 | 1:B:369:VAL:HG13 | 2.50 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:266:THR:CG2 | 1:C:273:VAL:HB | 2.50 | 0.41 |
| 1:C:288:MET:O | 1:C:292:ILE:HG13 | 2.20 | 0.41 |
| 1:D:225:LYS:NZ | 1:D:232:GLU:OE2 | 2.54 | 0.41 |
| 1:F:381:VAL:HG21 | 1:F:393:LYS:HA | 2.02 | 0.41 |
| 1:G:496:PRO:HB2 | 1:G:499:VAL:HG13 | 2.02 | 0.41 |
| 1:H:230:ILE:HB | 1:H:258:ALA:HA | 2.03 | 0.41 |
| 1:I:176:THR:CG2 | 1:I:177:VAL:N | 2.83 | 0.41 |
| 1:J:5:ASP:HB2 | 1:J:524:LEU:CD1 | 2.46 | 0.41 |
| 1:K:183:LEU:O | 1:K:184:GLN:CB | 2.55 | 0.41 |
| 1:K:413:ALA:H | 1:K:475:ASN:HD22 | 1.64 | 0.41 |
| 1:K:30:THR:HB | 1:K:51:LYS:O | 2.21 | 0.41 |
| 1:L:136:VAL:HA | 1:L:137:PRO:HD3 | 1.94 | 0.41 |
| 1:L:461:GLU:HB2 | 6:L:3097:HOH:O | 2.21 | 0.41 |
| 1:M:270:ILE:O | 1:M:271:VAL:CB | 2.69 | 0.41 |
| 1:N:457:ASN:HA | 4:N:1517:MPD:HM3 | 2.03 | 0.41 |
| 1:C:176:THR:HG21 | 1:C:333:ILE:CD1 | 2.34 | 0.41 |
| 1:C:31:LEU:HD12 | 1:C:31:LEU:HA | 1.83 | 0.41 |
| 1:D:349:ILE:HG21 | 1:D:369:VAL:HG13 | 2.03 | 0.41 |
| 1:D:381:VAL:HG21 | 1:D:393:LYS:HA | 2.03 | 0.41 |
| 1:E:326:ASN:ND2 | 1:E:329:THR:HB | 2.30 | 0.41 |
| 1:F:224:ASP:O | 1:F:225:LYS:HB3 | 2.21 | 0.41 |
| 1:G:429:LEU:HG | 1:G:440:ILE:HD13 | 2.02 | 0.41 |
| 1:H:221:LEU:HD11 | 1:H:301:ILE:HD12 | 2.03 | 0.41 |
| 1:H:242:LYS:C | 1:H:244:GLY:H | 2.24 | 0.41 |
| 1:I:352:GLN:HG2 | 1:I:352:GLN:H | 1.66 | 0.41 |
| 1:J:339:GLU:O | 1:J:343:GLN:HB2 | 2.20 | 0.41 |
| 1:L:413:ALA:CB | 1:L:417:VAL:HG22 | 2.51 | 0.41 |
| 1:N:199:TYR:C | 1:N:201:SER:H | 2.23 | 0.41 |
| 1:A:193:MET:HG3 | 1:A:371:LYS:HB3 | 2.03 | 0.41 |
| 1:D:16:MET:O | 1:D:20:VAL:HG13 | 2.21 | 0.41 |
| 1:D:219:PHE:HB3 | 1:D:317:LEU:HD23 | 2.03 | 0.41 |
| 1:E:344:GLY:O | 1:E:348:GLN:HG3 | 2.21 | 0.41 |
| 1:G:264:VAL:HG12 | 1:G:265:ASN:N | 2.36 | 0.41 |
| 1:I:16:MET:HB3 | 1:I:514:MET:HE1 | 2.02 | 0.41 |
| 1:J:124:VAL:HG21 | 1:J:508:ALA:CB | 2.51 | 0.41 |
| 1:K:176:THR:HG22 | 1:K:177:VAL:N | 2.36 | 0.41 |
| 1:K:225:LYS:HD2 | 1:K:226:LYS:O | 2.20 | 0.41 |
| 1:L:451:LEU:HD23 | 1:L:455:VAL:HG23 | 2.02 | 0.41 |
| 1:M:200:LEU:HG | 1:M:276:VAL:HA | 2.02 | 0.41 |
| 1:M:199:TYR:CD2 | 1:M:326:ASN:O | 2.74 | 0.41 |
| 1:N:240:VAL:HG11 | 1:N:247:LEU:HB2 | 2.03 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:24:ALA:O | 1:N:28:LYS:HG2 | 2.21 | 0.41 |
| 1:B:166:MET:HE2 | 1:B:171:LYS:HA | 2.03 | 0.40 |
| 1:B:413:ALA:CB | 1:B:417:VAL:HG22 | 2.50 | 0.40 |
| 1:D:221:LEU:HD23 | 1:D:249:ILE:HD12 | 2.03 | 0.40 |
| 1:D:230:ILE:HD13 | 1:D:261:THR:CG2 | 2.50 | 0.40 |
| 1:D:247:LEU:HD21 | 1:D:249:ILE:CD1 | 2.50 | 0.40 |
| 1:F:384:ALA:O | 1:F:385:THR:CG2 | 2.67 | 0.40 |
| 1:G:385:THR:OG1 | 1:G:388:GLU:HG3 | 2.20 | 0.40 |
| 1:K:134:LEU:HD12 | 1:K:412:VAL:HB | 2.03 | 0.40 |
| 1:K:232:GLU:HB3 | 1:K:309:LEU:HB2 | 2.03 | 0.40 |
| 1:L:70:GLY:HA2 | 1:L:73:MET:HE3 | 2.03 | 0.40 |
| 1:M:118:ARG:HD2 | 1:M:436:GLN:NE2 | 2.37 | 0.40 |
| 1:N:392:LYS:O | 1:N:396:VAL:HG23 | 2.21 | 0.40 |
| 1:N:472:GLY:HA3 | 1:N:476:TYR:HD2 | 1.86 | 0.40 |
| 1:A:266:THR:HG21 | 1:A:273:VAL:HB | 2.03 | 0.40 |
| 1:B:199:TYR:C | 1:B:201:SER:H | 2.23 | 0.40 |
| 1:B:242:LYS:C | 1:B:244:GLY:N | 2.75 | 0.40 |
| 1:C:183:LEU:O | 1:C:184:GLN:CB | 2.68 | 0.40 |
| 1:C:217:SER:N | 1:C:218:PRO:HD3 | 2.36 | 0.40 |
| 1:C:90:THR:O | 1:C:94:VAL:HG13 | 2.21 | 0.40 |
| 1:E:353:ILE:HD13 | 1:E:366:GLN:HG3 | 2.04 | 0.40 |
| 1:E:70:GLY:HA2 | 1:E:73:MET:HE2 | 2.01 | 0.40 |
| 1:F:39:VAL:HG12 | 1:G:69:MET:CE | 2.52 | 0.40 |
| 1:F:144:ILE:HG23 | 1:F:403:THR:HG21 | 2.03 | 0.40 |
| 1:A:228:SER:HB3 | 1:G:272:LYS:HZ3 | 1.86 | 0.40 |
| 1:G:85:ALA:HB1 | 1:G:499:VAL:HG12 | 2.02 | 0.40 |
| 1:I:451:LEU:O | 1:I:451:LEU:HD23 | 2.20 | 0.40 |
| 1:J:176:THR:HG22 | 1:J:177:VAL:N | 2.36 | 0.40 |
| 1:J:205:ILE:HG23 | 1:J:212:ALA:O | 2.21 | 0.40 |
| 1:K:284:ARG:NH1 | 6:K:3077:HOH:O | 2.53 | 0.40 |
| 1:L:23:LEU:CD2 | 1:L:74:VAL:HG22 | 2.51 | 0.40 |
| 1:L:241:ALA:C | 1:M:231:ARG:NH1 | 2.74 | 0.40 |
| 1:M:358:SER:HB3 | 1:M:361:ASP:OD1 | 2.20 | 0.40 |
| 1:B:16:MET:O | 1:B:20:VAL:HG13 | 2.21 | 0.40 |
| 1:B:16:MET:HB3 | 1:B:514:MET:HE1 | 2.02 | 0.40 |
| 1:C:68:ASN:O | 1:C:72:GLN:HG2 | 2.21 | 0.40 |
| 1:D:102:GLU:HB2 | 1:D:442:VAL:HG13 | 2.04 | 0.40 |
| 1:F:524:LEU:HD12 | 1:F:524:LEU:HA | 1.75 | 0.40 |
| 1:F:7:LYS:HE3 | 1:F:15:LYS:HE3 | 2.04 | 0.40 |
| 1:H:501:ARG:O | 1:H:505:GLN:HG3 | 2.21 | 0.40 |
| 1:H:23:LEU:CD2 | 1:H:74:VAL:HG22 | 2.51 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:100:ILE:O | 1:J:104:LEU:HG | 2.22 | 0.40 |
| 1:J:501:ARG:O | 1:J:505:GLN:HG3 | 2.21 | 0.40 |
| 1:L:201:SER:C | 1:L:202:PRO:O | 2.60 | 0.40 |
| 1:M:144:ILE:HD11 | 1:M:171:LYS:HE2 | 2.02 | 0.40 |
| 1:A:13:ARG:HD3 | 1:A:104:LEU:HD22 | 2.02 | 0.40 |
| 1:A:364:LYS:HD3 | 1:A:364:LYS:HA | 1.85 | 0.40 |
| 1:B:247:LEU:HB3 | 1:B:273:VAL:HG22 | 2.04 | 0.40 |
| 1:C:169:VAL:HG11 | 1:C:377:ALA:HB2 | 2.04 | 0.40 |
| 1:C:494:LEU:HD12 | 1:C:494:LEU:C | 2.41 | 0.40 |
| 1:D:144:ILE:HG23 | 1:D:403:THR:HG21 | 2.03 | 0.40 |
| 1:E:190:VAL:HG21 | 1:E:333:ILE:HG23 | 2.03 | 0.40 |
| 1:E:242:LYS:O | 1:E:244:GLY:N | 2.54 | 0.40 |
| 1:E:131:LEU:CD1 | 1:E:422:VAL:HG21 | 2.46 | 0.40 |
| 1:F:429:LEU:HG | 1:F:440:ILE:HD13 | 2.03 | 0.40 |
| 1:F:77:VAL:HG12 | 1:F:506:TYR:HB3 | 2.03 | 0.40 |
| 1:G:383:ALA:O | 1:G:384:ALA:CB | 2.69 | 0.40 |
| 1:G:381:VAL:HG21 | 1:G:393:LYS:HA | 2.04 | 0.40 |
| 1:H:524:LEU:HD12 | 1:H:524:LEU:HA | 1.82 | 0.40 |
| 1:K:146:GLN:O | 1:K:150:ILE:HG13 | 2.22 | 0.40 |
| 1:K:230:ILE:O | 1:K:230:ILE:HG12 | 2.21 | 0.40 |
| 1:K:339:GLU:O | 1:K:343:GLN:HB2 | 2.22 | 0.40 |
| 1:L:372:LEU:HA | 1:L:372:LEU:HD12 | 1.92 | 0.40 |
| 1:M:344:GLY:O | 1:M:347:ALA:HB3 | 2.21 | 0.40 |
| 1:M:71:ALA:O | 1:M:75:LYS:HB2 | 2.21 | 0.40 |
| 1:N:203:TYR:C | 1:N:205:ILE:N | 2.74 | 0.40 |
| 1:N:304:GLU:C | 1:N:306:GLY:H | 2.25 | 0.40 |
| 1:N:71:ALA:O | 1:N:75:LYS:HB2 | 2.22 | 0.40 |
| 1:C:144:ILE:HG23 | 1:C:403:THR:CG2 | 2.52 | 0.40 |
| 1:C:29:VAL:HG12 | 4:C:1514:MPD:H12 | 2.03 | 0.40 |
| 1:C:7:LYS:HE3 | 1:C:15:LYS:HE3 | 2.03 | 0.40 |
| 1:C:451:LEU:O | 1:C:451:LEU:HD23 | 2.22 | 0.40 |
| 1:E:185:ASP:HA | 1:E:380:LYS:O | 2.21 | 0.40 |
| 1:F:153:ASN:O | 1:F:154:SER:HB2 | 2.22 | 0.40 |
| 1:G:218:PRO:HD2 | 1:G:320:ALA:O | 2.22 | 0.40 |
| 1:H:18:ARG:HG3 | 1:H:67:GLU:CD | 2.42 | 0.40 |
| 1:I:282:GLY:O | 1:I:285:ARG:HB3 | 2.21 | 0.40 |
| 1:I:31:LEU:HD13 | 1:I:90:THR:HG21 | 2.04 | 0.40 |
| 1:K:290:GLN:O | 1:K:293:ALA:HB3 | 2.22 | 0.40 |
| 1:K:344:GLY:O | 1:K:347:ALA:HB3 | 2.21 | 0.40 |
| 1:L:287:ALA:HB1 | 1:L:368:ARG:HH12 | 1.84 | 0.40 |
| 1:L:65:LYS:H | 1:L:65:LYS:HG2 | 1.73 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:289:LEU:HD23 | 1:M:289:LEU:HA | 1.85 | 0.40 |
| 1:M:25:ASP:HA | 1:M:28:LYS:HE2 | 2.04 | 0.40 |
| 1:N:239:ALA:HB1 | 1:N:314:LEU:HG | 2.03 | 0.40 |
| 1:N:144:ILE:HG23 | 1:N:403:THR:HG21 | 2.02 | 0.40 |
| 1:N:429:LEU:HG | 1:N:440:ILE:HD13 | 2.03 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | A | 522/547 (95%) | 488 (94%) | 26 (5%) | 8 (2%) | 10 | 32 |
| 1 | B | 522/547 (95%) | 485 (93%) | 28 (5%) | 9 (2%) | 9 | 29 |
| 1 | C | 522/547 (95%) | 489 (94%) | 24 (5%) | 9 (2%) | 9 | 29 |
| 1 | D | 522/547 (95%) | 488 (94%) | 25 (5%) | 9 (2%) | 9 | 29 |
| 1 | E | 522/547 (95%) | 487 (93%) | 28 (5%) | 7 (1%) | 12 | 36 |
| 1 | F | 522/547 (95%) | 493 (94%) | 20 (4%) | 9 (2%) | 9 | 29 |
| 1 | G | 522/547 (95%) | 488 (94%) | 26 (5%) | 8 (2%) | 10 | 32 |
| 1 | H | 522/547 (95%) | 491 (94%) | 23 (4%) | 8 (2%) | 10 | 32 |
| 1 | I | 522/547 (95%) | 491 (94%) | 25 (5%) | 6 (1%) | 14 | 41 |
| 1 | J | 522/547 (95%) | 490 (94%) | 26 (5%) | 6 (1%) | 14 | 41 |
| 1 | K | 522/547 (95%) | 491 (94%) | 23 (4%) | 8 (2%) | 10 | 32 |
| 1 | L | 522/547 (95%) | 488 (94%) | 26 (5%) | 8 (2%) | 10 | 32 |
| 1 | M | 522/547 (95%) | 492 (94%) | 22 (4%) | 8 (2%) | 10 | 32 |
| 1 | N | 522/547 (95%) | 491 (94%) | 23 (4%) | 8 (2%) | 10 | 32 |
| All | All | 7308/7658 (95%) | 6852 (94%) | 345 (5%) | 111 (2%) | 10 | 32 |

All (111) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 184 | GLN |
| 1 | B | 183 | LEU |
| 1 | B | 184 | GLN |
| 1 | C | 183 | LEU |
| 1 | C | 184 | GLN |
| 1 | D | 183 | LEU |
| 1 | D | 184 | GLN |
| 1 | E | 183 | LEU |
| 1 | E | 184 | GLN |
| 1 | F | 183 | LEU |
| 1 | F | 184 | GLN |
| 1 | G | 183 | LEU |
| 1 | G | 184 | GLN |
| 1 | A | 183 | LEU |
| 1 | A | 256 | GLY |
| 1 | A | 385 | THR |
| 1 | B | 202 | PRO |
| 1 | B | 385 | THR |
| 1 | C | 256 | GLY |
| 1 | C | 385 | THR |
| 1 | D | 31 | LEU |
| 1 | D | 202 | PRO |
| 1 | D | 256 | GLY |
| 1 | D | 385 | THR |
| 1 | E | 202 | PRO |
| 1 | E | 385 | THR |
| 1 | F | 256 | GLY |
| 1 | F | 385 | THR |
| 1 | G | 256 | GLY |
| 1 | G | 385 | THR |
| 1 | H | 256 | GLY |
| 1 | H | 271 | VAL |
| 1 | I | 256 | GLY |
| 1 | J | 225 | LYS |
| 1 | J | 256 | GLY |
| 1 | K | 202 | PRO |
| 1 | K | 256 | GLY |
| 1 | L | 225 | LYS |
| 1 | L | 256 | GLY |
| 1 | M | 256 | GLY |
| 1 | M | 271 | VAL |
| 1 | N | 202 | PRO |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 225 | LYS |
| 1 | N | 256 | GLY |
| 1 | A | 202 | PRO |
| 1 | A | 271 | VAL |
| 1 | B | 256 | GLY |
| 1 | B | 383 | ALA |
| 1 | C | 202 | PRO |
| 1 | E | 271 | VAL |
| 1 | E | 383 | ALA |
| 1 | F | 225 | LYS |
| 1 | F | 271 | VAL |
| 1 | G | 202 | PRO |
| 1 | G | 271 | VAL |
| 1 | H | 184 | GLN |
| 1 | H | 202 | PRO |
| 1 | I | 184 | GLN |
| 1 | I | 271 | VAL |
| 1 | J | 184 | GLN |
| 1 | J | 202 | PRO |
| 1 | J | 271 | VAL |
| 1 | K | 9 | GLY |
| 1 | K | 184 | GLN |
| 1 | K | 225 | LYS |
| 1 | K | 271 | VAL |
| 1 | L | 184 | GLN |
| 1 | L | 202 | PRO |
| 1 | L | 271 | VAL |
| 1 | M | 202 | PRO |
| 1 | M | 225 | LYS |
| 1 | N | 184 | GLN |
| 1 | B | 225 | LYS |
| 1 | B | 271 | VAL |
| 1 | C | 225 | LYS |
| 1 | C | 271 | VAL |
| 1 | C | 383 | ALA |
| 1 | D | 271 | VAL |
| 1 | D | 383 | ALA |
| 1 | E | 256 | GLY |
| 1 | F | 202 | PRO |
| 1 | F | 383 | ALA |
| 1 | G | 383 | ALA |
| 1 | I | 9 | GLY |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 202 | PRO |
| 1 | I | 225 | LYS |
| 1 | M | 184 | GLN |
| 1 | M | 201 | SER |
| 1 | N | 271 | VAL |
| 1 | A | 383 | ALA |
| 1 | H | 31 | LEU |
| 1 | H | 225 | LYS |
| 1 | K | 230 | ILE |
| 1 | M | 9 | GLY |
| 1 | N | 230 | ILE |
| 1 | D | 225 | LYS |
| 1 | H | 9 | GLY |
| 1 | J | 9 | GLY |
| 1 | L | 9 | GLY |
| 1 | N | 9 | GLY |
| 1 | N | 201 | SER |
| 1 | B | 234 | LEU |
| 1 | G | 9 | GLY |
| 1 | L | 201 | SER |
| 1 | A | 9 | GLY |
| 1 | F | 9 | GLY |
| 1 | H | 230 | ILE |
| 1 | K | 201 | SER |
| 1 | L | 230 | ILE |
| 1 | C | 9 | GLY |
| 1 | M | 230 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | A | 404/414 (98%) | 393 (97%) | 11 (3%) | 44 | 75 |
| 1 | B | 404/414 (98%) | 393 (97%) | 11 (3%) | 44 | 75 |
| 1 | C | 404/414 (98%) | 391 (97%) | 13 (3%) | 39 | 71 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | D | 404/414 (98%) | 393 (97%) | 11 (3%) | 44 | 75 |
| 1 | E | 404/414 (98%) | 392 (97%) | 12 (3%) | 41 | 73 |
| 1 | F | 404/414 (98%) | 392 (97%) | 12 (3%) | 41 | 73 |
| 1 | G | 404/414 (98%) | 391 (97%) | 13 (3%) | 39 | 71 |
| 1 | H | 404/414 (98%) | 390 (96%) | 14 (4%) | 36 | 68 |
| 1 | I | 404/414 (98%) | 390 (96%) | 14 (4%) | 36 | 68 |
| 1 | J | 404/414 (98%) | 388 (96%) | 16 (4%) | 31 | 63 |
| 1 | K | 404/414 (98%) | 389 (96%) | 15 (4%) | 34 | 66 |
| 1 | L | 404/414 (98%) | 390 (96%) | 14 (4%) | 36 | 68 |
| 1 | M | 404/414 (98%) | 388 (96%) | 16 (4%) | 31 | 63 |
| 1 | N | 404/414 (98%) | 389 (96%) | 15 (4%) | 34 | 66 |
| All | All | 5656/5796 (98%) | 5469 (97%) | 187 (3%) | 38 | 70 |

All (187) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 129 | GLU |
| 1 | A | 131 | LEU |
| 1 | A | 134 | LEU |
| 1 | A | 177 | VAL |
| 1 | A | 284 | ARG |
| 1 | A | 329 | THR |
| 1 | A | 331 | THR |
| 1 | A | 361 | ASP |
| 1 | A | 398 | ASP |
| 1 | A | 404 | ARG |
| 1 | A | 524 | LEU |
| 1 | B | 74 | VAL |
| 1 | B | 94 | VAL |
| 1 | B | 129 | GLU |
| 1 | B | 134 | LEU |
| 1 | B | 177 | VAL |
| 1 | B | 284 | ARG |
| 1 | B | 328 | ASP |
| 1 | B | 361 | ASP |
| 1 | B | 398 | ASP |
| 1 | B | 404 | ARG |
| 1 | B | 524 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 74 | VAL |
| 1 | C | 129 | GLU |
| 1 | C | 134 | LEU |
| 1 | C | 177 | VAL |
| 1 | C | 183 | LEU |
| 1 | C | 284 | ARG |
| 1 | C | 328 | ASP |
| 1 | C | 329 | THR |
| 1 | C | 331 | THR |
| 1 | C | 361 | ASP |
| 1 | C | 398 | ASP |
| 1 | C | 404 | ARG |
| 1 | C | 524 | LEU |
| 1 | D | 74 | VAL |
| 1 | D | 134 | LEU |
| 1 | D | 177 | VAL |
| 1 | D | 284 | ARG |
| 1 | D | 328 | ASP |
| 1 | D | 329 | THR |
| 1 | D | 331 | THR |
| 1 | D | 361 | ASP |
| 1 | D | 398 | ASP |
| 1 | D | 404 | ARG |
| 1 | D | 524 | LEU |
| 1 | E | 129 | GLU |
| 1 | E | 131 | LEU |
| 1 | E | 134 | LEU |
| 1 | E | 177 | VAL |
| 1 | E | 199 | TYR |
| 1 | E | 218 | PRO |
| 1 | E | 284 | ARG |
| 1 | E | 331 | THR |
| 1 | E | 372 | LEU |
| 1 | E | 398 | ASP |
| 1 | E | 404 | ARG |
| 1 | E | 524 | LEU |
| 1 | F | 74 | VAL |
| 1 | F | 134 | LEU |
| 1 | F | 177 | VAL |
| 1 | F | 284 | ARG |
| 1 | F | 295 | LEU |
| 1 | F | 328 | ASP |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 329 | THR |
| 1 | F | 331 | THR |
| 1 | F | 361 | ASP |
| 1 | F | 398 | ASP |
| 1 | F | 404 | ARG |
| 1 | F | 524 | LEU |
| 1 | G | 74 | VAL |
| 1 | G | 129 | GLU |
| 1 | G | 134 | LEU |
| 1 | G | 177 | VAL |
| 1 | G | 183 | LEU |
| 1 | G | 284 | ARG |
| 1 | G | 328 | ASP |
| 1 | G | 329 | THR |
| 1 | G | 331 | THR |
| 1 | G | 361 | ASP |
| 1 | G | 398 | ASP |
| 1 | G | 404 | ARG |
| 1 | G | 524 | LEU |
| 1 | H | 20 | VAL |
| 1 | H | 74 | VAL |
| 1 | H | 76 | GLU |
| 1 | H | 89 | THR |
| 1 | H | 209 | GLU |
| 1 | H | 225 | LYS |
| 1 | H | 328 | ASP |
| 1 | H | 329 | THR |
| 1 | H | 331 | THR |
| 1 | H | 351 | GLN |
| 1 | H | 398 | ASP |
| 1 | H | 404 | ARG |
| 1 | H | 499 | VAL |
| 1 | H | 524 | LEU |
| 1 | I | 20 | VAL |
| 1 | I | 74 | VAL |
| 1 | I | 76 | GLU |
| 1 | I | 89 | THR |
| 1 | I | 209 | GLU |
| 1 | I | 225 | LYS |
| 1 | I | 328 | ASP |
| 1 | I | 329 | THR |
| 1 | I | 331 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 351 | GLN |
| 1 | I | 398 | ASP |
| 1 | I | 404 | ARG |
| 1 | I | 499 | VAL |
| 1 | I | 524 | LEU |
| 1 | J | 20 | VAL |
| 1 | J | 74 | VAL |
| 1 | J | 76 | GLU |
| 1 | J | 89 | THR |
| 1 | J | 94 | VAL |
| 1 | J | 225 | LYS |
| 1 | J | 289 | LEU |
| 1 | J | 328 | ASP |
| 1 | J | 329 | THR |
| 1 | J | 331 | THR |
| 1 | J | 351 | GLN |
| 1 | J | 372 | LEU |
| 1 | J | 398 | ASP |
| 1 | J | 404 | ARG |
| 1 | J | 499 | VAL |
| 1 | J | 524 | LEU |
| 1 | K | 20 | VAL |
| 1 | K | 74 | VAL |
| 1 | K | 76 | GLU |
| 1 | K | 89 | THR |
| 1 | K | 209 | GLU |
| 1 | K | 225 | LYS |
| 1 | K | 289 | LEU |
| 1 | K | 328 | ASP |
| 1 | K | 329 | THR |
| 1 | K | 331 | THR |
| 1 | K | 351 | GLN |
| 1 | K | 398 | ASP |
| 1 | K | 404 | ARG |
| 1 | K | 499 | VAL |
| 1 | K | 524 | LEU |
| 1 | L | 20 | VAL |
| 1 | L | 74 | VAL |
| 1 | L | 76 | GLU |
| 1 | L | 89 | THR |
| 1 | L | 209 | GLU |
| 1 | L | 225 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 328 | ASP |
| 1 | L | 329 | THR |
| 1 | L | 331 | THR |
| 1 | L | 351 | GLN |
| 1 | L | 398 | ASP |
| 1 | L | 404 | ARG |
| 1 | L | 499 | VAL |
| 1 | L | 524 | LEU |
| 1 | M | 20 | VAL |
| 1 | M | 74 | VAL |
| 1 | M | 76 | GLU |
| 1 | M | 89 | THR |
| 1 | M | 94 | VAL |
| 1 | M | 209 | GLU |
| 1 | M | 225 | LYS |
| 1 | M | 284 | ARG |
| 1 | M | 328 | ASP |
| 1 | M | 329 | THR |
| 1 | M | 331 | THR |
| 1 | M | 351 | GLN |
| 1 | M | 372 | LEU |
| 1 | M | 398 | ASP |
| 1 | M | 404 | ARG |
| 1 | M | 524 | LEU |
| 1 | N | 20 | VAL |
| 1 | N | 74 | VAL |
| 1 | N | 76 | GLU |
| 1 | N | 89 | THR |
| 1 | N | 94 | VAL |
| 1 | N | 209 | GLU |
| 1 | N | 225 | LYS |
| 1 | N | 328 | ASP |
| 1 | N | 329 | THR |
| 1 | N | 331 | THR |
| 1 | N | 351 | GLN |
| 1 | N | 398 | ASP |
| 1 | N | 404 | ARG |
| 1 | N | 499 | VAL |
| 1 | N | 524 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 37 | ASN |
| 1 | A | 146 | GLN |
| 1 | A | 265 | ASN |
| 1 | A | 319 | GLN |
| 1 | A | 326 | ASN |
| 1 | A | 351 | GLN |
| 1 | A | 366 | GLN |
| 1 | A | 475 | ASN |
| 1 | B | 10 | ASN |
| 1 | B | 37 | ASN |
| 1 | B | 146 | GLN |
| 1 | B | 265 | ASN |
| 1 | B | 326 | ASN |
| 1 | B | 351 | GLN |
| 1 | B | 366 | GLN |
| 1 | B | 475 | ASN |
| 1 | C | 37 | ASN |
| 1 | C | 146 | GLN |
| 1 | C | 229 | ASN |
| 1 | C | 265 | ASN |
| 1 | C | 326 | ASN |
| 1 | C | 351 | GLN |
| 1 | C | 366 | GLN |
| 1 | C | 475 | ASN |
| 1 | D | 37 | ASN |
| 1 | D | 146 | GLN |
| 1 | D | 265 | ASN |
| 1 | D | 326 | ASN |
| 1 | D | 351 | GLN |
| 1 | D | 366 | GLN |
| 1 | D | 475 | ASN |
| 1 | E | 37 | ASN |
| 1 | E | 146 | GLN |
| 1 | E | 265 | ASN |
| 1 | E | 319 | GLN |
| 1 | E | 326 | ASN |
| 1 | E | 366 | GLN |
| 1 | E | 475 | ASN |
| 1 | F | 10 | ASN |
| 1 | F | 37 | ASN |
| 1 | F | 146 | GLN |
| 1 | F | 229 | ASN |
| 1 | F | 265 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 326 | ASN |
| 1 | F | 366 | GLN |
| 1 | F | 475 | ASN |
| 1 | G | 37 | ASN |
| 1 | G | 146 | GLN |
| 1 | G | 265 | ASN |
| 1 | G | 326 | ASN |
| 1 | G | 343 | GLN |
| 1 | G | 351 | GLN |
| 1 | G | 366 | GLN |
| 1 | G | 475 | ASN |
| 1 | H | 37 | ASN |
| 1 | H | 146 | GLN |
| 1 | H | 265 | ASN |
| 1 | H | 290 | GLN |
| 1 | H | 319 | GLN |
| 1 | H | 351 | GLN |
| 1 | H | 475 | ASN |
| 1 | I | 37 | ASN |
| 1 | I | 146 | GLN |
| 1 | I | 265 | ASN |
| 1 | I | 348 | GLN |
| 1 | I | 351 | GLN |
| 1 | I | 475 | ASN |
| 1 | J | 37 | ASN |
| 1 | J | 265 | ASN |
| 1 | J | 351 | GLN |
| 1 | J | 475 | ASN |
| 1 | K | 37 | ASN |
| 1 | K | 146 | GLN |
| 1 | K | 265 | ASN |
| 1 | K | 348 | GLN |
| 1 | K | 351 | GLN |
| 1 | K | 475 | ASN |
| 1 | L | 37 | ASN |
| 1 | L | 146 | GLN |
| 1 | L | 229 | ASN |
| 1 | L | 265 | ASN |
| 1 | L | 348 | GLN |
| 1 | L | 351 | GLN |
| 1 | L | 475 | ASN |
| 1 | M | 10 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 37 | ASN |
| 1 | M | 146 | GLN |
| 1 | M | 265 | ASN |
| 1 | M | 351 | GLN |
| 1 | M | 475 | ASN |
| 1 | N | 37 | ASN |
| 1 | N | 229 | ASN |
| 1 | N | 265 | ASN |
| 1 | N | 326 | ASN |
| 1 | N | 351 | GLN |
| 1 | N | 475 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 14 are monoatomic - leaving 75 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 4 | MPD | K | 1527 | - | 7,7,7 | 0.47 | 0 | 9,10,10 | 0.78 | 0 |
| 2 | SO4 | N | 1146 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.09 | 0 |
| 4 | MPD | N | 1515 | - | 7,7,7 | 0.62 | 0 | 9,10,10 | 0.89 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | MPD | E | 1503 | - | 7,7,7 | 0.52 | 0 | 9,10,10 | 0.84 | 0 |
| 4 | MPD | J | 1529 | - | 7,7,7 | 0.47 | 0 | 9,10,10 | 0.75 | 0 |
| 4 | MPD | C | 1514 | - | 7,7,7 | 0.38 | 0 | 9,10,10 | 0.75 | 0 |
| 2 | SO4 | M | 1106 | - | 4,4,4 | 0.26 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | H | 1120 | - | 4,4,4 | 0.27 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | D | 1129 | - | 4,4,4 | 0.26 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | SO4 | D | 1112 | - | 4,4,4 | 0.31 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | SO4 | J | 1144 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 1113 | - | 4,4,4 | 0.26 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | SO4 | A | 1121 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.09 | 0 |
| 4 | MPD | H | 1516 | - | 7,7,7 | 0.45 | 0 | 9,10,10 | 0.83 | 0 |
| 4 | MPD | L | 1500 | - | 7,7,7 | 0.55 | 0 | 9,10,10 | 0.93 | 1 (11%) |
| 4 | MPD | I | 1524 | - | 7,7,7 | 0.50 | 0 | 9,10,10 | 0.82 | 0 |
| 2 | SO4 | H | 1142 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | D | 1110 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.08 | 0 |
| 4 | MPD | I | 1530 | - | 7,7,7 | 0.52 | 0 | 9,10,10 | 0.92 | 0 |
| 2 | SO4 | N | 1104 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.12 | 0 |
| 4 | MPD | A | 1507 | - | 7,7,7 | 0.60 | 0 | 9,10,10 | 0.84 | 0 |
| 2 | SO4 | M | 1105 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.09 | 0 |
| 4 | MPD | F | 1520 | - | 7,7,7 | 0.50 | 0 | 9,10,10 | 0.85 | 0 |
| 2 | SO4 | B | 1136 | - | 4,4,4 | 0.27 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | SO4 | L | 1117 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.08 | 0 |
| 4 | MPD | E | 1528 | - | 7,7,7 | 0.54 | 0 | 9,10,10 | 0.86 | 0 |
| 4 | MPD | G | 1509 | - | 7,7,7 | 0.50 | 0 | 9,10,10 | 0.82 | 0 |
| 4 | MPD | B | 1510 | - | 7,7,7 | 0.34 | 0 | 9,10,10 | 0.84 | 0 |
| 2 | SO4 | C | 1133 | - | 4,4,4 | 0.26 | 0 | 6,6,6 | 0.10 | 0 |
| 4 | MPD | E | 1502 | - | 7,7,7 | 0.49 | 0 | 9,10,10 | 0.78 | 0 |
| 2 | SO4 | C | 1137 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.08 | 0 |
| 5 | PEG | E | 2100 | - | 6,6,6 | 0.81 | 0 | 5,5,5 | 1.63 | 1 (20%) |
| 2 | SO4 | I | 1119 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | SO4 | M | 1126 | - | 4,4,4 | 0.24 | 0 | 6,6,6 | 0.10 | 0 |
| 4 | MPD | F | 1501 | - | 7,7,7 | 0.53 | 0 | 9,10,10 | 0.72 | 0 |
| 2 | SO4 | J | 1111 | - | 4,4,4 | 0.26 | 0 | 6,6,6 | 0.05 | 0 |
| 4 | MPD | E | 1521 | - | 7,7,7 | 0.58 | 0 | 9,10,10 | 0.86 | 0 |
| 2 | SO4 | B | 1114 | - | 4,4,4 | 0.27 | 0 | 6,6,6 | 0.05 | 0 |
| 4 | MPD | H | 1525 | - | 7,7,7 | 0.56 | 0 | 9,10,10 | 0.84 | 0 |
| 2 | SO4 | J | 1127 | - | 4,4,4 | 0.27 | 0 | 6,6,6 | 0.07 | 0 |
| 4 | MPD | E | 1504 | - | 7,7,7 | 0.49 | 0 | 9,10,10 | 0.92 | 0 |
| 2 | SO4 | C | 1101 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | B | 1130 | - | 4,4,4 | 0.27 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | SO4 | A | 1139 | - | 4,4,4 | 0.25 | 0 | 6,6,6 | 0.09 | 0 |
| 4 | MPD | A | 1511 | - | 7,7,7 | 0.54 | 0 | 9,10,10 | 0.86 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | SO4 | H | 1103 | - | 4,4,4 | 0.31 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | G | 1132 | - | 4,4,4 | 0.27 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 1125 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.07 | 0 |
| 4 | MPD | M | 1518 | - | 7,7,7 | 0.58 | 0 | 9,10,10 | 0.69 | 0 |
| 4 | MPD | G | 1519 | - | 7,7,7 | 0.49 | 0 | 9,10,10 | 0.76 | 0 |
| 2 | SO4 | A | 1115 | - | 4,4,4 | 0.25 | 0 | 6,6,6 | 0.07 | 0 |
| 4 | MPD | N | 1526 | - | 7,7,7 | 0.50 | 0 | 9,10,10 | 0.78 | 0 |
| 4 | MPD | K | 1506 | - | 7,7,7 | 0.64 | 0 | 9,10,10 | 0.73 | 0 |
| 4 | MPD | B | 1523 | - | 7,7,7 | 0.58 | 0 | 9,10,10 | 0.80 | 0 |
| 4 | MPD | D | 1508 | - | 7,7,7 | 0.49 | 0 | 9,10,10 | 0.75 | 0 |
| 2 | SO4 | K | 1134 | - | 4,4,4 | 0.30 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | SO4 | J | 1118 | - | 4,4,4 | 0.26 | 0 | 6,6,6 | 0.07 | 0 |
| 4 | MPD | B | 1512 | - | 7,7,7 | 0.49 | 0 | 9,10,10 | 0.77 | 0 |
| 2 | SO4 | F | 1141 | - | 4,4,4 | 0.30 | 0 | 6,6,6 | 0.05 | 0 |
| 4 | MPD | I | 1505 | - | 7,7,7 | 0.55 | 0 | 9,10,10 | 0.90 | 1 (11%) |
| 4 | MPD | N | 1517 | - | 7,7,7 | 0.53 | 0 | 9,10,10 | 0.78 | 0 |
| 2 | SO4 | D | 1138 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 1123 | - | 4,4,4 | 0.26 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 1140 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.10 | 0 |
| 4 | MPD | F | 1522 | - | 7,7,7 | 0.39 | 0 | 9,10,10 | 0.73 | 0 |
| 2 | SO4 | G | 1108 | - | 4,4,4 | 0.27 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | D | 1128 | - | 4,4,4 | 0.27 | 0 | 6,6,6 | 0.11 | 0 |
| 2 | SO4 | A | 1107 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | SO4 | C | 1124 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.08 | 0 |
| 4 | MPD | B | 1513 | - | 7,7,7 | 0.62 | 0 | 9,10,10 | 0.85 | 1 (11%) |
| 2 | SO4 | I | 1143 | - | 4,4,4 | 0.27 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | L | 1116 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | G | 1109 | - | 4,4,4 | 0.26 | 0 | 6,6,6 | 0.12 | 0 |
| 2 | SO4 | K | 1145 | - | 4,4,4 | 0.29 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | SO4 | B | 1135 | - | 4,4,4 | 0.28 | 0 | 6,6,6 | 0.05 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|-------|
| 4 | MPD | K | 1527 | - | - | 2/5/5/5 | - |
| 4 | MPD | N | 1515 | - | - | 0/5/5/5 | - |
| 4 | MPD | E | 1503 | - | - | 0/5/5/5 | - |
| 4 | MPD | J | 1529 | - | - | 0/5/5/5 | - |
| 4 | MPD | C | 1514 | - | - | 0/5/5/5 | - |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|-------|
| 4 | MPD | N | 1517 | - | - | 1/5/5/5 | - |
| 4 | MPD | H | 1516 | - | - | 0/5/5/5 | - |
| 4 | MPD | L | 1500 | - | - | 0/5/5/5 | - |
| 4 | MPD | I | 1524 | - | - | 0/5/5/5 | - |
| 4 | MPD | I | 1530 | - | - | 0/5/5/5 | - |
| 4 | MPD | A | 1507 | - | - | 0/5/5/5 | - |
| 4 | MPD | F | 1520 | - | - | 2/5/5/5 | - |
| 4 | MPD | E | 1528 | - | - | 0/5/5/5 | - |
| 4 | MPD | G | 1509 | - | - | 0/5/5/5 | - |
| 4 | MPD | B | 1510 | - | - | 0/5/5/5 | - |
| 4 | MPD | E | 1502 | - | - | 0/5/5/5 | - |
| 4 | MPD | H | 1525 | - | - | 0/5/5/5 | - |
| 4 | MPD | F | 1501 | - | - | 2/5/5/5 | - |
| 5 | PEG | E | 2100 | - | - | 1/4/4/4 | - |
| 4 | MPD | E | 1504 | - | - | 0/5/5/5 | - |
| 4 | MPD | A | 1511 | - | - | 0/5/5/5 | - |
| 4 | MPD | E | 1521 | - | - | 0/5/5/5 | - |
| 4 | MPD | F | 1522 | - | - | 1/5/5/5 | - |
| 4 | MPD | G | 1519 | - | - | 0/5/5/5 | - |
| 4 | MPD | N | 1526 | - | - | 0/5/5/5 | - |
| 4 | MPD | K | 1506 | - | - | 1/5/5/5 | - |
| 4 | MPD | B | 1523 | - | - | 0/5/5/5 | - |
| 4 | MPD | D | 1508 | - | - | 0/5/5/5 | - |
| 4 | MPD | B | 1512 | - | - | 0/5/5/5 | - |
| 4 | MPD | I | 1505 | - | - | 0/5/5/5 | - |
| 4 | MPD | M | 1518 | - | - | 2/5/5/5 | - |
| 4 | MPD | B | 1513 | - | - | 2/5/5/5 | - |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 5 | E | 2100 | PEG | O2-C2-C1 | 2.61 | 121.54 | 110.07 |
| 4 | I | 1505 | MPD | O4-C4-C3 | 2.11 | 119.88 | 111.36 |
| 4 | B | 1513 | MPD | O4-C4-C3 | 2.02 | 119.52 | 111.36 |
| 4 | L | 1500 | MPD | O4-C4-C3 | 2.01 | 119.49 | 111.36 |

There are no chirality outliers.

All (14) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 4 | F | 1520 | MPD | C1-C2-C3-C4 |
| 4 | F | 1520 | MPD | O2-C2-C3-C4 |
| 5 | E | 2100 | PEG | O1-C1-C2-O2 |
| 4 | K | 1506 | MPD | O2-C2-C3-C4 |
| 4 | F | 1522 | MPD | CM-C2-C3-C4 |
| 4 | B | 1513 | MPD | C1-C2-C3-C4 |
| 4 | F | 1501 | MPD | C1-C2-C3-C4 |
| 4 | K | 1527 | MPD | C1-C2-C3-C4 |
| 4 | N | 1517 | MPD | CM-C2-C3-C4 |
| 4 | M | 1518 | MPD | C1-C2-C3-C4 |
| 4 | B | 1513 | MPD | O2-C2-C3-C4 |
| 4 | F | 1501 | MPD | O2-C2-C3-C4 |
| 4 | K | 1527 | MPD | O2-C2-C3-C4 |
| 4 | M | 1518 | MPD | O2-C2-C3-C4 |

There are no ring outliers.

14 monomers are involved in 27 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | N | 1146 | SO4 | 1 | 0 |
| 4 | N | 1515 | MPD | 5 | 0 |
| 4 | C | 1514 | MPD | 2 | 0 |
| 4 | H | 1516 | MPD | 2 | 0 |
| 2 | B | 1136 | SO4 | 2 | 0 |
| 4 | G | 1509 | MPD | 1 | 0 |
| 4 | B | 1510 | MPD | 2 | 0 |
| 4 | E | 1502 | MPD | 1 | 0 |
| 4 | M | 1518 | MPD | 3 | 0 |
| 4 | N | 1526 | MPD | 2 | 0 |
| 4 | K | 1506 | MPD | 2 | 0 |
| 2 | F | 1141 | SO4 | 1 | 0 |
| 4 | N | 1517 | MPD | 2 | 0 |
| 4 | F | 1522 | MPD | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1 | A | 524/547 (95%) | -0.23 | 4 (0%) 86 86 | 15, 40, 73, 90 | 0 |
| 1 | B | 524/547 (95%) | -0.03 | 15 (2%) 51 48 | 15, 43, 75, 91 | 0 |
| 1 | C | 524/547 (95%) | -0.15 | 12 (2%) 60 59 | 17, 43, 75, 90 | 0 |
| 1 | D | 524/547 (95%) | -0.27 | 4 (0%) 86 86 | 15, 41, 73, 90 | 0 |
| 1 | E | 524/547 (95%) | -0.23 | 4 (0%) 86 86 | 17, 42, 74, 90 | 0 |
| 1 | F | 524/547 (95%) | -0.21 | 7 (1%) 77 77 | 16, 41, 75, 90 | 0 |
| 1 | G | 524/547 (95%) | -0.28 | 2 (0%) 92 92 | 16, 40, 73, 88 | 0 |
| 1 | H | 524/547 (95%) | -0.05 | 8 (1%) 73 73 | 20, 48, 89, 101 | 0 |
| 1 | I | 524/547 (95%) | -0.18 | 6 (1%) 80 81 | 21, 49, 89, 101 | 0 |
| 1 | J | 524/547 (95%) | -0.18 | 4 (0%) 86 86 | 19, 48, 89, 102 | 0 |
| 1 | K | 524/547 (95%) | -0.12 | 8 (1%) 73 73 | 20, 48, 89, 102 | 0 |
| 1 | L | 524/547 (95%) | 0.17 | 46 (8%) 10 7 | 19, 49, 91, 103 | 0 |
| 1 | M | 524/547 (95%) | 0.01 | 24 (4%) 32 29 | 20, 49, 90, 103 | 0 |
| 1 | N | 524/547 (95%) | -0.12 | 9 (1%) 70 70 | 21, 49, 89, 102 | 0 |
| All | All | 7336/7658 (95%) | -0.13 | 153 (2%) 63 62 | 15, 45, 84, 103 | 0 |

All (153) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | L | 313 | THR | 6.3 |
| 1 | L | 203 | TYR | 5.7 |
| 1 | L | 312 | ALA | 5.2 |
| 1 | M | 44 | PHE | 4.9 |
| 1 | L | 236 | VAL | 4.9 |
| 1 | L | 266 | THR | 4.8 |
| 1 | L | 353 | ILE | 4.5 |
| 1 | E | 44 | PHE | 4.5 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | D | 44 | PHE | 4.4 |
| 1 | H | 44 | PHE | 4.4 |
| 1 | L | 301 | ILE | 4.3 |
| 1 | L | 355 | GLU | 4.3 |
| 1 | M | 360 | TYR | 4.2 |
| 1 | C | 44 | PHE | 4.2 |
| 1 | C | 313 | THR | 4.1 |
| 1 | L | 311 | LYS | 4.0 |
| 1 | F | 305 | ILE | 3.9 |
| 1 | L | 210 | THR | 3.9 |
| 1 | L | 309 | LEU | 3.9 |
| 1 | B | 44 | PHE | 3.9 |
| 1 | L | 314 | LEU | 3.8 |
| 1 | L | 201 | SER | 3.7 |
| 1 | K | 44 | PHE | 3.6 |
| 1 | C | 203 | TYR | 3.6 |
| 1 | M | 310 | GLU | 3.6 |
| 1 | B | 266 | THR | 3.6 |
| 1 | N | 203 | TYR | 3.6 |
| 1 | L | 354 | GLU | 3.5 |
| 1 | N | 44 | PHE | 3.5 |
| 1 | G | 44 | PHE | 3.5 |
| 1 | M | 201 | SER | 3.5 |
| 1 | J | 44 | PHE | 3.5 |
| 1 | L | 357 | THR | 3.4 |
| 1 | L | 231 | ARG | 3.4 |
| 1 | B | 203 | TYR | 3.4 |
| 1 | K | 360 | TYR | 3.4 |
| 1 | L | 271 | VAL | 3.3 |
| 1 | A | 44 | PHE | 3.3 |
| 1 | L | 233 | MET | 3.3 |
| 1 | M | 243 | ALA | 3.2 |
| 1 | C | 243 | ALA | 3.2 |
| 1 | N | 243 | ALA | 3.2 |
| 1 | M | 238 | GLU | 3.2 |
| 1 | F | 203 | TYR | 3.1 |
| 1 | M | 353 | ILE | 3.1 |
| 1 | M | 203 | TYR | 3.1 |
| 1 | L | 234 | LEU | 3.1 |
| 1 | L | 299 | THR | 3.1 |
| 1 | M | 266 | THR | 3.1 |
| 1 | J | 305 | ILE | 3.0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | I | 357 | THR | 3.0 |
| 1 | B | 284 | ARG | 3.0 |
| 1 | L | 268 | ARG | 3.0 |
| 1 | H | 306 | GLY | 3.0 |
| 1 | C | 306 | GLY | 2.9 |
| 1 | F | 356 | ALA | 2.9 |
| 1 | L | 235 | PRO | 2.9 |
| 1 | B | 353 | ILE | 2.9 |
| 1 | K | 236 | VAL | 2.9 |
| 1 | H | 305 | ILE | 2.9 |
| 1 | N | 356 | ALA | 2.9 |
| 1 | F | 44 | PHE | 2.8 |
| 1 | A | 43 | SER | 2.8 |
| 1 | N | 360 | TYR | 2.8 |
| 1 | I | 284 | ARG | 2.7 |
| 1 | B | 272 | LYS | 2.7 |
| 1 | C | 311 | LYS | 2.7 |
| 1 | K | 238 | GLU | 2.7 |
| 1 | L | 366 | GLN | 2.7 |
| 1 | L | 238 | GLU | 2.7 |
| 1 | D | 203 | TYR | 2.7 |
| 1 | K | 356 | ALA | 2.7 |
| 1 | L | 307 | MET | 2.6 |
| 1 | C | 43 | SER | 2.6 |
| 1 | L | 356 | ALA | 2.6 |
| 1 | L | 269 | GLY | 2.6 |
| 1 | C | 356 | ALA | 2.6 |
| 1 | E | 244 | GLY | 2.6 |
| 1 | M | 268 | ARG | 2.6 |
| 1 | M | 362 | ARG | 2.5 |
| 1 | M | 342 | ILE | 2.5 |
| 1 | M | 217 | SER | 2.5 |
| 1 | H | 308 | GLU | 2.5 |
| 1 | A | 305 | ILE | 2.5 |
| 1 | H | 43 | SER | 2.5 |
| 1 | I | 44 | PHE | 2.5 |
| 1 | B | 355 | GLU | 2.4 |
| 1 | L | 352 | GLN | 2.4 |
| 1 | M | 356 | ALA | 2.4 |
| 1 | M | 294 | THR | 2.4 |
| 1 | E | 271 | VAL | 2.4 |
| 1 | H | 209 | GLU | 2.4 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | J | 209 | GLU | 2.4 |
| 1 | F | 308 | GLU | 2.4 |
| 1 | N | 268 | ARG | 2.4 |
| 1 | N | 43 | SER | 2.4 |
| 1 | J | 284 | ARG | 2.4 |
| 1 | I | 366 | GLN | 2.3 |
| 1 | K | 315 | GLU | 2.3 |
| 1 | L | 44 | PHE | 2.3 |
| 1 | M | 384 | ALA | 2.3 |
| 1 | L | 255 | GLU | 2.3 |
| 1 | B | 347 | ALA | 2.3 |
| 1 | G | 384 | ALA | 2.3 |
| 1 | B | 43 | SER | 2.3 |
| 1 | M | 152 | ALA | 2.3 |
| 1 | K | 43 | SER | 2.3 |
| 1 | L | 358 | SER | 2.3 |
| 1 | B | 356 | ALA | 2.3 |
| 1 | N | 284 | ARG | 2.3 |
| 1 | L | 308 | GLU | 2.3 |
| 1 | L | 381 | VAL | 2.3 |
| 1 | B | 349 | ILE | 2.3 |
| 1 | L | 229 | ASN | 2.2 |
| 1 | M | 240 | VAL | 2.2 |
| 1 | M | 43 | SER | 2.2 |
| 1 | C | 256 | GLY | 2.2 |
| 1 | M | 354 | GLU | 2.2 |
| 1 | L | 242 | LYS | 2.2 |
| 1 | L | 214 | GLU | 2.2 |
| 1 | K | 357 | THR | 2.2 |
| 1 | L | 200 | LEU | 2.2 |
| 1 | L | 302 | SER | 2.2 |
| 1 | M | 258 | ALA | 2.2 |
| 1 | M | 343 | GLN | 2.2 |
| 1 | I | 360 | TYR | 2.2 |
| 1 | M | 271 | VAL | 2.2 |
| 1 | D | 43 | SER | 2.2 |
| 1 | B | 354 | GLU | 2.2 |
| 1 | H | 363 | GLU | 2.2 |
| 1 | I | 305 | ILE | 2.1 |
| 1 | L | 316 | ASP | 2.1 |
| 1 | B | 489 | ILE | 2.1 |
| 1 | C | 284 | ARG | 2.1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | F | 357 | THR | 2.1 |
| 1 | L | 243 | ALA | 2.1 |
| 1 | D | 484 | GLU | 2.1 |
| 1 | L | 272 | LYS | 2.1 |
| 1 | L | 310 | GLU | 2.1 |
| 1 | C | 305 | ILE | 2.1 |
| 1 | H | 210 | THR | 2.1 |
| 1 | L | 341 | ALA | 2.0 |
| 1 | M | 239 | ALA | 2.0 |
| 1 | B | 357 | THR | 2.0 |
| 1 | L | 259 | LEU | 2.0 |
| 1 | L | 205 | ILE | 2.0 |
| 1 | L | 305 | ILE | 2.0 |
| 1 | F | 355 | GLU | 2.0 |
| 1 | B | 351 | GLN | 2.0 |
| 1 | C | 362 | ARG | 2.0 |
| 1 | N | 183 | LEU | 2.0 |
| 1 | E | 360 | TYR | 2.0 |
| 1 | A | 208 | PRO | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2 | SO4 | A | 1115 | 5/5 | 0.58 | 0.49 | 157,157,158,158 | 0 |
| 5 | PEG | E | 2100 | 7/7 | 0.69 | 0.23 | 83,86,88,89 | 0 |
| 3 | K | H | 3030 | 1/1 | 0.74 | 0.29 | 86,86,86,86 | 0 |
| 4 | MPD | N | 1526 | 8/8 | 0.74 | 0.42 | 85,86,87,87 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3 | K | I | 3040 | 1/1 | 0.74 | 0.21 | 94,94,94,94 | 0 |
| 4 | MPD | I | 1524 | 8/8 | 0.75 | 0.28 | 75,80,83,83 | 0 |
| 2 | SO4 | L | 1117 | 5/5 | 0.76 | 0.42 | 146,146,147,147 | 0 |
| 3 | K | M | 3080 | 1/1 | 0.77 | 0.19 | 87,87,87,87 | 0 |
| 4 | MPD | D | 1508 | 8/8 | 0.78 | 0.38 | 78,80,81,81 | 0 |
| 2 | SO4 | B | 1135 | 5/5 | 0.78 | 0.31 | 137,138,139,139 | 0 |
| 2 | SO4 | M | 1106 | 5/5 | 0.78 | 0.30 | 147,147,147,147 | 0 |
| 4 | MPD | E | 1521 | 8/8 | 0.79 | 0.30 | 80,81,84,84 | 0 |
| 3 | K | J | 3060 | 1/1 | 0.79 | 0.16 | 78,78,78,78 | 0 |
| 3 | K | F | 3120 | 1/1 | 0.79 | 0.24 | 81,81,81,81 | 0 |
| 2 | SO4 | C | 1133 | 5/5 | 0.80 | 0.31 | 139,139,140,140 | 0 |
| 2 | SO4 | C | 1124 | 5/5 | 0.81 | 0.41 | 133,133,134,134 | 0 |
| 2 | SO4 | G | 1132 | 5/5 | 0.81 | 0.28 | 145,146,146,146 | 0 |
| 3 | K | B | 3140 | 1/1 | 0.81 | 0.18 | 70,70,70,70 | 0 |
| 2 | SO4 | D | 1129 | 5/5 | 0.82 | 0.30 | 144,144,144,144 | 0 |
| 2 | SO4 | D | 1138 | 5/5 | 0.83 | 0.36 | 134,134,134,135 | 0 |
| 2 | SO4 | N | 1146 | 5/5 | 0.83 | 0.32 | 135,135,136,136 | 0 |
| 4 | MPD | B | 1512 | 8/8 | 0.83 | 0.35 | 69,72,73,74 | 0 |
| 2 | SO4 | A | 1139 | 5/5 | 0.83 | 0.31 | 124,124,125,125 | 0 |
| 4 | MPD | F | 1522 | 8/8 | 0.84 | 0.40 | 70,73,74,75 | 0 |
| 3 | K | A | 3010 | 1/1 | 0.84 | 0.29 | 88,88,88,88 | 0 |
| 4 | MPD | K | 1527 | 8/8 | 0.84 | 0.34 | 99,101,102,102 | 0 |
| 2 | SO4 | K | 1145 | 5/5 | 0.84 | 0.31 | 127,127,128,128 | 0 |
| 2 | SO4 | B | 1113 | 5/5 | 0.85 | 0.24 | 112,113,114,114 | 0 |
| 2 | SO4 | D | 1110 | 5/5 | 0.85 | 0.27 | 113,114,115,115 | 0 |
| 4 | MPD | E | 1502 | 8/8 | 0.85 | 0.29 | 73,75,79,81 | 0 |
| 2 | SO4 | M | 1105 | 5/5 | 0.86 | 0.38 | 124,125,125,125 | 0 |
| 4 | MPD | F | 1520 | 8/8 | 0.86 | 0.31 | 41,47,56,57 | 0 |
| 3 | K | C | 3100 | 1/1 | 0.86 | 0.25 | 78,78,78,78 | 0 |
| 4 | MPD | I | 1505 | 8/8 | 0.86 | 0.36 | 63,66,68,68 | 0 |
| 2 | SO4 | B | 1136 | 5/5 | 0.87 | 0.47 | 130,130,130,130 | 0 |
| 4 | MPD | H | 1525 | 8/8 | 0.87 | 0.25 | 74,75,75,75 | 0 |
| 2 | SO4 | J | 1111 | 5/5 | 0.87 | 0.21 | 111,112,112,112 | 0 |
| 4 | MPD | E | 1528 | 8/8 | 0.87 | 0.31 | 63,65,69,70 | 0 |
| 4 | MPD | G | 1519 | 8/8 | 0.87 | 0.26 | 57,59,60,60 | 0 |
| 2 | SO4 | C | 1137 | 5/5 | 0.87 | 0.34 | 139,140,140,140 | 0 |
| 2 | SO4 | M | 1126 | 5/5 | 0.87 | 0.23 | 115,115,116,116 | 0 |
| 2 | SO4 | N | 1104 | 5/5 | 0.88 | 0.23 | 108,108,108,108 | 0 |
| 2 | SO4 | F | 1141 | 5/5 | 0.88 | 0.30 | 103,104,104,104 | 0 |
| 2 | SO4 | B | 1130 | 5/5 | 0.88 | 0.46 | 132,133,133,133 | 0 |
| 2 | SO4 | J | 1144 | 5/5 | 0.88 | 0.27 | 129,129,130,131 | 0 |
| 4 | MPD | N | 1517 | 8/8 | 0.88 | 0.33 | 67,69,70,71 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2 | SO4 | H | 1103 | 5/5 | 0.88 | 0.18 | 116,116,117,117 | 0 |
| 3 | K | D | 3020 | 1/1 | 0.88 | 0.13 | 65,65,65,65 | 0 |
| 2 | SO4 | E | 1123 | 5/5 | 0.88 | 0.31 | 137,137,137,137 | 0 |
| 2 | SO4 | E | 1140 | 5/5 | 0.88 | 0.35 | 135,135,136,136 | 0 |
| 4 | MPD | I | 1530 | 8/8 | 0.88 | 0.30 | 58,59,62,62 | 0 |
| 2 | SO4 | D | 1128 | 5/5 | 0.88 | 0.33 | 118,118,118,119 | 0 |
| 2 | SO4 | C | 1101 | 5/5 | 0.89 | 0.27 | 101,102,103,103 | 0 |
| 3 | K | L | 3070 | 1/1 | 0.89 | 0.13 | 71,71,71,71 | 0 |
| 2 | SO4 | G | 1108 | 5/5 | 0.89 | 0.25 | 116,117,117,118 | 0 |
| 4 | MPD | F | 1501 | 8/8 | 0.89 | 0.37 | 54,59,66,68 | 0 |
| 4 | MPD | B | 1510 | 8/8 | 0.89 | 0.36 | 76,76,77,77 | 0 |
| 3 | K | G | 3130 | 1/1 | 0.89 | 0.36 | 79,79,79,79 | 0 |
| 4 | MPD | C | 1514 | 8/8 | 0.89 | 0.28 | 59,60,66,66 | 0 |
| 4 | MPD | A | 1507 | 8/8 | 0.89 | 0.26 | 56,59,60,62 | 0 |
| 3 | K | K | 3050 | 1/1 | 0.89 | 0.15 | 91,91,91,91 | 0 |
| 2 | SO4 | H | 1142 | 5/5 | 0.90 | 0.28 | 120,120,121,121 | 0 |
| 2 | SO4 | F | 1125 | 5/5 | 0.90 | 0.16 | 110,111,111,111 | 0 |
| 4 | MPD | G | 1509 | 8/8 | 0.90 | 0.32 | 55,57,62,65 | 0 |
| 2 | SO4 | B | 1114 | 5/5 | 0.90 | 0.21 | 130,130,131,132 | 0 |
| 2 | SO4 | A | 1107 | 5/5 | 0.90 | 0.21 | 128,129,129,129 | 0 |
| 4 | MPD | E | 1504 | 8/8 | 0.90 | 0.31 | 52,53,57,59 | 0 |
| 2 | SO4 | L | 1116 | 5/5 | 0.90 | 0.33 | 114,115,115,115 | 0 |
| 4 | MPD | M | 1518 | 8/8 | 0.91 | 0.28 | 64,65,65,66 | 0 |
| 4 | MPD | B | 1523 | 8/8 | 0.91 | 0.35 | 77,77,79,79 | 0 |
| 2 | SO4 | H | 1120 | 5/5 | 0.91 | 0.37 | 107,108,109,109 | 0 |
| 4 | MPD | N | 1515 | 8/8 | 0.91 | 0.23 | 67,69,70,70 | 0 |
| 2 | SO4 | K | 1134 | 5/5 | 0.91 | 0.21 | 109,109,109,110 | 0 |
| 2 | SO4 | I | 1143 | 5/5 | 0.91 | 0.29 | 120,121,121,121 | 0 |
| 4 | MPD | L | 1500 | 8/8 | 0.91 | 0.29 | 43,46,49,49 | 0 |
| 2 | SO4 | I | 1119 | 5/5 | 0.92 | 0.31 | 105,106,106,107 | 0 |
| 3 | K | E | 3110 | 1/1 | 0.92 | 0.18 | 80,80,80,80 | 0 |
| 4 | MPD | B | 1513 | 8/8 | 0.92 | 0.31 | 45,51,55,56 | 0 |
| 4 | MPD | A | 1511 | 8/8 | 0.93 | 0.25 | 42,43,45,45 | 0 |
| 4 | MPD | K | 1506 | 8/8 | 0.93 | 0.22 | 46,50,50,51 | 0 |
| 2 | SO4 | J | 1127 | 5/5 | 0.93 | 0.31 | 137,137,137,138 | 0 |
| 3 | K | N | 3090 | 1/1 | 0.93 | 0.14 | 67,67,67,67 | 0 |
| 2 | SO4 | A | 1121 | 5/5 | 0.94 | 0.18 | 98,98,99,99 | 0 |
| 2 | SO4 | D | 1112 | 5/5 | 0.94 | 0.16 | 88,90,90,90 | 0 |
| 4 | MPD | H | 1516 | 8/8 | 0.94 | 0.16 | 48,49,49,49 | 0 |
| 2 | SO4 | G | 1109 | 5/5 | 0.94 | 0.14 | 85,85,86,86 | 0 |
| 2 | SO4 | J | 1118 | 5/5 | 0.95 | 0.26 | 104,104,104,105 | 0 |
| 4 | MPD | E | 1503 | 8/8 | 0.95 | 0.36 | 56,56,59,59 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4 | MPD | J | 1529 | 8/8 | 0.96 | 0.27 | 55,56,57,57 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.