



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:57 am GMT

PDB ID : 1GQ2
Title : MALIC ENZYME FROM PIGEON LIVER
Authors : Yang, Z.; Zhang, H.; Liang, T.
Deposited on : 2001-11-19
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

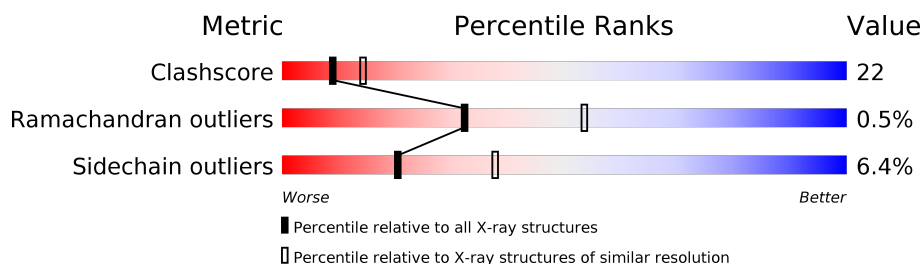
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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)) |
|-----------------------|-----------------------------|---|
| Clashscore | 112137 | 4554 (2.50-2.50) |
| Ramachandran outliers | 110173 | 4463 (2.50-2.50) |
| Sidechain outliers | 110143 | 4465 (2.50-2.50) |










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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 555 | |
| 1 | B | 555 | |
| 1 | C | 555 | |
| 1 | D | 555 | |
| 1 | E | 555 | |
| 1 | F | 555 | |
| 1 | G | 555 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | H | 555 |  62%35%. |
| 1 | I | 555 |  64%33%. |
| 1 | J | 555 |  64%33%. |
| 1 | K | 555 |  58%39%. |
| 1 | L | 555 |  58%38%. |
| 1 | M | 555 |  63%34%. |
| 1 | N | 555 |  60%36%. |
| 1 | O | 555 |  62%35%. |
| 1 | P | 555 |  64%32%. |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3 | OXL | C | 1582 | - | - | X | - |
| 3 | OXL | D | 1582 | - | - | X | - |

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 71519 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 MALIC ENZYME.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|----|---------|---------|-------|
| 1 | A | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | B | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | C | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | D | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | E | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | F | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | G | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | H | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | I | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | J | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | K | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | L | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | M | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | N | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | O | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4345 | 2772 | 742 | 806 | 11 | 14 | | | |
| 1 | P | 555 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 4346 | 2772 | 742 | 807 | 11 | 14 | | | |

There are 224 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| A | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| A | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| A | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| A | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| A | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| A | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| A | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| A | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| A | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| A | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| A | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| A | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| A | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| A | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| B | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| C | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| D | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| D | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| D | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| D | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| D | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| D | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| D | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| D | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| D | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| D | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| D | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| D | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| D | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| D | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| E | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| F | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| G | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| G | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| G | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| G | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| G | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| G | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| G | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| G | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| G | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| G | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| G | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| G | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| G | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| G | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| H | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| I | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| J | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| J | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| J | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| J | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| J | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| J | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| J | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| J | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| J | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| J | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| J | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| J | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| J | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| J | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| K | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| L | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |

Continued on next page...

Continued from previous page...

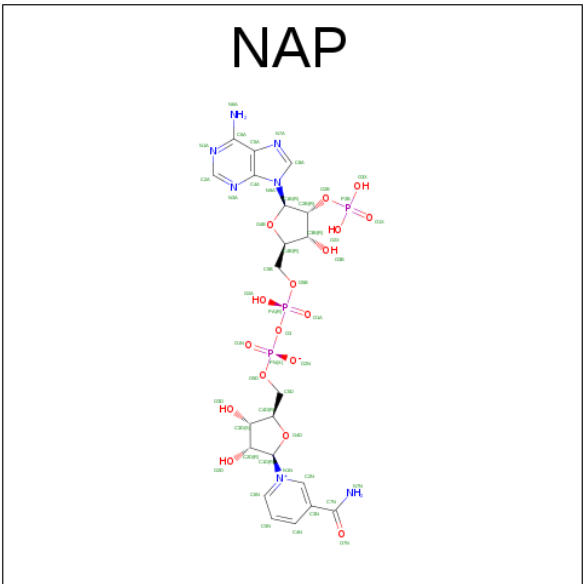
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| M | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| M | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| M | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| M | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| M | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| M | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| M | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| M | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| M | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| M | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| M | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| M | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| M | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| M | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| N | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| O | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| P | 38 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| P | 86 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| P | 108 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| P | 146 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| P | 177 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| P | 202 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| P | 239 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| P | 248 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| P | 325 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| P | 327 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| P | 343 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| P | 374 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| P | 407 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |
| P | 577 | MSE | MET | MODIFIED RESIDUE | UNP P40927 |

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



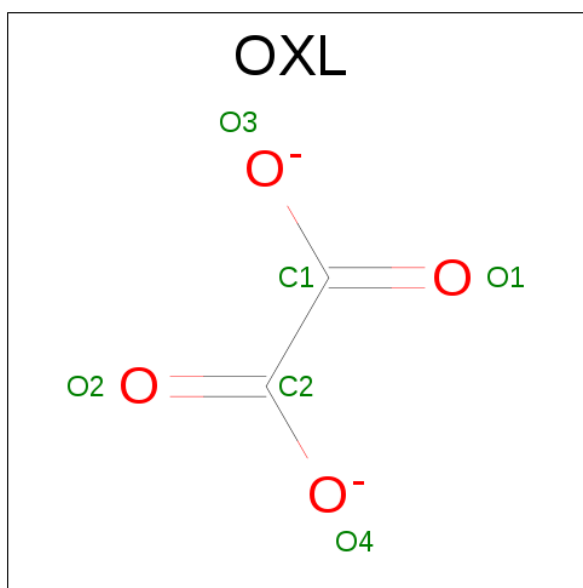
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | H | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | I | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | J | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | K | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | L | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | M | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | N | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | O | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |
| 2 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | | |

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 3 | A | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | B | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | C | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | D | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | E | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | F | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | G | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | H | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | I | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | J | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | K | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | L | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | M | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | N | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | O | 1 | Total C O 6 2 4 | 0 | 0 |
| 3 | P | 1 | Total C O 6 2 4 | 0 | 0 |

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4 | P | 1 | Total Mn 1 1 | 0 | 0 |
| 4 | G | 1 | Total Mn 1 1 | 0 | 0 |
| 4 | J | 1 | Total Mn 1 1 | 0 | 0 |
| 4 | D | 1 | Total Mn 1 1 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 4 | K | 1 | Total 1 | Mn 1 | 0 | 0 |
| 4 | E | 1 | Total 1 | Mn 1 | 0 | 0 |
| 4 | H | 1 | Total 1 | Mn 1 | 0 | 0 |
| 4 | B | 1 | Total 1 | Mn 1 | 0 | 0 |
| 4 | I | 1 | Total 1 | Mn 1 | 0 | 0 |
| 4 | C | 1 | Total 1 | Mn 1 | 0 | 0 |
| 4 | A | 1 | Total 1 | Mn 1 | 0 | 0 |
| 4 | N | 1 | Total 1 | Mn 1 | 0 | 0 |
| 4 | O | 1 | Total 1 | Mn 1 | 0 | 0 |
| 4 | L | 1 | Total 1 | Mn 1 | 0 | 0 |
| 4 | F | 1 | Total 1 | Mn 1 | 0 | 0 |
| 4 | M | 1 | Total 1 | Mn 1 | 0 | 0 |

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 5 | P | 3 | Total 3 | Cl 3 | 0 | 0 |
| 5 | G | 1 | Total 1 | Cl 1 | 0 | 0 |
| 5 | J | 2 | Total 2 | Cl 2 | 0 | 0 |
| 5 | K | 1 | Total 1 | Cl 1 | 0 | 0 |
| 5 | E | 3 | Total 3 | Cl 3 | 0 | 0 |
| 5 | H | 1 | Total 1 | Cl 1 | 0 | 0 |
| 5 | B | 1 | Total 1 | Cl 1 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 5 | I | 5 | Total 5 | Cl 5 | 0 | 0 |
| 5 | C | 4 | Total 4 | Cl 4 | 0 | 0 |
| 5 | N | 2 | Total 2 | Cl 2 | 0 | 0 |
| 5 | O | 4 | Total 4 | Cl 4 | 0 | 0 |
| 5 | L | 1 | Total 1 | Cl 1 | 0 | 0 |
| 5 | F | 2 | Total 2 | Cl 2 | 0 | 0 |
| 5 | M | 3 | Total 3 | Cl 3 | 0 | 0 |

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 6 | P | 5 | Total 5 | Na 5 | 0 | 0 |
| 6 | G | 1 | Total 1 | Na 1 | 0 | 0 |
| 6 | J | 2 | Total 2 | Na 2 | 0 | 0 |
| 6 | D | 2 | Total 2 | Na 2 | 0 | 0 |
| 6 | K | 1 | Total 1 | Na 1 | 0 | 0 |
| 6 | H | 5 | Total 5 | Na 5 | 0 | 0 |
| 6 | I | 2 | Total 2 | Na 2 | 0 | 0 |
| 6 | C | 4 | Total 4 | Na 4 | 0 | 0 |
| 6 | N | 1 | Total 1 | Na 1 | 0 | 0 |
| 6 | O | 4 | Total 4 | Na 4 | 0 | 0 |
| 6 | L | 1 | Total 1 | Na 1 | 0 | 0 |
| 6 | F | 2 | Total 2 | Na 2 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 6 | M | 6 | Total 6 | Na 6 | 0 | 0 |

- Molecule 7 is water.

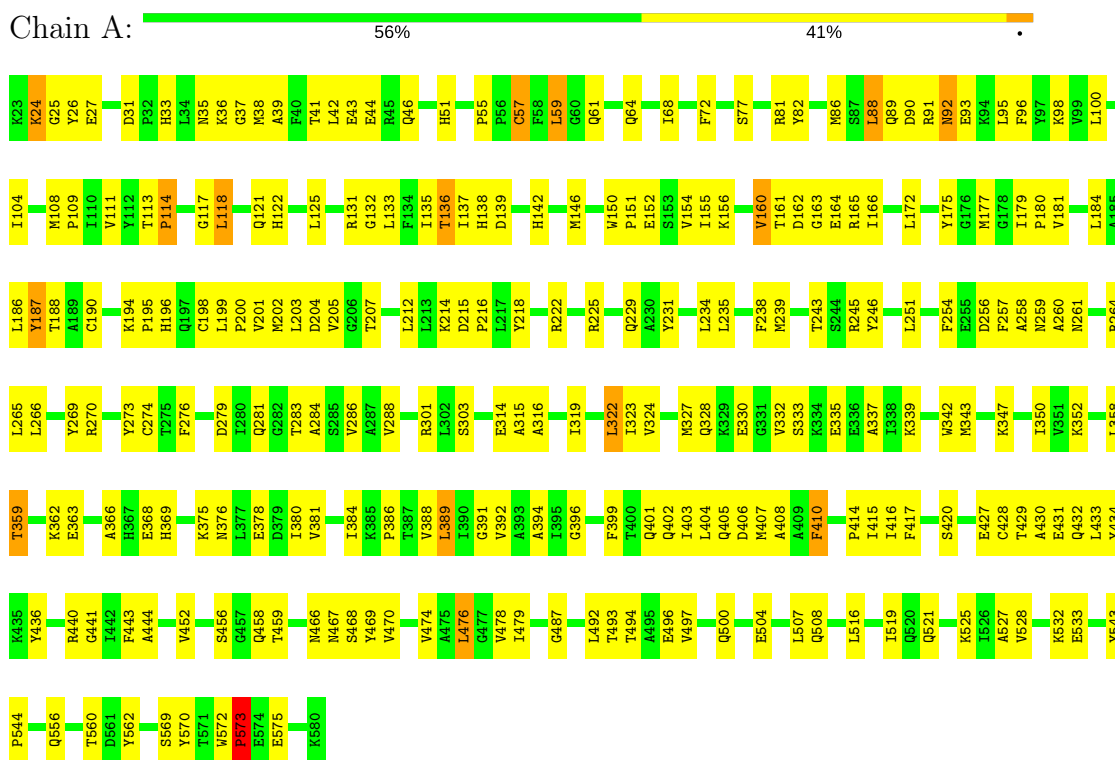
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 7 | A | 35 | Total 35 | O 35 | 0 | 0 |
| 7 | B | 42 | Total 42 | O 42 | 0 | 0 |
| 7 | C | 77 | Total 77 | O 77 | 0 | 0 |
| 7 | D | 49 | Total 49 | O 49 | 0 | 0 |
| 7 | E | 58 | Total 58 | O 58 | 0 | 0 |
| 7 | F | 78 | Total 78 | O 78 | 0 | 0 |
| 7 | G | 65 | Total 65 | O 65 | 0 | 0 |
| 7 | H | 77 | Total 77 | O 77 | 0 | 0 |
| 7 | I | 80 | Total 80 | O 80 | 0 | 0 |
| 7 | J | 63 | Total 63 | O 63 | 0 | 0 |
| 7 | K | 41 | Total 41 | O 41 | 0 | 0 |
| 7 | L | 75 | Total 75 | O 75 | 0 | 0 |
| 7 | M | 81 | Total 81 | O 81 | 0 | 0 |
| 7 | N | 71 | Total 71 | O 71 | 0 | 0 |
| 7 | O | 78 | Total 78 | O 78 | 0 | 0 |
| 7 | P | 79 | Total 79 | O 79 | 0 | 0 |

3 Residue-property plots

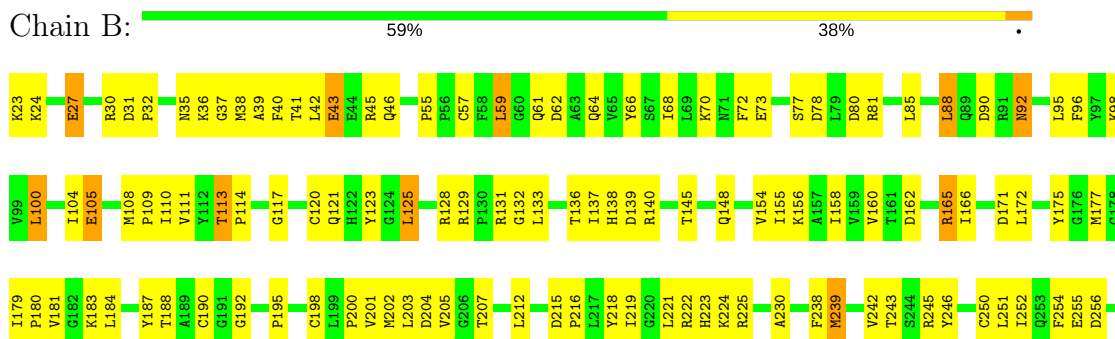
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

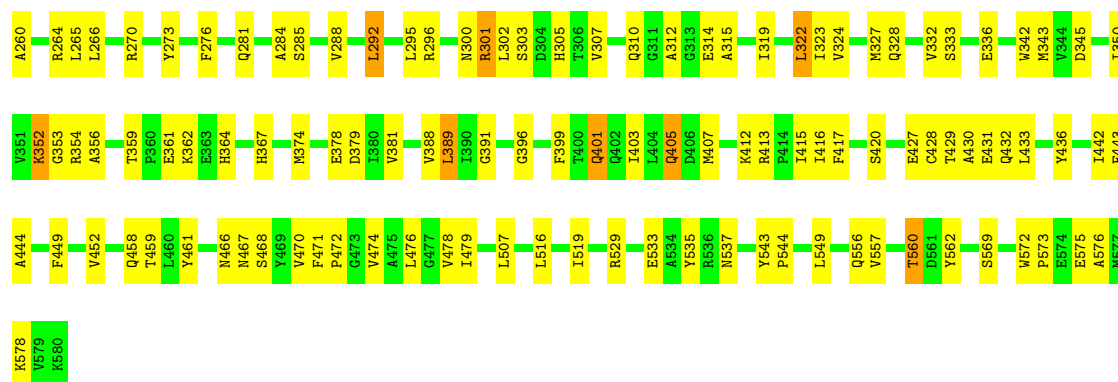
Note EDS was not executed.

• Molecule 1: MALIC ENZYME



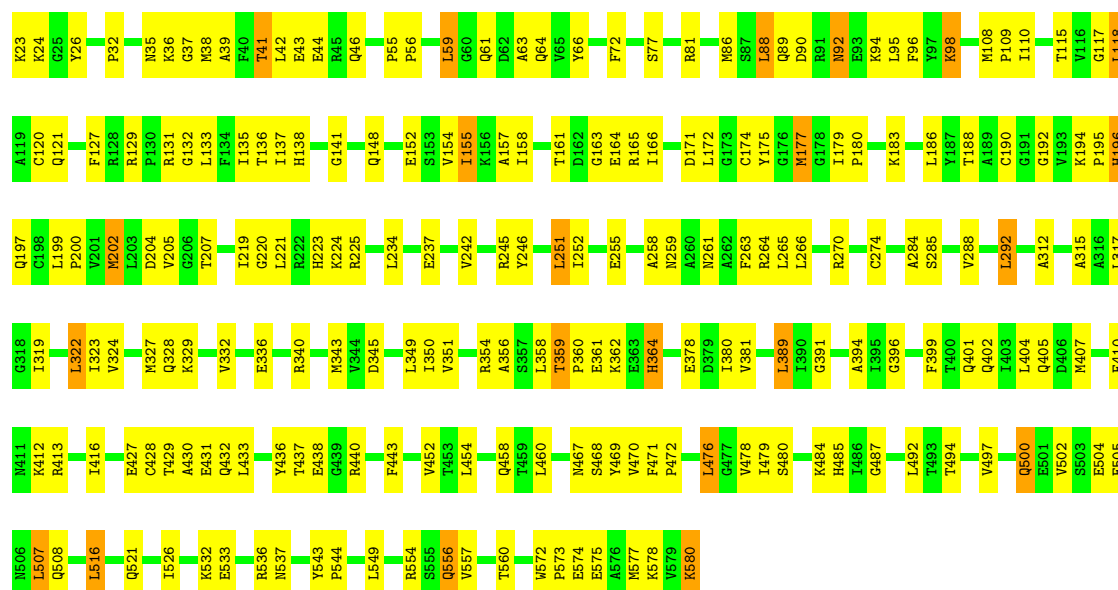
• Molecule 1: MALIC ENZYME





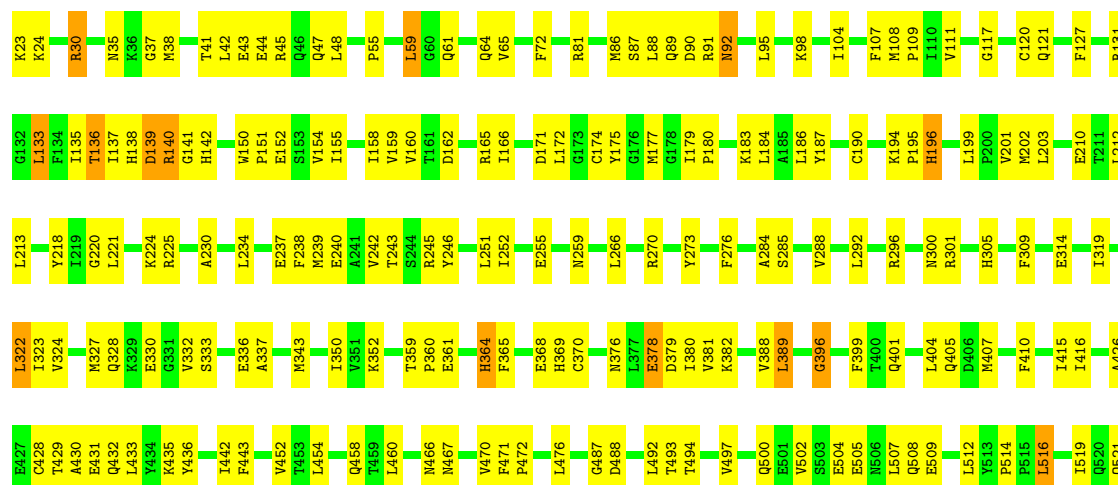
• Molecule 1: MALIC ENZYME

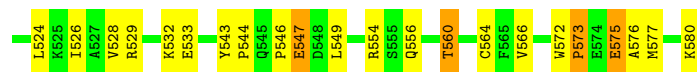
Chain C: 62% 34%



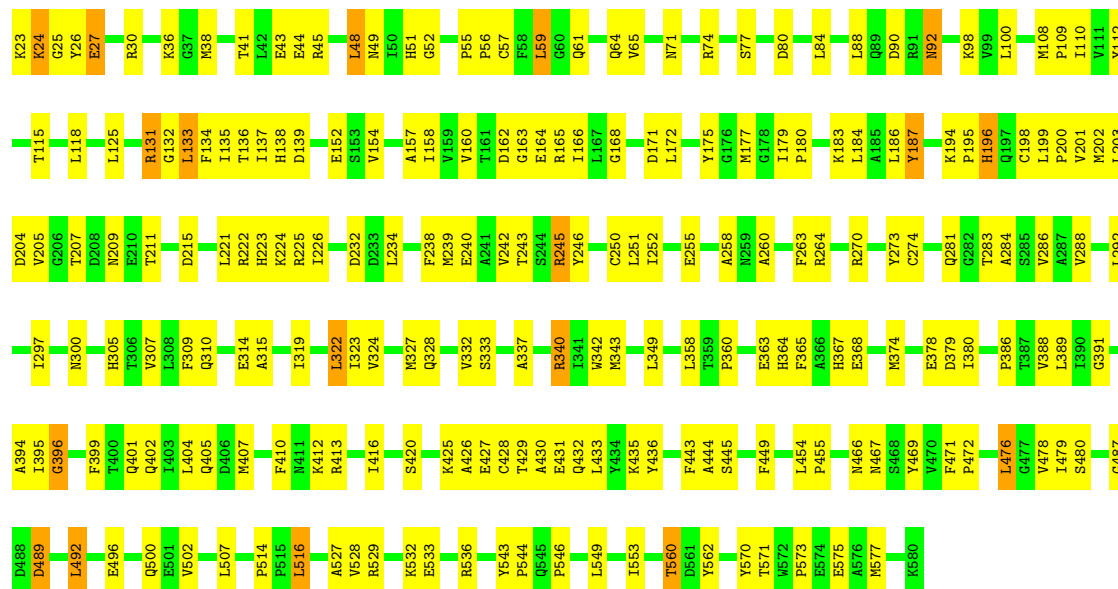
• Molecule 1: MALIC ENZYME

Chain D: 61% 35%

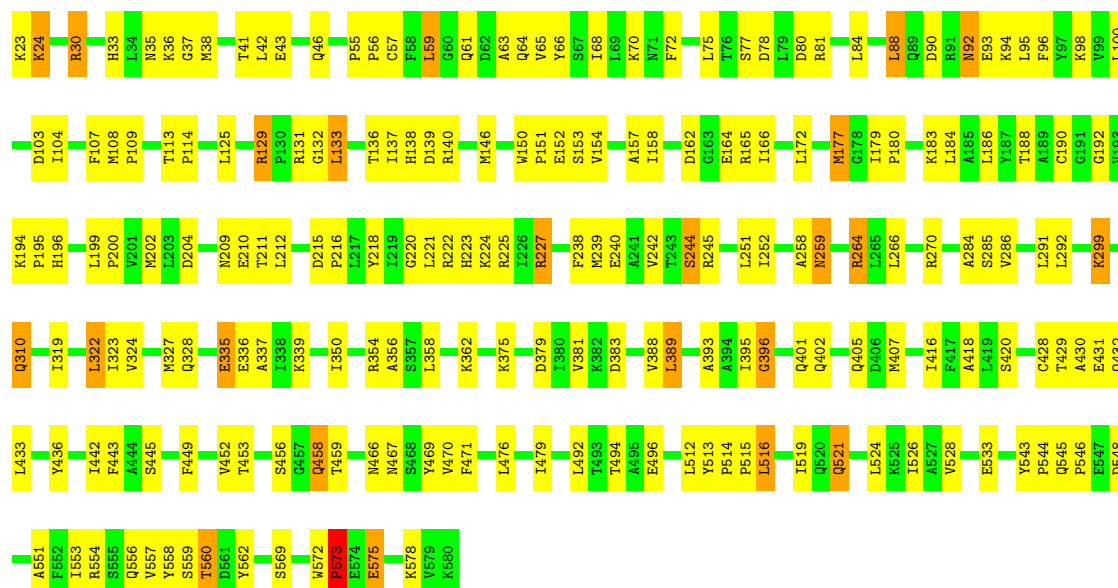




• Molecule 1: MALIC ENZYME

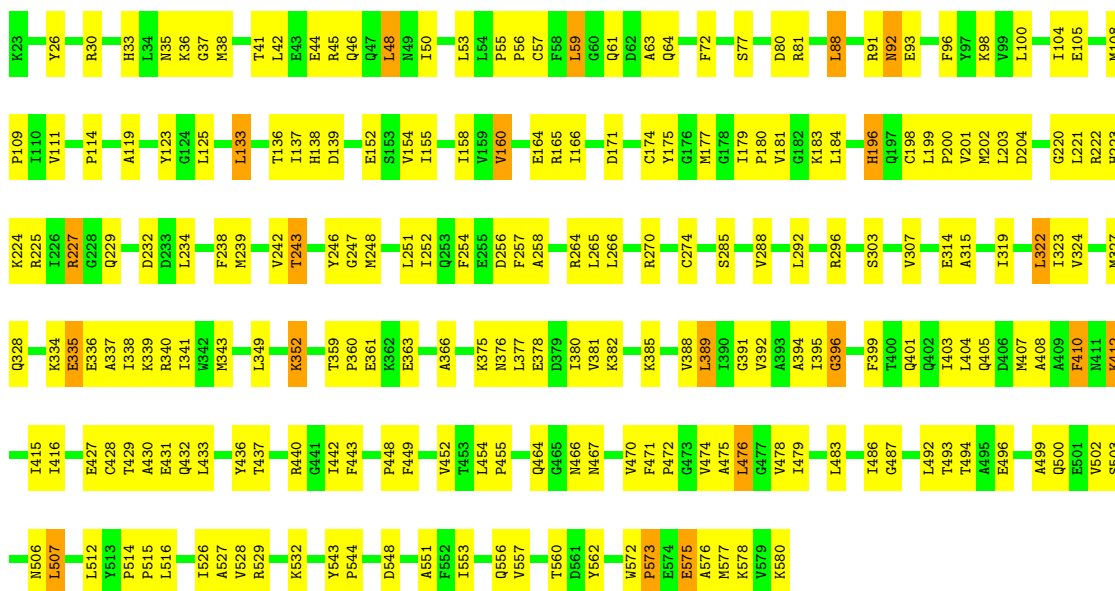


• Molecule 1: MALIC ENZYME



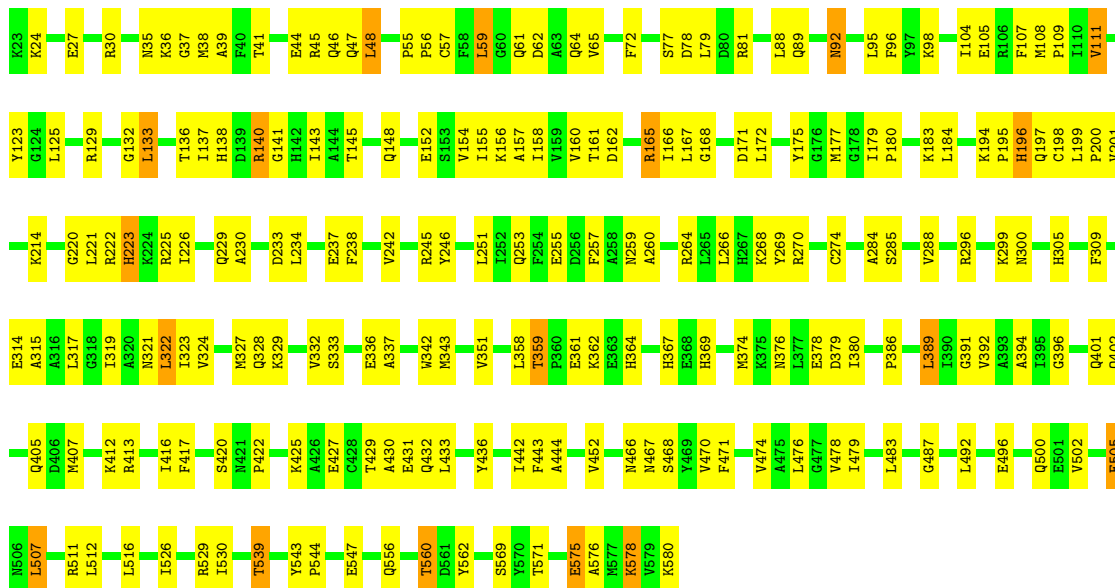
• Molecule 1: MALIC ENZYME





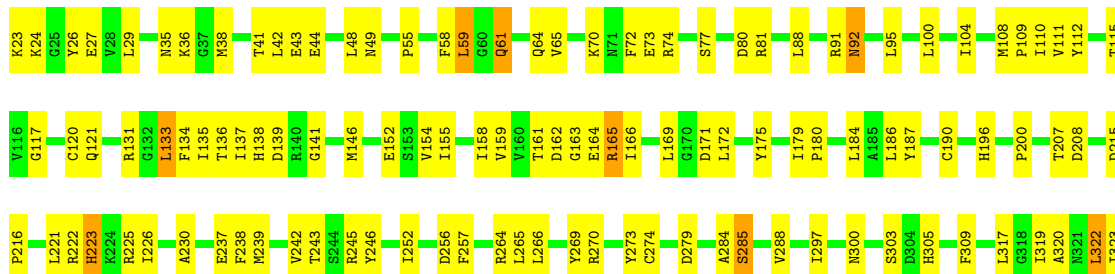
• Molecule 1: MALIC ENZYME

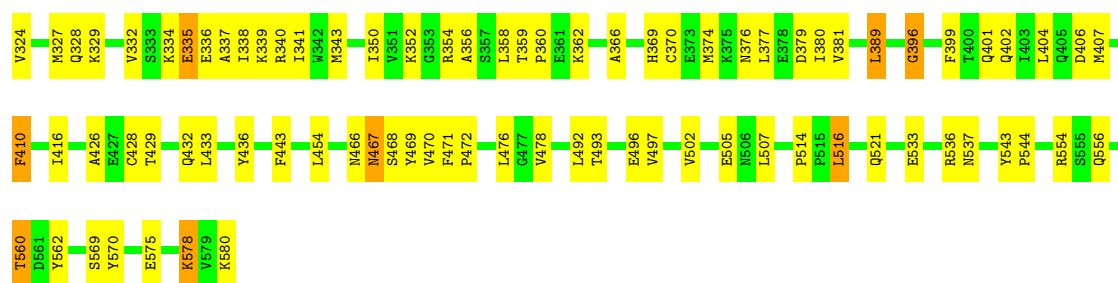
Chain H: 62% 35%



• Molecule 1: MALIC ENZYME

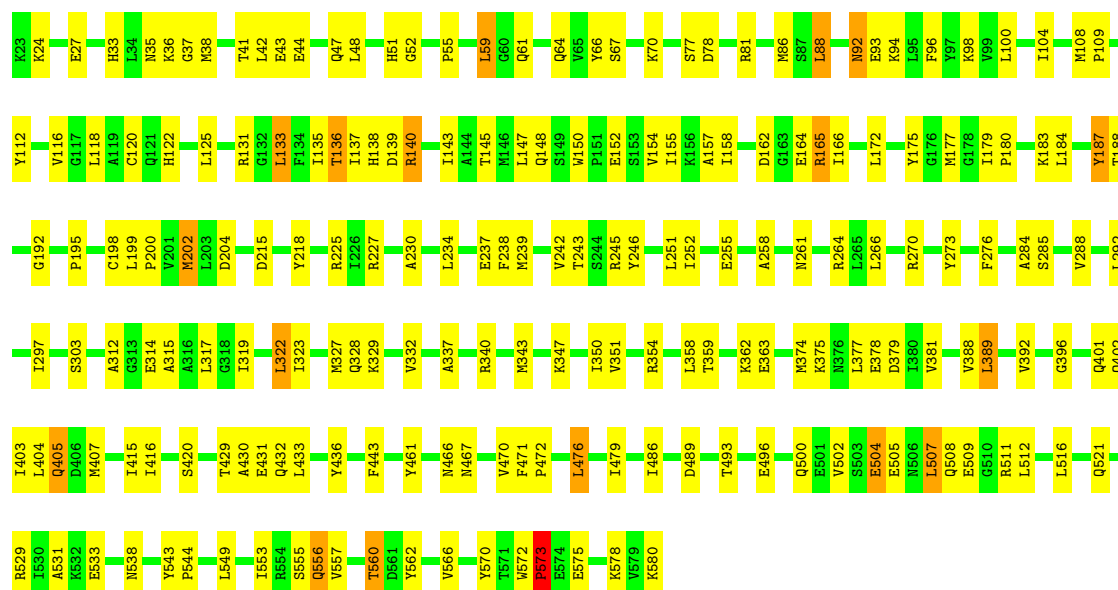
Chain I: 64% 33%





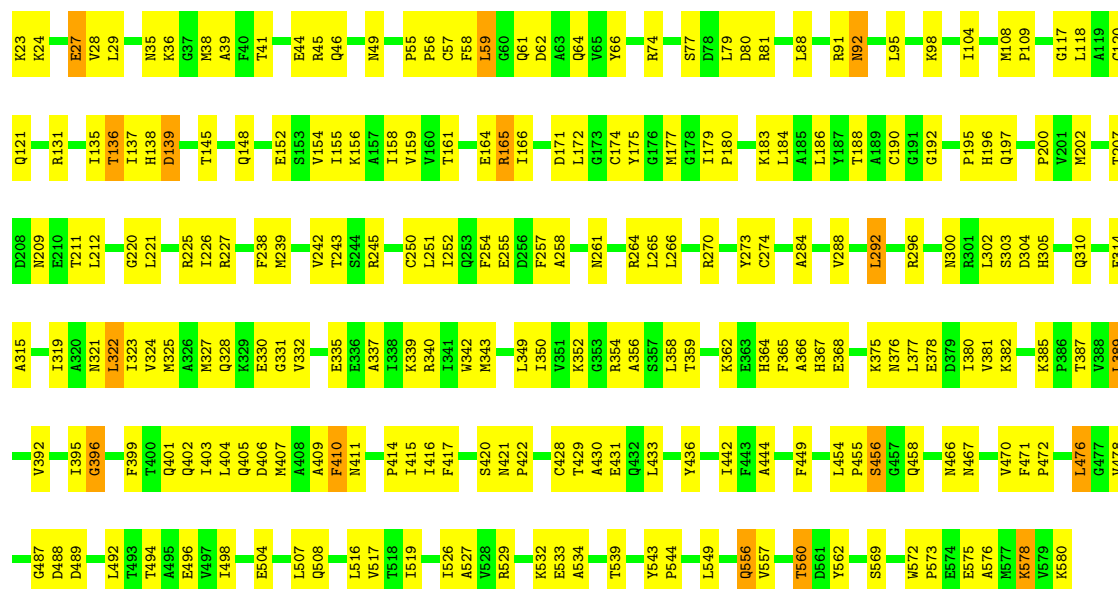
• Molecule 1: MALIC ENZYME

Chain J: 64% 33%

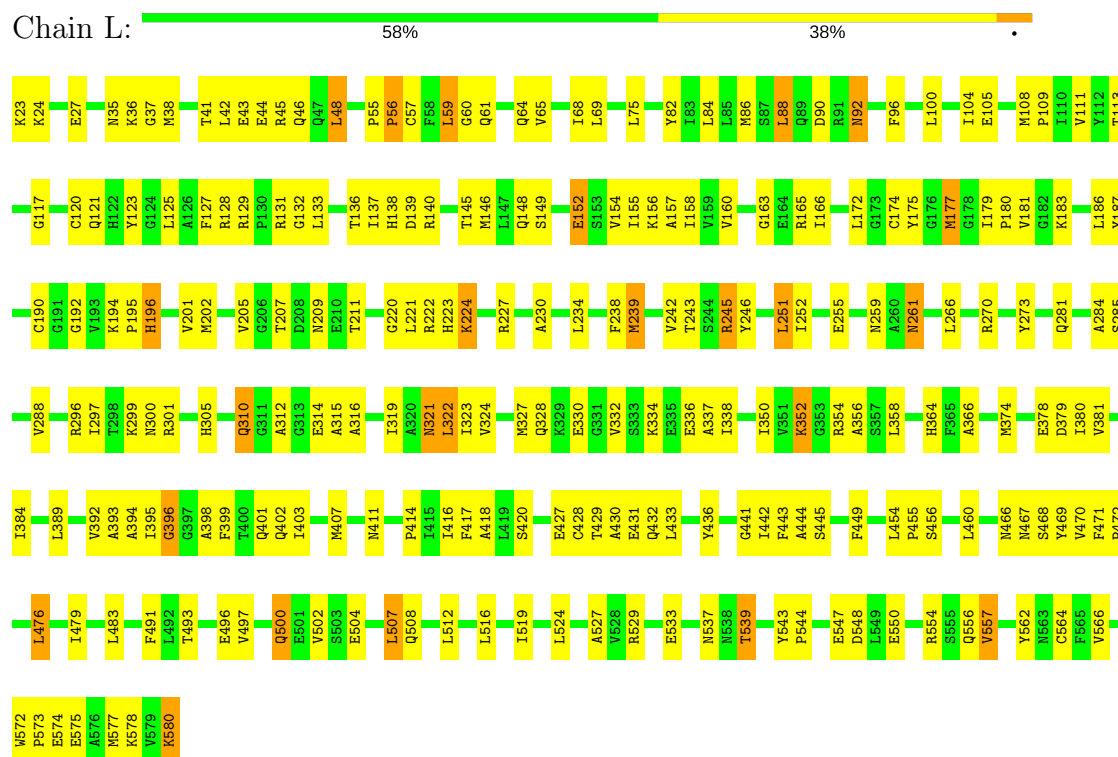


• Molecule 1: MALIC ENZYME

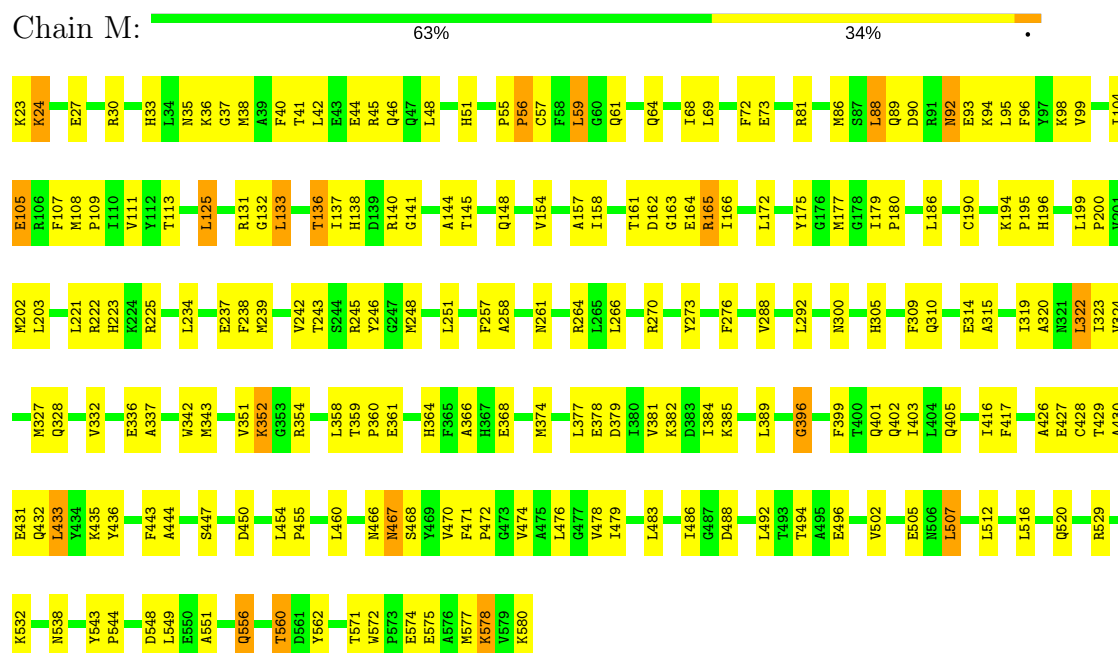
Chain K: 58% 39%



• Molecule 1: MALIC ENZYME

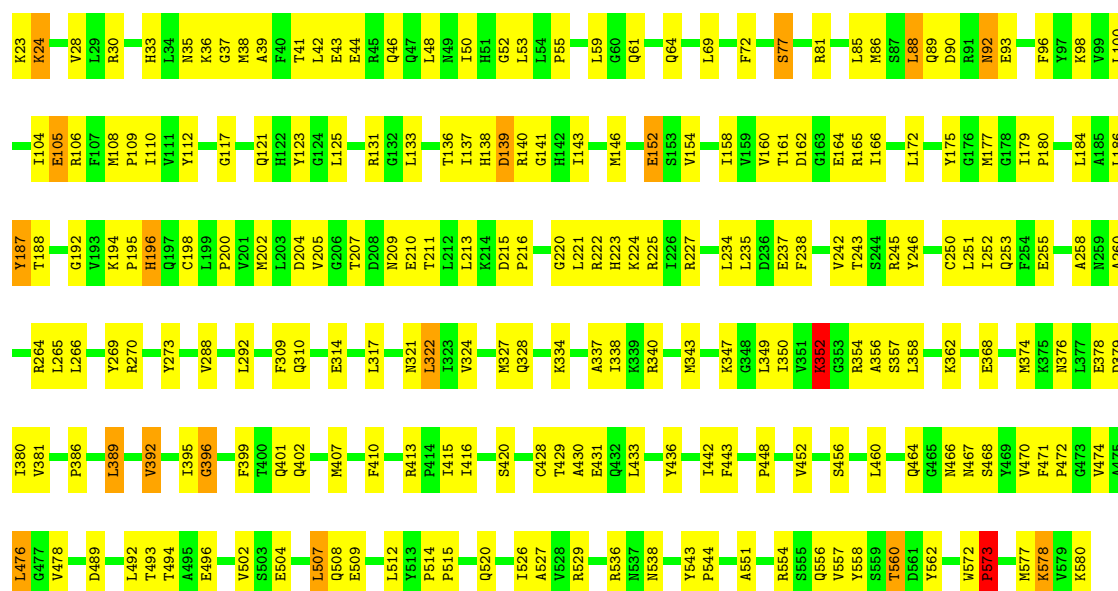


• Molecule 1: MALIC ENZYME



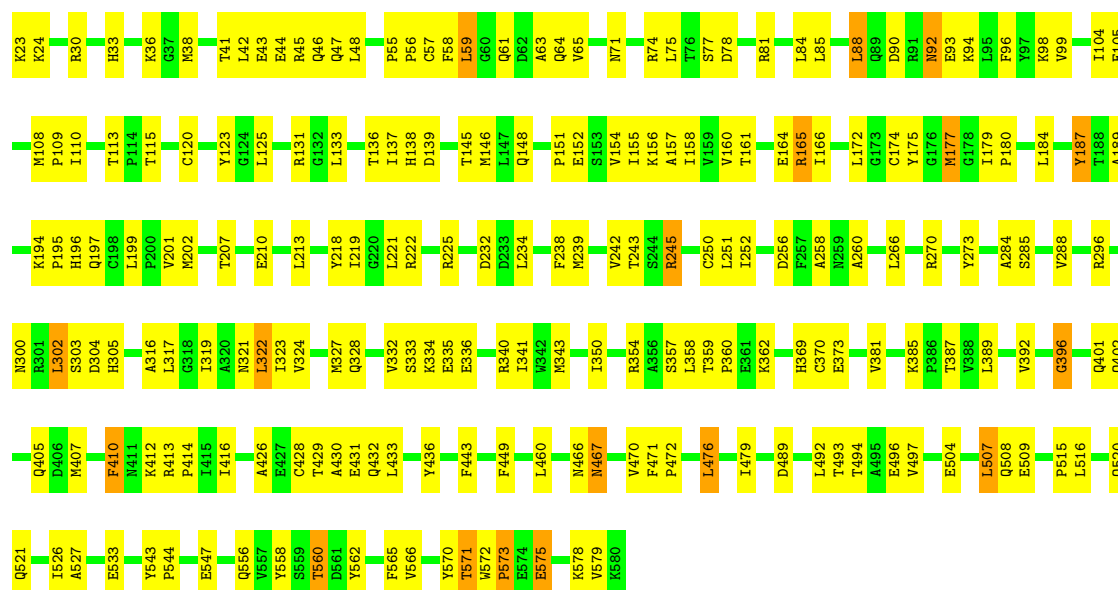
• Molecule 1: MALIC ENZYME





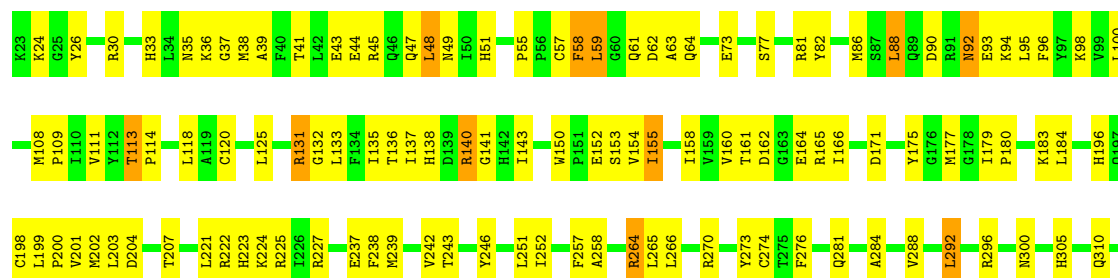
• Molecule 1: MALIC ENZYME

Chain O: 62% 35%



• Molecule 1: MALIC ENZYME

Chain P: 64% 32%



| | | |
|------|------|------|
| I319 | T429 | P544 |
| A430 | A430 | R554 |
| E431 | E431 | S555 |
| Q432 | Q432 | Q556 |
| L433 | L433 | V557 |
| K327 | E438 | Y558 |
| V332 | F443 | S559 |
| E336 | L454 | T560 |
| A337 | P455 | D561 |
| R340 | L460 | Y562 |
| T341 | N466 | V566 |
| W342 | N467 | W572 |
| I350 | S468 | P573 |
| L358 | F471 | E574 |
| K362 | P472 | E575 |
| E363 | G473 | K578 |
| H364 | L476 | V579 |
| H367 | G477 | K580 |
| V478 | V478 | |
| G487 | G487 | |
| N376 | L492 | |
| D379 | T493 | |
| I380 | E496 | |
| V381 | V497 | |
| K385 | Q500 | |
| V388 | E501 | |
| L389 | V502 | |
| S503 | S503 | |
| E504 | E504 | |
| F399 | L507 | |
| T400 | Q508 | |
| Q401 | L516 | |
| Q402 | I519 | |
| I403 | Q520 | |
| L404 | Q521 | |
| Q405 | Q521 | |
| D406 | L524 | |
| H407 | A527 | |
| F410 | V528 | |
| N411 | R529 | |
| I415 | I530 | |
| I416 | E533 | |
| A426 | Y543 | |
| E427 | | |
| C428 | | |

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 124.15Å 140.86Å 167.08Å 90.05° 87.16° 75.63° | Depositor |
| Resolution (Å) | 10.00 – 2.50 | Depositor |
| % Data completeness (in resolution range) | 83.0 (10.00-2.50) | Depositor |
| R_{merge} | 0.08 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.210 , 0.256 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 71519 | wwPDB-VP |
| Average B, all atoms (Å ²) | 18.0 | wwPDB-VP |

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: OXL, NA, NAP, MN, CL

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 | 0.39 | 0/4420 | 0.61 | 0/5962 |
| 1 | B | 0.38 | 0/4420 | 0.61 | 0/5962 |
| 1 | C | 0.40 | 0/4420 | 0.62 | 1/5962 (0.0%) |
| 1 | D | 0.40 | 0/4420 | 0.62 | 0/5962 |
| 1 | E | 0.38 | 0/4420 | 0.61 | 0/5962 |
| 1 | F | 0.40 | 0/4420 | 0.63 | 1/5962 (0.0%) |
| 1 | G | 0.39 | 0/4420 | 0.62 | 0/5962 |
| 1 | H | 0.41 | 0/4420 | 0.62 | 0/5962 |
| 1 | I | 0.40 | 0/4420 | 0.63 | 0/5962 |
| 1 | J | 0.40 | 0/4420 | 0.61 | 0/5962 |
| 1 | K | 0.39 | 0/4420 | 0.61 | 0/5962 |
| 1 | L | 0.39 | 0/4420 | 0.62 | 0/5962 |
| 1 | M | 0.41 | 0/4420 | 0.63 | 0/5962 |
| 1 | N | 0.40 | 0/4420 | 0.63 | 1/5962 (0.0%) |
| 1 | O | 0.39 | 0/4420 | 0.62 | 0/5962 |
| 1 | P | 0.39 | 0/4421 | 0.62 | 0/5962 |
| All | All | 0.39 | 0/70721 | 0.62 | 3/95392 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | C | 251 | LEU | CA-CB-CG | 5.19 | 127.24 | 115.30 |
| 1 | F | 310 | GLN | N-CA-C | -5.11 | 97.21 | 111.00 |
| 1 | N | 352 | LYS | N-CA-C | 5.09 | 124.75 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4345 | 0 | 4366 | 230 | 0 |
| 1 | B | 4345 | 0 | 4366 | 216 | 0 |
| 1 | C | 4345 | 0 | 4366 | 219 | 0 |
| 1 | D | 4345 | 0 | 4366 | 196 | 0 |
| 1 | E | 4345 | 0 | 4366 | 189 | 0 |
| 1 | F | 4345 | 0 | 4366 | 193 | 0 |
| 1 | G | 4345 | 0 | 4366 | 197 | 0 |
| 1 | H | 4345 | 0 | 4366 | 178 | 0 |
| 1 | I | 4345 | 0 | 4366 | 181 | 0 |
| 1 | J | 4345 | 0 | 4366 | 200 | 0 |
| 1 | K | 4345 | 0 | 4366 | 208 | 0 |
| 1 | L | 4345 | 0 | 4366 | 227 | 0 |
| 1 | M | 4345 | 0 | 4366 | 188 | 0 |
| 1 | N | 4345 | 0 | 4366 | 207 | 0 |
| 1 | O | 4345 | 0 | 4366 | 226 | 0 |
| 1 | P | 4346 | 0 | 4366 | 194 | 0 |
| 2 | A | 48 | 0 | 25 | 4 | 0 |
| 2 | B | 48 | 0 | 25 | 4 | 0 |
| 2 | C | 48 | 0 | 25 | 2 | 0 |
| 2 | D | 48 | 0 | 25 | 2 | 0 |
| 2 | E | 48 | 0 | 25 | 3 | 0 |
| 2 | F | 48 | 0 | 25 | 2 | 0 |
| 2 | G | 48 | 0 | 25 | 3 | 0 |
| 2 | H | 48 | 0 | 25 | 3 | 0 |
| 2 | I | 48 | 0 | 25 | 3 | 0 |
| 2 | J | 48 | 0 | 25 | 4 | 0 |
| 2 | K | 48 | 0 | 25 | 5 | 0 |
| 2 | L | 48 | 0 | 25 | 5 | 0 |
| 2 | M | 48 | 0 | 25 | 3 | 0 |
| 2 | N | 48 | 0 | 25 | 3 | 0 |
| 2 | O | 48 | 0 | 25 | 2 | 0 |
| 2 | P | 48 | 0 | 25 | 1 | 0 |
| 3 | A | 6 | 0 | 0 | 1 | 0 |
| 3 | B | 6 | 0 | 0 | 1 | 0 |
| 3 | C | 6 | 0 | 0 | 3 | 0 |
| 3 | D | 6 | 0 | 0 | 2 | 0 |
| 3 | E | 6 | 0 | 0 | 1 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | F | 6 | 0 | 0 | 1 | 0 |
| 3 | G | 6 | 0 | 0 | 1 | 0 |
| 3 | H | 6 | 0 | 0 | 1 | 0 |
| 3 | I | 6 | 0 | 0 | 0 | 0 |
| 3 | J | 6 | 0 | 0 | 1 | 0 |
| 3 | K | 6 | 0 | 0 | 1 | 0 |
| 3 | L | 6 | 0 | 0 | 1 | 0 |
| 3 | M | 6 | 0 | 0 | 0 | 0 |
| 3 | N | 6 | 0 | 0 | 1 | 0 |
| 3 | O | 6 | 0 | 0 | 0 | 0 |
| 3 | P | 6 | 0 | 0 | 1 | 0 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | C | 1 | 0 | 0 | 0 | 0 |
| 4 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | E | 1 | 0 | 0 | 0 | 0 |
| 4 | F | 1 | 0 | 0 | 0 | 0 |
| 4 | G | 1 | 0 | 0 | 0 | 0 |
| 4 | H | 1 | 0 | 0 | 0 | 0 |
| 4 | I | 1 | 0 | 0 | 0 | 0 |
| 4 | J | 1 | 0 | 0 | 0 | 0 |
| 4 | K | 1 | 0 | 0 | 0 | 0 |
| 4 | L | 1 | 0 | 0 | 0 | 0 |
| 4 | M | 1 | 0 | 0 | 0 | 0 |
| 4 | N | 1 | 0 | 0 | 0 | 0 |
| 4 | O | 1 | 0 | 0 | 0 | 0 |
| 4 | P | 1 | 0 | 0 | 0 | 0 |
| 5 | B | 1 | 0 | 0 | 0 | 0 |
| 5 | C | 4 | 0 | 0 | 1 | 0 |
| 5 | E | 3 | 0 | 0 | 1 | 0 |
| 5 | F | 2 | 0 | 0 | 1 | 0 |
| 5 | G | 1 | 0 | 0 | 0 | 0 |
| 5 | H | 1 | 0 | 0 | 0 | 0 |
| 5 | I | 5 | 0 | 0 | 1 | 0 |
| 5 | J | 2 | 0 | 0 | 0 | 0 |
| 5 | K | 1 | 0 | 0 | 0 | 0 |
| 5 | L | 1 | 0 | 0 | 0 | 0 |
| 5 | M | 3 | 0 | 0 | 1 | 0 |
| 5 | N | 2 | 0 | 0 | 1 | 0 |
| 5 | O | 4 | 0 | 0 | 3 | 0 |
| 5 | P | 3 | 0 | 0 | 3 | 0 |
| 6 | C | 4 | 0 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6 | D | 2 | 0 | 0 | 0 | 0 |
| 6 | F | 2 | 0 | 0 | 0 | 0 |
| 6 | G | 1 | 0 | 0 | 0 | 0 |
| 6 | H | 5 | 0 | 0 | 0 | 0 |
| 6 | I | 2 | 0 | 0 | 0 | 0 |
| 6 | J | 2 | 0 | 0 | 0 | 0 |
| 6 | K | 1 | 0 | 0 | 0 | 0 |
| 6 | L | 1 | 0 | 0 | 0 | 0 |
| 6 | M | 6 | 0 | 0 | 0 | 0 |
| 6 | N | 1 | 0 | 0 | 0 | 0 |
| 6 | O | 4 | 0 | 0 | 0 | 0 |
| 6 | P | 5 | 0 | 0 | 0 | 0 |
| 7 | A | 35 | 0 | 0 | 6 | 0 |
| 7 | B | 42 | 0 | 0 | 6 | 0 |
| 7 | C | 77 | 0 | 0 | 7 | 0 |
| 7 | D | 49 | 0 | 0 | 2 | 0 |
| 7 | E | 58 | 0 | 0 | 5 | 0 |
| 7 | F | 78 | 0 | 0 | 6 | 0 |
| 7 | G | 65 | 0 | 0 | 6 | 0 |
| 7 | H | 77 | 0 | 0 | 7 | 0 |
| 7 | I | 80 | 0 | 0 | 7 | 0 |
| 7 | J | 63 | 0 | 0 | 3 | 0 |
| 7 | K | 41 | 0 | 0 | 5 | 0 |
| 7 | L | 75 | 0 | 0 | 7 | 0 |
| 7 | M | 81 | 0 | 0 | 7 | 0 |
| 7 | N | 71 | 0 | 0 | 7 | 0 |
| 7 | O | 78 | 0 | 0 | 8 | 0 |
| 7 | P | 79 | 0 | 0 | 4 | 0 |
| All | All | 71519 | 0 | 70256 | 3151 | 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 22.

All (3151) 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:H:136:THR:HG22 | 1:H:138:HIS:H | 1.08 | 1.17 |
| 1:N:136:THR:HG22 | 1:N:138:HIS:H | 1.04 | 1.17 |
| 1:K:98:LYS:HD3 | 1:K:560:THR:HG21 | 1.30 | 1.14 |
| 1:F:136:THR:HG22 | 1:F:138:HIS:H | 1.10 | 1.13 |
| 1:B:136:THR:HG22 | 1:B:138:HIS:H | 1.06 | 1.13 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:416:ILE:HG13 | 1:G:433:LEU:HD21 | 1.24 | 1.13 |
| 1:N:381:VAL:HG13 | 1:N:407:MSE:HE2 | 1.30 | 1.13 |
| 1:M:429:THR:HB | 1:M:432:GLN:HG3 | 1.34 | 1.10 |
| 1:E:136:THR:HG22 | 1:E:138:HIS:H | 1.06 | 1.10 |
| 1:O:323:ILE:HG22 | 1:O:327:MSE:HE2 | 1.25 | 1.10 |
| 1:K:136:THR:HG23 | 1:K:138:HIS:H | 1.08 | 1.10 |
| 1:P:136:THR:HG22 | 1:P:138:HIS:H | 1.04 | 1.09 |
| 1:C:136:THR:HG22 | 1:C:138:HIS:H | 1.08 | 1.09 |
| 1:A:327:MSE:HE3 | 1:A:337:ALA:HB1 | 1.33 | 1.08 |
| 1:C:323:ILE:HG22 | 1:C:327:MSE:HE2 | 1.36 | 1.08 |
| 1:C:494:THR:HG23 | 1:C:526:ILE:HD12 | 1.35 | 1.08 |
| 1:I:136:THR:HG22 | 1:I:138:HIS:H | 1.09 | 1.08 |
| 1:D:160:VAL:HG12 | 1:D:201:VAL:HB | 1.30 | 1.07 |
| 1:A:177:MSE:HE1 | 1:A:200:PRO:HB2 | 1.35 | 1.07 |
| 1:O:136:THR:HG22 | 1:O:138:HIS:H | 1.12 | 1.07 |
| 1:A:386:PRO:HG2 | 1:A:407:MSE:HE1 | 1.13 | 1.07 |
| 1:L:136:THR:HG22 | 1:L:138:HIS:H | 1.04 | 1.06 |
| 1:L:327:MSE:HE3 | 1:L:337:ALA:HB1 | 1.38 | 1.05 |
| 1:K:327:MSE:HE3 | 1:K:337:ALA:HB1 | 1.39 | 1.04 |
| 1:P:160:VAL:HG22 | 1:P:201:VAL:HB | 1.40 | 1.04 |
| 1:M:136:THR:HG23 | 1:M:138:HIS:H | 1.17 | 1.03 |
| 1:E:386:PRO:HG2 | 1:E:407:MSE:HE1 | 1.36 | 1.03 |
| 1:G:136:THR:HG22 | 1:G:138:HIS:H | 1.24 | 1.03 |
| 1:J:136:THR:HG22 | 1:J:138:HIS:H | 1.20 | 1.01 |
| 1:P:327:MSE:HE3 | 1:P:337:ALA:HB1 | 1.40 | 1.01 |
| 1:O:104:ILE:HG13 | 1:O:108:MSE:HE3 | 1.38 | 1.00 |
| 1:N:327:MSE:HE3 | 1:N:337:ALA:HB1 | 1.40 | 1.00 |
| 1:G:177:MSE:HE1 | 1:G:200:PRO:HB2 | 1.42 | 1.00 |
| 1:C:416:ILE:HG13 | 1:C:433:LEU:HD21 | 1.40 | 0.99 |
| 1:M:429:THR:H | 1:M:432:GLN:HE21 | 1.04 | 0.98 |
| 1:B:416:ILE:HG13 | 1:B:433:LEU:HD21 | 1.39 | 0.98 |
| 1:N:36:LYS:HG2 | 1:N:39:ALA:HB3 | 1.45 | 0.98 |
| 1:E:24:LYS:HG2 | 1:E:25:GLY:N | 1.77 | 0.97 |
| 1:H:327:MSE:HE3 | 1:H:337:ALA:HB1 | 1.44 | 0.97 |
| 1:E:24:LYS:HZ2 | 1:E:49:ASN:HD22 | 1.00 | 0.97 |
| 1:N:504:GLU:HG3 | 1:N:508:GLN:HE21 | 1.30 | 0.96 |
| 1:L:416:ILE:HG13 | 1:L:433:LEU:HD21 | 1.48 | 0.96 |
| 1:M:238:PHE:HD2 | 1:M:239:MSE:HE2 | 1.29 | 0.96 |
| 1:L:261:ASN:H | 1:L:261:ASN:HD22 | 1.11 | 0.95 |
| 1:L:145:THR:O | 1:L:148:GLN:HG2 | 1.65 | 0.95 |
| 1:H:359:THR:HG22 | 1:H:362:LYS:H | 1.31 | 0.95 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:386:PRO:HG2 | 1:H:407:MSE:HE1 | 1.47 | 0.95 |
| 1:P:136:THR:HG22 | 1:P:138:HIS:N | 1.81 | 0.94 |
| 1:F:177:MSE:HE3 | 1:F:177:MSE:HA | 1.49 | 0.94 |
| 1:K:136:THR:HG23 | 1:K:138:HIS:N | 1.81 | 0.94 |
| 1:P:504:GLU:HG3 | 1:P:508:GLN:HE22 | 1.30 | 0.94 |
| 1:J:136:THR:CG2 | 1:J:138:HIS:H | 1.80 | 0.94 |
| 1:L:136:THR:HG22 | 1:L:138:HIS:N | 1.82 | 0.94 |
| 1:P:416:ILE:HG13 | 1:P:433:LEU:HD21 | 1.49 | 0.94 |
| 1:D:136:THR:HG23 | 1:D:138:HIS:H | 1.31 | 0.94 |
| 1:D:547:GLU:H | 1:D:547:GLU:CD | 1.65 | 0.94 |
| 1:P:36:LYS:HG2 | 1:P:39:ALA:HB3 | 1.50 | 0.93 |
| 1:E:24:LYS:HZ2 | 1:E:49:ASN:ND2 | 1.64 | 0.93 |
| 1:O:160:VAL:HG22 | 1:O:201:VAL:HB | 1.51 | 0.93 |
| 1:I:429:THR:HG23 | 1:I:432:GLN:H | 1.33 | 0.93 |
| 1:L:261:ASN:HD22 | 1:L:261:ASN:N | 1.67 | 0.93 |
| 1:M:454:LEU:HD11 | 1:M:460:LEU:HG | 1.51 | 0.93 |
| 1:A:41:THR:HB | 1:A:44:GLU:HG3 | 1.51 | 0.92 |
| 1:E:327:MSE:HE3 | 1:E:337:ALA:HB1 | 1.50 | 0.92 |
| 1:G:378:GLU:HA | 1:G:403:ILE:HD11 | 1.51 | 0.92 |
| 1:A:42:LEU:HD23 | 1:C:577:MSE:HE3 | 1.50 | 0.91 |
| 1:G:164:GLU:HG2 | 1:G:258:ALA:HB2 | 1.51 | 0.91 |
| 1:A:36:LYS:HG2 | 1:A:39:ALA:HB3 | 1.52 | 0.91 |
| 1:C:23:LYS:HG2 | 1:C:24:LYS:H | 1.34 | 0.91 |
| 1:I:136:THR:HG22 | 1:I:138:HIS:N | 1.85 | 0.91 |
| 1:O:401:GLN:HG2 | 1:O:405:GLN:HE21 | 1.33 | 0.91 |
| 1:B:98:LYS:HD3 | 1:B:560:THR:HG21 | 1.50 | 0.91 |
| 1:C:136:THR:HG22 | 1:C:138:HIS:N | 1.87 | 0.90 |
| 1:F:429:THR:H | 1:F:432:GLN:NE2 | 1.69 | 0.90 |
| 1:A:570:TYR:H | 1:C:46:GLN:HE22 | 1.19 | 0.89 |
| 1:D:23:LYS:HG2 | 1:D:24:LYS:H | 1.36 | 0.89 |
| 1:B:140:ARG:HH12 | 1:B:230:ALA:HB1 | 1.38 | 0.89 |
| 1:K:416:ILE:HG13 | 1:K:433:LEU:HD21 | 1.53 | 0.89 |
| 1:N:136:THR:HG22 | 1:N:138:HIS:N | 1.87 | 0.89 |
| 1:N:389:LEU:HG | 1:N:407:MSE:HE3 | 1.54 | 0.89 |
| 1:J:429:THR:HB | 1:J:432:GLN:HG2 | 1.54 | 0.88 |
| 1:L:239:MSE:HA | 1:L:239:MSE:HE2 | 1.55 | 0.88 |
| 1:O:136:THR:HB | 1:O:139:ASP:OD2 | 1.73 | 0.88 |
| 1:O:412:LYS:HB2 | 1:O:412:LYS:NZ | 1.88 | 0.88 |
| 1:E:136:THR:HG22 | 1:E:138:HIS:N | 1.89 | 0.88 |
| 1:M:578:LYS:NZ | 1:M:580:LYS:HB2 | 1.89 | 0.88 |
| 1:E:429:THR:HG22 | 1:E:431:GLU:H | 1.37 | 0.88 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:222:ARG:HG3 | 1:G:222:ARG:HH11 | 1.39 | 0.88 |
| 1:N:98:LYS:HD3 | 1:N:560:THR:HG21 | 1.55 | 0.88 |
| 1:D:324:VAL:HG12 | 1:D:328:GLN:HE21 | 1.39 | 0.87 |
| 1:L:104:ILE:HG13 | 1:L:108:MSE:HE3 | 1.56 | 0.87 |
| 1:A:466:ASN:HA | 2:A:1581:NAP:H72N | 1.39 | 0.87 |
| 1:G:560:THR:HG23 | 7:G:2062:HOH:O | 1.74 | 0.87 |
| 1:J:416:ILE:HG13 | 1:J:433:LEU:HD21 | 1.57 | 0.87 |
| 1:A:358:LEU:HD23 | 1:A:363:GLU:HG3 | 1.56 | 0.87 |
| 1:E:98:LYS:HD3 | 1:E:560:THR:HG21 | 1.56 | 0.87 |
| 1:O:238:PHE:CD2 | 1:O:239:MSE:HE3 | 2.09 | 0.87 |
| 1:B:239:MSE:HE1 | 1:B:252:ILE:HG12 | 1.56 | 0.86 |
| 1:A:238:PHE:HD2 | 1:A:239:MSE:HE2 | 1.38 | 0.86 |
| 1:L:429:THR:HB | 1:L:432:GLN:HG3 | 1.57 | 0.86 |
| 1:J:466:ASN:HA | 2:J:1581:NAP:H72N | 1.38 | 0.86 |
| 1:P:136:THR:CG2 | 1:P:138:HIS:H | 1.87 | 0.86 |
| 1:F:572:TRP:O | 1:F:573:PRO:O | 1.94 | 0.86 |
| 1:G:136:THR:HG22 | 1:G:138:HIS:N | 1.91 | 0.86 |
| 1:A:569:SER:HA | 1:C:46:GLN:NE2 | 1.91 | 0.86 |
| 1:H:575:GLU:O | 1:H:578:LYS:HG2 | 1.73 | 0.86 |
| 1:J:136:THR:HG22 | 1:J:138:HIS:N | 1.90 | 0.85 |
| 1:P:143:ILE:HD12 | 1:P:237:GLU:HG2 | 1.58 | 0.85 |
| 1:C:36:LYS:HG2 | 1:C:39:ALA:HB3 | 1.56 | 0.85 |
| 1:K:239:MSE:HA | 1:K:239:MSE:HE2 | 1.56 | 0.85 |
| 1:N:416:ILE:HG13 | 1:N:433:LEU:HD21 | 1.57 | 0.85 |
| 1:G:575:GLU:HG2 | 1:G:576:ALA:N | 1.88 | 0.85 |
| 1:M:433:LEU:HG | 1:M:443:PHE:HB2 | 1.59 | 0.85 |
| 1:A:572:TRP:O | 1:A:573:PRO:O | 1.94 | 0.85 |
| 1:B:239:MSE:HE2 | 1:B:239:MSE:HA | 1.56 | 0.85 |
| 1:G:429:THR:H | 1:G:432:GLN:NE2 | 1.75 | 0.85 |
| 1:I:327:MSE:HE3 | 1:I:337:ALA:HB1 | 1.55 | 0.85 |
| 1:O:239:MSE:HA | 1:O:239:MSE:HE2 | 1.59 | 0.84 |
| 1:O:41:THR:HB | 1:O:44:GLU:HG3 | 1.58 | 0.84 |
| 1:I:133:LEU:HD22 | 1:I:135:ILE:HG13 | 1.58 | 0.84 |
| 1:A:136:THR:CG2 | 1:A:138:HIS:H | 1.91 | 0.84 |
| 1:M:327:MSE:HE3 | 1:M:337:ALA:HB1 | 1.59 | 0.84 |
| 1:M:24:LYS:HB2 | 1:M:24:LYS:NZ | 1.89 | 0.84 |
| 1:N:24:LYS:HG2 | 1:P:24:LYS:NZ | 1.93 | 0.84 |
| 1:H:416:ILE:HG13 | 1:H:433:LEU:HD21 | 1.57 | 0.84 |
| 1:M:401:GLN:O | 1:M:405:GLN:HG3 | 1.77 | 0.84 |
| 1:B:136:THR:HB | 1:B:139:ASP:OD1 | 1.78 | 0.83 |
| 1:J:572:TRP:O | 1:J:573:PRO:O | 1.96 | 0.83 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:129:ARG:HH11 | 1:F:129:ARG:HG3 | 1.42 | 0.83 |
| 1:N:381:VAL:CG1 | 1:N:407:MSE:HE2 | 2.07 | 0.83 |
| 1:E:340:ARG:HH11 | 1:E:340:ARG:HB3 | 1.44 | 0.83 |
| 1:J:327:MSE:HE3 | 1:J:337:ALA:HB1 | 1.57 | 0.83 |
| 1:B:352:LYS:HE2 | 1:B:353:GLY:H | 1.42 | 0.83 |
| 1:B:41:THR:HG22 | 1:B:43:GLU:H | 1.43 | 0.83 |
| 1:G:378:GLU:HA | 1:G:403:ILE:CD1 | 2.09 | 0.83 |
| 1:K:152:GLU:OE2 | 1:K:154:VAL:HG12 | 1.78 | 0.83 |
| 7:N:2067:HOH:O | 1:O:222:ARG:HD2 | 1.77 | 0.83 |
| 1:A:359:THR:HG22 | 1:A:362:LYS:HE2 | 1.61 | 0.83 |
| 1:D:35:ASN:ND2 | 1:D:37:GLY:H | 1.77 | 0.83 |
| 1:J:98:LYS:HD3 | 1:J:560:THR:HG21 | 1.60 | 0.83 |
| 1:K:164:GLU:HG2 | 1:K:258:ALA:HB2 | 1.60 | 0.83 |
| 1:L:132:GLY:HA3 | 1:L:177:MSE:HE1 | 1.58 | 0.83 |
| 1:G:324:VAL:HG12 | 1:G:328:GLN:HE21 | 1.43 | 0.83 |
| 1:B:301:ARG:NH1 | 1:B:301:ARG:HB3 | 1.94 | 0.82 |
| 1:A:316:ALA:HB1 | 1:A:343:MSE:CE | 2.10 | 0.82 |
| 1:J:578:LYS:HE2 | 1:J:580:LYS:HE3 | 1.61 | 0.82 |
| 1:F:238:PHE:CD2 | 1:F:239:MSE:HE3 | 2.14 | 0.82 |
| 1:L:136:THR:CG2 | 1:L:138:HIS:H | 1.90 | 0.82 |
| 1:D:238:PHE:CD2 | 1:D:239:MSE:HE2 | 2.15 | 0.82 |
| 1:D:23:LYS:HG2 | 1:D:24:LYS:N | 1.92 | 0.82 |
| 1:I:136:THR:CG2 | 1:I:138:HIS:H | 1.93 | 0.82 |
| 1:D:359:THR:HG22 | 1:D:361:GLU:H | 1.44 | 0.82 |
| 1:J:238:PHE:CD2 | 1:J:239:MSE:HE2 | 2.15 | 0.82 |
| 1:F:239:MSE:HE2 | 1:F:239:MSE:HA | 1.61 | 0.81 |
| 1:I:350:ILE:HG23 | 1:I:358:LEU:HD11 | 1.60 | 0.81 |
| 1:O:59:LEU:HD13 | 1:O:64:GLN:HG3 | 1.61 | 0.81 |
| 1:A:26:TYR:HB2 | 7:A:2002:HOH:O | 1.79 | 0.81 |
| 1:F:433:LEU:HG | 1:F:443:PHE:CD1 | 2.15 | 0.81 |
| 1:J:359:THR:HG23 | 1:J:362:LYS:H | 1.43 | 0.81 |
| 1:B:136:THR:HG22 | 1:B:138:HIS:N | 1.92 | 0.81 |
| 1:F:88:LEU:HD21 | 1:F:95:LEU:HD12 | 1.62 | 0.81 |
| 1:L:466:ASN:HA | 2:L:1581:NAP:H72N | 1.44 | 0.81 |
| 1:O:429:THR:HB | 1:O:432:GLN:HG2 | 1.63 | 0.81 |
| 1:D:136:THR:HG23 | 1:D:138:HIS:N | 1.96 | 0.81 |
| 1:L:35:ASN:ND2 | 1:L:37:GLY:H | 1.79 | 0.81 |
| 1:I:429:THR:HG22 | 1:I:432:GLN:CG | 2.10 | 0.81 |
| 1:L:381:VAL:CG1 | 1:L:407:MSE:HE1 | 2.11 | 0.81 |
| 1:P:504:GLU:HG3 | 1:P:508:GLN:NE2 | 1.95 | 0.81 |
| 1:F:136:THR:HG23 | 1:F:221:LEU:HD11 | 1.61 | 0.80 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:154:VAL:HG12 | 7:H:2026:HOH:O | 1.81 | 0.80 |
| 1:K:98:LYS:HD3 | 1:K:560:THR:CG2 | 2.11 | 0.80 |
| 1:B:98:LYS:HD3 | 1:B:560:THR:CG2 | 2.11 | 0.80 |
| 1:D:327:MSE:HE3 | 1:D:337:ALA:HB1 | 1.63 | 0.80 |
| 1:H:288:VAL:HG21 | 1:H:322:LEU:HB3 | 1.64 | 0.80 |
| 1:O:23:LYS:O | 1:O:24:LYS:HG3 | 1.81 | 0.80 |
| 1:A:98:LYS:HD3 | 1:A:560:THR:HG21 | 1.61 | 0.80 |
| 1:N:340:ARG:HD3 | 7:N:2043:HOH:O | 1.81 | 0.80 |
| 1:N:386:PRO:HG2 | 1:N:407:MSE:HE1 | 1.62 | 0.80 |
| 1:D:133:LEU:HD13 | 1:D:135:ILE:HD11 | 1.63 | 0.80 |
| 1:K:36:LYS:HG2 | 1:K:39:ALA:HB3 | 1.64 | 0.80 |
| 1:M:24:LYS:HD2 | 1:O:24:LYS:HZ2 | 1.47 | 0.80 |
| 1:O:177:MSE:CE | 1:O:177:MSE:HA | 2.12 | 0.79 |
| 1:F:136:THR:HG22 | 1:F:138:HIS:N | 1.94 | 0.79 |
| 1:M:104:ILE:HG13 | 1:M:108:MSE:HE3 | 1.63 | 0.79 |
| 1:D:41:THR:HG22 | 1:D:43:GLU:H | 1.45 | 0.79 |
| 1:H:92:ASN:C | 1:H:92:ASN:HD22 | 1.85 | 0.79 |
| 1:P:41:THR:HG22 | 1:P:43:GLU:H | 1.47 | 0.79 |
| 1:A:177:MSE:CE | 1:A:181:VAL:HG23 | 2.13 | 0.79 |
| 1:O:136:THR:HG23 | 1:O:221:LEU:HD11 | 1.63 | 0.79 |
| 1:F:416:ILE:HG13 | 1:F:433:LEU:HD21 | 1.63 | 0.79 |
| 1:J:104:ILE:HG13 | 1:J:108:MSE:HE3 | 1.65 | 0.79 |
| 1:D:416:ILE:HG13 | 1:D:433:LEU:HD21 | 1.65 | 0.78 |
| 1:K:415:ILE:CD1 | 1:K:442:ILE:HD12 | 2.14 | 0.78 |
| 1:K:238:PHE:CD2 | 1:K:239:MSE:HE3 | 2.19 | 0.78 |
| 1:H:136:THR:HG22 | 1:H:138:HIS:N | 1.92 | 0.78 |
| 1:N:572:TRP:O | 1:N:573:PRO:O | 2.02 | 0.78 |
| 1:O:328:GLN:NE2 | 1:O:334:LYS:HD2 | 1.98 | 0.78 |
| 1:G:136:THR:CG2 | 1:G:138:HIS:H | 1.94 | 0.78 |
| 1:H:378:GLU:OE2 | 1:H:402:GLN:HB3 | 1.84 | 0.78 |
| 1:M:92:ASN:HD22 | 1:M:92:ASN:C | 1.85 | 0.78 |
| 1:O:433:LEU:HD12 | 1:O:443:PHE:HB2 | 1.64 | 0.78 |
| 1:D:572:TRP:O | 1:D:573:PRO:O | 2.02 | 0.77 |
| 1:H:36:LYS:HG2 | 1:H:39:ALA:HB3 | 1.65 | 0.77 |
| 1:I:41:THR:HB | 1:I:44:GLU:HG3 | 1.66 | 0.77 |
| 1:E:160:VAL:HG12 | 1:E:201:VAL:HB | 1.65 | 0.77 |
| 1:G:396:GLY:HA3 | 7:G:2041:HOH:O | 1.84 | 0.77 |
| 1:H:575:GLU:HG2 | 1:H:576:ALA:N | 1.97 | 0.77 |
| 1:J:225:ARG:HB2 | 1:J:227:ARG:NH1 | 2.00 | 0.77 |
| 1:O:136:THR:HG22 | 1:O:138:HIS:N | 1.96 | 0.77 |
| 1:F:299:LYS:HB3 | 1:F:299:LYS:NZ | 2.00 | 0.77 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:238:PHE:HD2 | 1:D:239:MSE:HE2 | 1.49 | 0.77 |
| 1:E:239:MSE:HE2 | 1:E:239:MSE:HA | 1.65 | 0.77 |
| 1:G:137:ILE:HA | 1:G:234:LEU:HD22 | 1.66 | 0.77 |
| 1:I:238:PHE:CD2 | 1:I:239:MSE:HE3 | 2.20 | 0.77 |
| 1:N:104:ILE:HG12 | 1:N:108:MSE:HE3 | 1.67 | 0.76 |
| 1:N:324:VAL:HG12 | 1:N:328:GLN:HE21 | 1.49 | 0.76 |
| 1:C:38:MSE:HB2 | 1:C:59:LEU:HD11 | 1.67 | 0.76 |
| 1:M:416:ILE:HB | 1:M:433:LEU:HD21 | 1.68 | 0.76 |
| 1:O:47:GLN:HE22 | 1:O:566:VAL:HG13 | 1.49 | 0.76 |
| 1:G:177:MSE:HE3 | 1:G:181:VAL:HG23 | 1.68 | 0.76 |
| 1:C:429:THR:HB | 1:C:432:GLN:HG3 | 1.68 | 0.76 |
| 1:E:238:PHE:CD2 | 1:E:239:MSE:HE3 | 2.21 | 0.76 |
| 1:M:202:MSE:HE3 | 1:M:203:LEU:C | 2.06 | 0.76 |
| 1:O:179:ILE:HB | 1:O:180:PRO:HD3 | 1.68 | 0.76 |
| 1:C:88:LEU:HD13 | 1:C:96:PHE:HA | 1.69 | 0.75 |
| 1:G:238:PHE:HD2 | 1:G:239:MSE:HE2 | 1.51 | 0.75 |
| 1:P:47:GLN:HE22 | 1:P:566:VAL:HG13 | 1.50 | 0.75 |
| 1:A:136:THR:HG22 | 1:A:138:HIS:H | 1.49 | 0.75 |
| 1:L:261:ASN:ND2 | 1:L:261:ASN:H | 1.85 | 0.75 |
| 1:K:466:ASN:HA | 2:K:1581:NAP:H72N | 1.51 | 0.75 |
| 1:M:429:THR:HG22 | 1:M:431:GLU:H | 1.50 | 0.75 |
| 1:E:288:VAL:HG21 | 1:E:322:LEU:HB3 | 1.67 | 0.75 |
| 1:O:41:THR:O | 1:O:45:ARG:HG3 | 1.87 | 0.75 |
| 1:F:179:ILE:HB | 1:F:180:PRO:HD3 | 1.68 | 0.75 |
| 1:B:41:THR:HG22 | 1:B:43:GLU:N | 2.01 | 0.75 |
| 1:F:23:LYS:N | 1:F:24:LYS:HZ3 | 1.85 | 0.75 |
| 1:M:323:ILE:HG22 | 1:M:327:MSE:HE2 | 1.68 | 0.75 |
| 1:N:334:LYS:O | 1:N:338:ILE:HD12 | 1.87 | 0.75 |
| 1:N:504:GLU:HG3 | 1:N:508:GLN:NE2 | 2.01 | 0.75 |
| 1:J:179:ILE:HB | 1:J:180:PRO:HD3 | 1.69 | 0.74 |
| 1:A:238:PHE:CD2 | 1:A:239:MSE:HE2 | 2.21 | 0.74 |
| 1:I:92:ASN:C | 1:I:92:ASN:HD22 | 1.88 | 0.74 |
| 1:L:550:GLU:O | 1:L:554:ARG:HG3 | 1.88 | 0.74 |
| 1:F:227:ARG:HH11 | 1:F:227:ARG:HG3 | 1.52 | 0.74 |
| 1:I:239:MSE:HE1 | 1:I:252:ILE:HG21 | 1.69 | 0.74 |
| 1:O:321:ASN:HB2 | 7:O:2055:HOH:O | 1.84 | 0.74 |
| 1:F:350:ILE:HD11 | 1:F:362:LYS:HD3 | 1.69 | 0.74 |
| 1:M:136:THR:HG23 | 1:M:138:HIS:N | 1.99 | 0.74 |
| 1:L:132:GLY:HA3 | 1:L:177:MSE:CE | 2.16 | 0.74 |
| 1:A:504:GLU:HG3 | 1:A:508:GLN:HE21 | 1.52 | 0.74 |
| 1:J:270:ARG:HH11 | 1:J:270:ARG:HG2 | 1.52 | 0.74 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:324:VAL:HA | 1:O:327:MSE:HE3 | 1.69 | 0.74 |
| 1:C:136:THR:CG2 | 1:C:138:HIS:H | 1.96 | 0.74 |
| 1:G:238:PHE:CD2 | 1:G:239:MSE:HE2 | 2.22 | 0.74 |
| 1:L:310:GLN:HE22 | 1:L:393:ALA:HB3 | 1.52 | 0.74 |
| 1:B:104:ILE:HG13 | 1:B:108:MSE:HE3 | 1.70 | 0.74 |
| 1:G:227:ARG:HH11 | 1:G:227:ARG:HG3 | 1.53 | 0.74 |
| 1:N:136:THR:HG23 | 1:N:221:LEU:HD11 | 1.68 | 0.74 |
| 1:O:266:LEU:O | 1:O:270:ARG:HB2 | 1.88 | 0.74 |
| 1:N:429:THR:HG22 | 1:N:431:GLU:H | 1.53 | 0.73 |
| 1:E:297:ILE:HD11 | 1:E:507:LEU:HD12 | 1.69 | 0.73 |
| 1:I:429:THR:HG22 | 1:I:432:GLN:HG3 | 1.69 | 0.73 |
| 1:O:412:LYS:HZ3 | 1:O:412:LYS:HB2 | 1.51 | 0.73 |
| 7:A:2016:HOH:O | 1:D:580:LYS:HG2 | 1.87 | 0.73 |
| 1:O:381:VAL:HG13 | 1:O:407:MSE:HE1 | 1.69 | 0.73 |
| 1:A:431:GLU:OE2 | 1:A:452:VAL:HG22 | 1.88 | 0.73 |
| 1:B:136:THR:HG23 | 1:B:221:LEU:HD11 | 1.70 | 0.73 |
| 1:D:155:ILE:HD13 | 1:D:246:TYR:CE2 | 2.22 | 0.73 |
| 1:O:47:GLN:NE2 | 1:O:566:VAL:HG13 | 2.04 | 0.73 |
| 1:A:335:GLU:HG2 | 1:A:339:LYS:HE3 | 1.71 | 0.73 |
| 1:L:350:ILE:HG23 | 1:L:358:LEU:HD11 | 1.71 | 0.73 |
| 1:M:288:VAL:HG21 | 1:M:322:LEU:HB3 | 1.71 | 0.73 |
| 1:E:98:LYS:HD3 | 1:E:560:THR:CG2 | 2.18 | 0.73 |
| 1:F:42:LEU:O | 1:F:46:GLN:HG3 | 1.88 | 0.73 |
| 1:O:146:MSE:HE3 | 1:P:51:HIS:CD2 | 2.23 | 0.73 |
| 1:F:183:LYS:HE2 | 5:F:1586:CL:CL | 2.26 | 0.73 |
| 1:F:401:GLN:HG2 | 1:F:436:TYR:CZ | 2.23 | 0.73 |
| 1:M:148:GLN:HG3 | 1:M:245:ARG:HH21 | 1.54 | 0.73 |
| 1:M:377:LEU:O | 1:M:381:VAL:HG23 | 1.88 | 0.73 |
| 1:P:429:THR:HG22 | 1:P:431:GLU:H | 1.52 | 0.73 |
| 1:A:270:ARG:HH12 | 1:A:487:GLY:HA2 | 1.54 | 0.72 |
| 1:O:327:MSE:HB3 | 1:O:332:VAL:HG11 | 1.71 | 0.72 |
| 1:O:429:THR:HB | 7:O:2063:HOH:O | 1.89 | 0.72 |
| 1:D:61:GLN:HG2 | 1:D:98:LYS:HG2 | 1.69 | 0.72 |
| 1:G:324:VAL:HG12 | 1:G:328:GLN:NE2 | 2.04 | 0.72 |
| 1:N:386:PRO:CG | 1:N:407:MSE:HE1 | 2.18 | 0.72 |
| 1:G:389:LEU:HD12 | 1:G:407:MSE:HE3 | 1.70 | 0.72 |
| 1:M:578:LYS:HZ2 | 1:M:580:LYS:HB2 | 1.55 | 0.72 |
| 1:N:164:GLU:HG2 | 1:N:258:ALA:HB2 | 1.70 | 0.72 |
| 1:E:429:THR:HG22 | 1:E:431:GLU:N | 2.04 | 0.72 |
| 1:M:578:LYS:HZ1 | 1:M:580:LYS:HD3 | 1.54 | 0.72 |
| 1:A:386:PRO:CG | 1:A:407:MSE:HE1 | 2.07 | 0.72 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:266:LEU:O | 1:D:270:ARG:HB2 | 1.89 | 0.72 |
| 1:D:38:MSE:HB2 | 1:D:59:LEU:HD11 | 1.71 | 0.72 |
| 1:E:164:GLU:HG2 | 1:E:258:ALA:HB2 | 1.71 | 0.72 |
| 1:D:92:ASN:HD22 | 1:D:92:ASN:C | 1.92 | 0.72 |
| 1:F:98:LYS:HD3 | 1:F:560:THR:HG21 | 1.70 | 0.72 |
| 1:G:222:ARG:NH1 | 1:G:222:ARG:HG3 | 2.04 | 0.72 |
| 1:A:155:ILE:HD13 | 1:A:199:LEU:HB2 | 1.70 | 0.72 |
| 1:L:227:ARG:HG3 | 1:L:227:ARG:HH11 | 1.55 | 0.72 |
| 1:N:466:ASN:HA | 2:N:1581:NAP:H72N | 1.54 | 0.72 |
| 1:B:389:LEU:HD12 | 1:B:407:MSE:HE3 | 1.71 | 0.72 |
| 1:E:378:GLU:OE2 | 1:E:402:GLN:HB3 | 1.88 | 0.72 |
| 1:F:61:GLN:O | 1:F:65:VAL:HG23 | 1.90 | 0.72 |
| 1:J:140:ARG:HH11 | 1:J:140:ARG:HB3 | 1.55 | 0.72 |
| 1:J:266:LEU:O | 1:J:270:ARG:HB2 | 1.89 | 0.72 |
| 1:C:41:THR:HG22 | 1:C:44:GLU:H | 1.55 | 0.71 |
| 1:N:136:THR:CG2 | 1:N:138:HIS:H | 1.95 | 0.71 |
| 1:B:301:ARG:HH11 | 1:B:301:ARG:HB3 | 1.54 | 0.71 |
| 1:E:163:GLY:HA2 | 1:E:166:ILE:HD11 | 1.70 | 0.71 |
| 1:K:59:LEU:HD13 | 1:K:64:GLN:HG3 | 1.70 | 0.71 |
| 1:F:266:LEU:O | 1:F:270:ARG:HB2 | 1.90 | 0.71 |
| 1:A:569:SER:HA | 1:C:46:GLN:HE21 | 1.53 | 0.71 |
| 1:J:238:PHE:HD2 | 1:J:239:MSE:HE2 | 1.52 | 0.71 |
| 1:P:41:THR:HG22 | 1:P:43:GLU:N | 2.04 | 0.71 |
| 1:P:454:LEU:HB3 | 1:P:455:PRO:HD2 | 1.71 | 0.71 |
| 1:B:239:MSE:HA | 1:B:239:MSE:CE | 2.20 | 0.71 |
| 1:J:350:ILE:HG23 | 1:J:358:LEU:HD11 | 1.73 | 0.71 |
| 1:J:354:ARG:HB3 | 1:J:358:LEU:HD21 | 1.71 | 0.71 |
| 1:O:402:GLN:HG3 | 7:O:2057:HOH:O | 1.90 | 0.71 |
| 1:A:164:GLU:HG2 | 1:A:258:ALA:HB2 | 1.72 | 0.71 |
| 1:I:359:THR:HG23 | 1:I:362:LYS:H | 1.56 | 0.71 |
| 1:O:327:MSE:O | 1:O:332:VAL:HG12 | 1.89 | 0.71 |
| 1:O:61:GLN:O | 1:O:65:VAL:HG23 | 1.91 | 0.71 |
| 1:L:92:ASN:C | 1:L:92:ASN:HD22 | 1.93 | 0.71 |
| 1:D:389:LEU:HD12 | 1:D:407:MSE:HE3 | 1.73 | 0.71 |
| 1:G:177:MSE:CE | 1:G:200:PRO:HB2 | 2.20 | 0.71 |
| 1:N:538:ASN:HB3 | 7:N:2058:HOH:O | 1.88 | 0.71 |
| 1:J:225:ARG:HB2 | 1:J:227:ARG:HH12 | 1.55 | 0.71 |
| 1:H:107:PHE:O | 1:H:111:VAL:HG23 | 1.91 | 0.71 |
| 1:P:88:LEU:HD13 | 1:P:96:PHE:HA | 1.72 | 0.71 |
| 1:D:359:THR:HG23 | 1:D:360:PRO:HD2 | 1.73 | 0.70 |
| 1:J:41:THR:HG22 | 1:J:43:GLU:H | 1.56 | 0.70 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:165:ARG:HD2 | 1:H:165:ARG:O | 1.91 | 0.70 |
| 1:P:61:GLN:NE2 | 1:P:98:LYS:HE3 | 2.05 | 0.70 |
| 1:E:49:ASN:HB3 | 7:E:2003:HOH:O | 1.90 | 0.70 |
| 1:M:238:PHE:CD2 | 1:M:239:MSE:HE2 | 2.19 | 0.70 |
| 1:O:177:MSE:HE2 | 1:O:177:MSE:HA | 1.73 | 0.70 |
| 1:B:66:TYR:CE1 | 1:B:70:LYS:HD3 | 2.26 | 0.70 |
| 1:H:160:VAL:HG22 | 1:H:201:VAL:HB | 1.73 | 0.70 |
| 1:A:265:LEU:HD22 | 1:A:269:TYR:HE1 | 1.55 | 0.70 |
| 1:B:104:ILE:HG13 | 1:B:108:MSE:CE | 2.20 | 0.70 |
| 1:I:92:ASN:ND2 | 1:I:95:LEU:H | 1.90 | 0.70 |
| 1:P:401:GLN:O | 1:P:405:GLN:HG3 | 1.90 | 0.70 |
| 1:P:94:LYS:HD3 | 1:P:558:TYR:OH | 1.91 | 0.70 |
| 1:G:359:THR:HG22 | 1:G:361:GLU:H | 1.56 | 0.70 |
| 1:M:24:LYS:HZ2 | 1:O:24:LYS:HD3 | 1.55 | 0.70 |
| 1:M:578:LYS:HZ1 | 1:M:580:LYS:HB2 | 1.57 | 0.70 |
| 1:C:401:GLN:O | 1:C:405:GLN:HG3 | 1.92 | 0.70 |
| 1:G:307:VAL:HG12 | 1:G:388:VAL:HB | 1.73 | 0.70 |
| 1:H:136:THR:HG23 | 1:H:221:LEU:HD11 | 1.74 | 0.70 |
| 1:A:136:THR:HG22 | 1:A:138:HIS:N | 2.05 | 0.70 |
| 1:C:533:GLU:OE2 | 1:C:536:ARG:HD2 | 1.90 | 0.70 |
| 1:J:140:ARG:HB3 | 1:J:140:ARG:NH1 | 2.06 | 0.70 |
| 1:F:177:MSE:HA | 1:F:177:MSE:CE | 2.20 | 0.69 |
| 1:A:104:ILE:CG1 | 1:A:108:MSE:HE3 | 2.22 | 0.69 |
| 1:G:160:VAL:HG12 | 1:G:201:VAL:HB | 1.74 | 0.69 |
| 1:I:533:GLU:HA | 1:I:536:ARG:NH1 | 2.06 | 0.69 |
| 1:J:429:THR:HG22 | 1:J:431:GLU:H | 1.58 | 0.69 |
| 1:K:305:HIS:O | 1:K:340:ARG:HD2 | 1.92 | 0.69 |
| 1:K:381:VAL:HG11 | 1:K:407:MSE:HE1 | 1.75 | 0.69 |
| 1:M:42:LEU:O | 1:M:46:GLN:HG3 | 1.92 | 0.69 |
| 1:M:578:LYS:NZ | 1:M:580:LYS:HD3 | 2.07 | 0.69 |
| 1:O:41:THR:HG22 | 1:O:43:GLU:H | 1.58 | 0.69 |
| 1:H:41:THR:O | 1:H:45:ARG:HG3 | 1.92 | 0.69 |
| 1:L:502:VAL:HG11 | 1:L:507:LEU:HD13 | 1.74 | 0.69 |
| 1:M:578:LYS:NZ | 1:M:580:LYS:CB | 2.54 | 0.69 |
| 1:O:288:VAL:HG21 | 1:O:322:LEU:HB3 | 1.73 | 0.69 |
| 1:A:560:THR:HG22 | 7:A:2006:HOH:O | 1.92 | 0.69 |
| 1:G:35:ASN:ND2 | 1:G:37:GLY:H | 1.91 | 0.69 |
| 1:J:133:LEU:HD13 | 1:J:135:ILE:HD11 | 1.74 | 0.69 |
| 1:L:401:GLN:HB2 | 1:L:436:TYR:CD1 | 2.27 | 0.69 |
| 1:F:259:ASN:HD22 | 1:F:259:ASN:C | 1.92 | 0.69 |
| 1:I:521:GLN:HG2 | 7:I:2064:HOH:O | 1.93 | 0.69 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:I:72:PHE:CZ | 1:I:81:ARG:HD3 | 2.27 | 0.69 |
| 1:K:183:LYS:HE3 | 1:K:255:GLU:CD | 2.13 | 0.69 |
| 1:L:239:MSE:HA | 1:L:239:MSE:CE | 2.22 | 0.69 |
| 1:F:41:THR:HG22 | 1:F:43:GLU:H | 1.58 | 0.69 |
| 1:H:401:GLN:O | 1:H:405:GLN:HG3 | 1.91 | 0.69 |
| 1:N:98:LYS:HD3 | 1:N:560:THR:CG2 | 2.23 | 0.69 |
| 1:B:466:ASN:HA | 2:B:1581:NAP:H72N | 1.57 | 0.69 |
| 1:E:137:ILE:HA | 1:E:234:LEU:HD22 | 1.75 | 0.69 |
| 1:L:483:LEU:HD12 | 1:L:539:THR:HB | 1.74 | 0.69 |
| 1:O:385:LYS:HB2 | 1:O:385:LYS:NZ | 2.08 | 0.69 |
| 1:F:212:LEU:HD13 | 1:F:218:TYR:CE1 | 2.28 | 0.69 |
| 1:L:381:VAL:HG11 | 1:L:407:MSE:HE1 | 1.73 | 0.69 |
| 1:M:41:THR:O | 1:M:45:ARG:HG3 | 1.93 | 0.69 |
| 1:N:24:LYS:HG2 | 1:P:24:LYS:HZ2 | 1.57 | 0.69 |
| 1:B:467:ASN:ND2 | 3:B:1582:OXL:O2 | 2.26 | 0.69 |
| 1:N:140:ARG:NH1 | 1:N:140:ARG:HB3 | 2.07 | 0.69 |
| 1:D:529:ARG:HA | 1:D:532:LYS:HE3 | 1.73 | 0.68 |
| 1:E:454:LEU:HB3 | 1:E:455:PRO:HD2 | 1.74 | 0.68 |
| 1:P:92:ASN:C | 1:P:92:ASN:HD22 | 1.95 | 0.68 |
| 1:M:136:THR:CG2 | 1:M:138:HIS:H | 2.02 | 0.68 |
| 1:A:429:THR:HG22 | 1:A:430:ALA:N | 2.07 | 0.68 |
| 1:G:378:GLU:CA | 1:G:403:ILE:HD11 | 2.24 | 0.68 |
| 1:M:429:THR:N | 1:M:432:GLN:HE21 | 1.84 | 0.68 |
| 1:P:133:LEU:HD22 | 1:P:135:ILE:HG13 | 1.75 | 0.68 |
| 1:E:489:ASP:HB3 | 7:E:2049:HOH:O | 1.93 | 0.68 |
| 1:F:129:ARG:NH1 | 1:F:129:ARG:HG3 | 2.05 | 0.68 |
| 1:G:327:MSE:CE | 1:G:337:ALA:HA | 2.23 | 0.68 |
| 1:L:38:MSE:SE | 1:L:55:PRO:HG2 | 2.44 | 0.68 |
| 1:O:88:LEU:HD13 | 1:O:96:PHE:HA | 1.73 | 0.68 |
| 1:C:532:LYS:HD2 | 1:C:549:LEU:HD12 | 1.75 | 0.68 |
| 1:J:343:MSE:HB2 | 1:J:350:ILE:HD12 | 1.75 | 0.68 |
| 1:L:24:LYS:HG2 | 1:L:48:LEU:HD12 | 1.75 | 0.68 |
| 1:G:158:ILE:HD12 | 1:G:242:VAL:HG11 | 1.75 | 0.68 |
| 1:G:442:ILE:HG22 | 1:G:512:LEU:HD11 | 1.75 | 0.68 |
| 1:O:433:LEU:CD1 | 1:O:443:PHE:HB2 | 2.24 | 0.68 |
| 1:L:381:VAL:HG13 | 1:L:407:MSE:HE1 | 1.75 | 0.68 |
| 1:P:429:THR:HG22 | 1:P:431:GLU:N | 2.08 | 0.68 |
| 1:A:98:LYS:HD3 | 1:A:560:THR:CG2 | 2.23 | 0.68 |
| 1:C:133:LEU:HD22 | 1:C:135:ILE:HG13 | 1.74 | 0.68 |
| 1:G:41:THR:O | 1:G:45:ARG:HG3 | 1.93 | 0.68 |
| 1:K:266:LEU:O | 1:K:270:ARG:HB2 | 1.94 | 0.68 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:171:ASP:OD2 | 1:E:225:ARG:HD2 | 1.94 | 0.68 |
| 1:G:266:LEU:O | 1:G:270:ARG:HB2 | 1.93 | 0.68 |
| 1:M:266:LEU:O | 1:M:270:ARG:HB2 | 1.93 | 0.68 |
| 1:I:329:LYS:HD3 | 1:I:492:LEU:HD21 | 1.75 | 0.67 |
| 1:I:77:SER:O | 1:I:81:ARG:HG3 | 1.93 | 0.67 |
| 1:J:104:ILE:CG1 | 1:J:108:MSE:HE3 | 2.22 | 0.67 |
| 1:B:260:ALA:O | 1:B:264:ARG:HG2 | 1.94 | 0.67 |
| 1:C:416:ILE:HG13 | 1:C:433:LEU:CD2 | 2.21 | 0.67 |
| 1:F:453:THR:HG22 | 1:F:459:THR:OG1 | 1.94 | 0.67 |
| 1:G:528:VAL:HG12 | 1:G:532:LYS:HE2 | 1.76 | 0.67 |
| 1:I:466:ASN:HA | 2:I:1581:NAP:H72N | 1.58 | 0.67 |
| 1:K:161:THR:HA | 1:K:257:PHE:CE1 | 2.29 | 0.67 |
| 1:L:429:THR:HG23 | 1:L:449:PHE:CE2 | 2.29 | 0.67 |
| 1:G:88:LEU:HD13 | 1:G:96:PHE:HA | 1.74 | 0.67 |
| 1:H:154:VAL:O | 1:H:154:VAL:HG13 | 1.94 | 0.67 |
| 1:J:556:GLN:HE21 | 1:J:556:GLN:N | 1.92 | 0.67 |
| 1:K:401:GLN:O | 1:K:405:GLN:HG3 | 1.95 | 0.67 |
| 1:K:381:VAL:CG1 | 1:K:407:MSE:HE1 | 2.24 | 0.67 |
| 1:A:570:TYR:N | 1:C:46:GLN:HE22 | 1.93 | 0.67 |
| 1:F:336:GLU:HG2 | 7:F:2050:HOH:O | 1.92 | 0.67 |
| 1:N:448:PRO:HD3 | 1:N:464:GLN:HE22 | 1.57 | 0.67 |
| 1:N:354:ARG:HB3 | 1:N:358:LEU:HD21 | 1.75 | 0.67 |
| 1:N:381:VAL:HG13 | 1:N:407:MSE:CE | 2.19 | 0.67 |
| 1:A:266:LEU:O | 1:A:270:ARG:HB2 | 1.94 | 0.67 |
| 1:I:502:VAL:HG12 | 1:I:507:LEU:HD22 | 1.74 | 0.67 |
| 1:J:136:THR:HB | 1:J:139:ASP:OD2 | 1.95 | 0.67 |
| 1:B:433:LEU:HG | 1:B:443:PHE:CD1 | 2.30 | 0.67 |
| 1:G:327:MSE:HE1 | 1:G:337:ALA:HA | 1.76 | 0.67 |
| 1:G:385:LYS:HA | 1:G:410:PHE:CE2 | 2.29 | 0.67 |
| 1:J:35:ASN:ND2 | 1:J:37:GLY:H | 1.92 | 0.67 |
| 1:J:502:VAL:HG12 | 1:J:507:LEU:HD22 | 1.76 | 0.67 |
| 1:G:202:MSE:HE3 | 1:G:203:LEU:C | 2.15 | 0.67 |
| 1:G:243:THR:HG22 | 1:G:248:MSE:HA | 1.75 | 0.67 |
| 1:P:137:ILE:O | 1:P:140:ARG:HG2 | 1.94 | 0.67 |
| 1:D:494:THR:HG22 | 1:D:526:ILE:HG23 | 1.77 | 0.67 |
| 1:K:165:ARG:O | 1:K:165:ARG:HD2 | 1.95 | 0.67 |
| 1:D:245:ARG:HG2 | 1:D:246:TYR:CD2 | 2.30 | 0.66 |
| 1:L:429:THR:H | 1:L:432:GLN:HE21 | 1.43 | 0.66 |
| 1:O:401:GLN:HG2 | 1:O:405:GLN:NE2 | 2.07 | 0.66 |
| 1:P:154:VAL:O | 1:P:154:VAL:HG13 | 1.94 | 0.66 |
| 1:M:38:MSE:SE | 1:M:55:PRO:HG2 | 2.46 | 0.66 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:359:THR:HG22 | 1:A:362:LYS:CE | 2.24 | 0.66 |
| 1:C:163:GLY:HA2 | 1:C:166:ILE:HD11 | 1.77 | 0.66 |
| 1:K:335:GLU:HG2 | 1:K:339:LYS:HZ2 | 1.59 | 0.66 |
| 1:P:389:LEU:HD12 | 1:P:407:MSE:HE3 | 1.78 | 0.66 |
| 1:H:466:ASN:HA | 2:H:1581:NAP:H72N | 1.59 | 0.66 |
| 1:I:239:MSE:HE2 | 1:I:239:MSE:HA | 1.75 | 0.66 |
| 1:B:429:THR:HB | 1:B:432:GLN:HG2 | 1.76 | 0.66 |
| 1:E:469:TYR:OH | 1:E:516:LEU:HD13 | 1.95 | 0.66 |
| 1:G:401:GLN:O | 1:G:405:GLN:HG3 | 1.96 | 0.66 |
| 1:I:578:LYS:NZ | 1:L:222:ARG:HD3 | 2.11 | 0.66 |
| 1:J:59:LEU:HD13 | 1:J:64:GLN:HG2 | 1.78 | 0.66 |
| 1:L:239:MSE:HE1 | 1:L:252:ILE:HG12 | 1.78 | 0.66 |
| 1:L:378:GLU:HA | 1:L:403:ILE:CD1 | 2.25 | 0.66 |
| 1:I:429:THR:CG2 | 1:I:432:GLN:HG3 | 2.25 | 0.66 |
| 1:J:184:LEU:HD22 | 1:J:198:CYS:HB3 | 1.78 | 0.66 |
| 1:M:177:MSE:O | 1:M:180:PRO:HD2 | 1.96 | 0.66 |
| 1:M:402:GLN:HB3 | 7:M:2046:HOH:O | 1.94 | 0.66 |
| 1:O:416:ILE:HG13 | 1:O:433:LEU:HD21 | 1.78 | 0.66 |
| 1:P:300:ASN:OD1 | 1:P:305:HIS:HE1 | 1.78 | 0.66 |
| 1:C:266:LEU:O | 1:C:270:ARG:HB2 | 1.95 | 0.66 |
| 1:D:239:MSE:SE | 1:D:252:ILE:HD13 | 2.46 | 0.66 |
| 1:G:179:ILE:HB | 1:G:180:PRO:HD3 | 1.77 | 0.66 |
| 1:L:41:THR:O | 1:L:45:ARG:HG3 | 1.96 | 0.66 |
| 1:M:92:ASN:ND2 | 1:M:95:LEU:H | 1.94 | 0.66 |
| 1:A:288:VAL:HG21 | 1:A:322:LEU:HB3 | 1.76 | 0.66 |
| 1:O:429:THR:HG23 | 1:O:449:PHE:CE2 | 2.31 | 0.66 |
| 1:D:47:GLN:NE2 | 1:D:566:VAL:HG13 | 2.11 | 0.66 |
| 1:G:391:GLY:HA3 | 1:G:427:GLU:HG2 | 1.78 | 0.66 |
| 1:H:391:GLY:HA3 | 1:H:427:GLU:HG2 | 1.77 | 0.66 |
| 1:K:415:ILE:HD13 | 1:K:442:ILE:HD12 | 1.78 | 0.66 |
| 1:I:222:ARG:HH11 | 1:L:580:LYS:HE2 | 1.59 | 0.66 |
| 1:A:324:VAL:HG12 | 1:A:328:GLN:HE21 | 1.61 | 0.66 |
| 1:B:24:LYS:NZ | 1:D:24:LYS:HD3 | 2.11 | 0.66 |
| 1:D:332:VAL:HG13 | 1:D:336:GLU:HB2 | 1.78 | 0.66 |
| 1:I:416:ILE:HG13 | 1:I:433:LEU:HD21 | 1.78 | 0.66 |
| 1:K:154:VAL:HG13 | 1:K:154:VAL:O | 1.95 | 0.66 |
| 1:P:47:GLN:NE2 | 1:P:566:VAL:HG13 | 2.10 | 0.66 |
| 1:B:288:VAL:HG21 | 1:B:322:LEU:HB3 | 1.79 | 0.65 |
| 1:L:310:GLN:NE2 | 1:L:393:ALA:HB3 | 2.10 | 0.65 |
| 1:A:108:MSE:SE | 1:A:516:LEU:HD21 | 2.46 | 0.65 |
| 1:D:504:GLU:HG3 | 1:D:508:GLN:NE2 | 2.10 | 0.65 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:454:LEU:HB3 | 1:L:455:PRO:HD2 | 1.77 | 0.65 |
| 1:M:352:LYS:HD2 | 1:M:366:ALA:O | 1.97 | 0.65 |
| 1:B:190:CYS:HB3 | 1:B:519:ILE:HG12 | 1.77 | 0.65 |
| 1:D:296:ARG:HB2 | 1:D:507:LEU:HD21 | 1.76 | 0.65 |
| 1:O:157:ALA:HB2 | 1:O:479:ILE:HD11 | 1.79 | 0.65 |
| 1:P:454:LEU:HD21 | 1:P:460:LEU:HD11 | 1.77 | 0.65 |
| 1:J:504:GLU:O | 1:J:508:GLN:HG3 | 1.96 | 0.65 |
| 1:L:165:ARG:HD2 | 1:L:165:ARG:O | 1.95 | 0.65 |
| 1:N:270:ARG:HH11 | 1:N:270:ARG:HG2 | 1.61 | 0.65 |
| 1:O:166:ILE:HA | 1:O:256:ASP:OD2 | 1.97 | 0.65 |
| 1:B:416:ILE:CG1 | 1:B:433:LEU:HD21 | 2.19 | 0.65 |
| 1:C:137:ILE:HA | 1:C:234:LEU:HD22 | 1.78 | 0.65 |
| 1:D:41:THR:O | 1:D:45:ARG:HG3 | 1.96 | 0.65 |
| 1:J:125:LEU:O | 1:J:125:LEU:HD23 | 1.96 | 0.65 |
| 1:L:502:VAL:CG1 | 1:L:507:LEU:HD13 | 2.26 | 0.65 |
| 1:N:179:ILE:HB | 1:N:180:PRO:HD3 | 1.77 | 0.65 |
| 1:D:546:PRO:HB2 | 1:D:549:LEU:HD23 | 1.79 | 0.65 |
| 1:F:327:MSE:HE3 | 1:F:337:ALA:HB1 | 1.79 | 0.65 |
| 1:I:578:LYS:C | 1:I:578:LYS:HD2 | 2.16 | 0.65 |
| 1:K:319:ILE:O | 1:K:323:ILE:HG13 | 1.97 | 0.65 |
| 1:M:474:VAL:O | 1:M:478:VAL:HG23 | 1.97 | 0.65 |
| 1:A:202:MSE:HE3 | 1:A:203:LEU:C | 2.16 | 0.65 |
| 1:J:389:LEU:HD12 | 1:J:407:MSE:HE3 | 1.78 | 0.65 |
| 1:N:288:VAL:HG21 | 1:N:322:LEU:HB3 | 1.78 | 0.65 |
| 1:E:391:GLY:HA3 | 1:E:427:GLU:HG2 | 1.79 | 0.65 |
| 1:F:92:ASN:C | 1:F:92:ASN:HD22 | 2.00 | 0.65 |
| 1:L:136:THR:HB | 1:L:139:ASP:OD2 | 1.96 | 0.65 |
| 1:N:35:ASN:ND2 | 1:N:37:GLY:H | 1.95 | 0.65 |
| 1:E:133:LEU:HD22 | 1:E:135:ILE:HG13 | 1.78 | 0.65 |
| 1:I:429:THR:CG2 | 1:I:432:GLN:H | 2.09 | 0.65 |
| 1:J:347:LYS:O | 1:J:375:LYS:NZ | 2.30 | 0.65 |
| 1:J:476:LEU:HD21 | 1:J:553:ILE:HG23 | 1.77 | 0.65 |
| 1:K:456:SER:OG | 1:K:458:GLN:HG2 | 1.97 | 0.65 |
| 1:C:188:THR:HG21 | 1:C:195:PRO:HG3 | 1.78 | 0.65 |
| 1:C:389:LEU:HD13 | 1:C:399:PHE:CZ | 2.31 | 0.65 |
| 1:C:429:THR:HG22 | 1:C:431:GLU:H | 1.60 | 0.65 |
| 1:K:498:ILE:HD11 | 1:K:526:ILE:HD11 | 1.79 | 0.65 |
| 1:C:572:TRP:HB2 | 1:C:577:MSE:HG3 | 1.78 | 0.64 |
| 1:G:467:ASN:ND2 | 3:G:1582:OXL:O2 | 2.29 | 0.64 |
| 1:I:243:THR:HG21 | 1:I:273:TYR:CD2 | 2.32 | 0.64 |
| 1:I:155:ILE:HD12 | 1:I:246:TYR:CZ | 2.31 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:401:GLN:HG2 | 1:J:436:TYR:CZ | 2.32 | 0.64 |
| 1:P:572:TRP:O | 1:P:573:PRO:O | 2.14 | 0.64 |
| 1:H:158:ILE:HD12 | 1:H:242:VAL:HG11 | 1.80 | 0.64 |
| 1:J:98:LYS:HD3 | 1:J:560:THR:CG2 | 2.27 | 0.64 |
| 1:M:72:PHE:CZ | 1:M:81:ARG:HD3 | 2.33 | 0.64 |
| 1:N:416:ILE:CG1 | 1:N:433:LEU:HD21 | 2.26 | 0.64 |
| 1:A:184:LEU:HD12 | 1:A:200:PRO:HB3 | 1.79 | 0.64 |
| 1:D:572:TRP:HB2 | 1:D:577:MSE:HG3 | 1.78 | 0.64 |
| 1:G:548:ASP:OD2 | 1:G:551:ALA:HB2 | 1.96 | 0.64 |
| 1:M:24:LYS:HD2 | 1:O:24:LYS:NZ | 2.12 | 0.64 |
| 1:N:166:ILE:HD12 | 1:N:179:ILE:HG13 | 1.78 | 0.64 |
| 1:K:416:ILE:CG1 | 1:K:433:LEU:HD21 | 2.25 | 0.64 |
| 1:L:454:LEU:HD21 | 1:L:460:LEU:HG | 1.78 | 0.64 |
| 1:M:104:ILE:CG1 | 1:M:108:MSE:HE3 | 2.27 | 0.64 |
| 1:N:265:LEU:HD22 | 1:N:269:TYR:HE1 | 1.61 | 0.64 |
| 1:N:573:PRO:O | 1:N:577:MSE:HE2 | 1.97 | 0.64 |
| 1:C:179:ILE:HB | 1:C:180:PRO:HD3 | 1.80 | 0.64 |
| 1:D:98:LYS:HD3 | 1:D:560:THR:HG21 | 1.80 | 0.64 |
| 1:I:133:LEU:CD2 | 1:I:135:ILE:HG13 | 2.27 | 0.64 |
| 1:O:75:LEU:HD11 | 1:O:84:LEU:HD22 | 1.78 | 0.64 |
| 1:P:266:LEU:O | 1:P:270:ARG:HB2 | 1.98 | 0.64 |
| 1:A:352:LYS:HG2 | 1:A:366:ALA:O | 1.97 | 0.64 |
| 1:H:389:LEU:HB2 | 1:H:407:MSE:HE2 | 1.80 | 0.64 |
| 1:K:378:GLU:HA | 1:K:403:ILE:CD1 | 2.27 | 0.64 |
| 1:L:416:ILE:CG1 | 1:L:433:LEU:HD21 | 2.26 | 0.64 |
| 1:M:466:ASN:HA | 2:M:1581:NAP:H72N | 1.63 | 0.64 |
| 1:A:350:ILE:HD11 | 1:A:362:LYS:HD2 | 1.79 | 0.64 |
| 1:G:155:ILE:HD13 | 1:G:246:TYR:CE2 | 2.32 | 0.64 |
| 1:A:335:GLU:O | 1:A:339:LYS:HG3 | 1.98 | 0.64 |
| 1:C:108:MSE:HE2 | 1:C:186:LEU:HD13 | 1.80 | 0.64 |
| 1:D:98:LYS:HD3 | 1:D:560:THR:CG2 | 2.28 | 0.64 |
| 1:E:416:ILE:HG13 | 1:E:433:LEU:HD21 | 1.79 | 0.64 |
| 1:H:222:ARG:HH11 | 1:H:222:ARG:HG3 | 1.61 | 0.64 |
| 1:J:41:THR:HB | 1:J:44:GLU:HG3 | 1.78 | 0.64 |
| 1:N:266:LEU:O | 1:N:270:ARG:HB2 | 1.97 | 0.64 |
| 1:A:104:ILE:HG13 | 1:A:108:MSE:HE3 | 1.80 | 0.64 |
| 1:A:92:ASN:HD22 | 1:A:92:ASN:C | 1.99 | 0.64 |
| 1:B:62:ASP:HB2 | 7:B:2004:HOH:O | 1.98 | 0.64 |
| 1:I:335:GLU:O | 1:I:339:LYS:HG3 | 1.98 | 0.64 |
| 1:I:352:LYS:HE2 | 1:I:366:ALA:O | 1.98 | 0.64 |
| 1:J:164:GLU:HG2 | 1:J:258:ALA:HB2 | 1.80 | 0.64 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:L:429:THR:HG22 | 1:L:431:GLU:H | 1.62 | 0.64 |
| 1:N:429:THR:HG22 | 1:N:430:ALA:N | 2.12 | 0.64 |
| 1:G:416:ILE:CG1 | 1:G:433:LEU:HD21 | 2.16 | 0.63 |
| 1:M:186:LEU:HD22 | 1:M:190:CYS:SG | 2.38 | 0.63 |
| 1:B:238:PHE:CD2 | 1:B:239:MSE:HE3 | 2.33 | 0.63 |
| 1:G:72:PHE:CZ | 1:G:81:ARG:HD3 | 2.34 | 0.63 |
| 1:K:335:GLU:HG2 | 1:K:339:LYS:NZ | 2.13 | 0.63 |
| 1:M:429:THR:HG22 | 1:M:431:GLU:N | 2.12 | 0.63 |
| 1:O:466:ASN:HA | 2:O:1581:NAP:H72N | 1.64 | 0.63 |
| 1:P:416:ILE:CG1 | 1:P:433:LEU:HD21 | 2.26 | 0.63 |
| 1:B:300:ASN:HD21 | 1:B:305:HIS:CE1 | 2.16 | 0.63 |
| 1:D:352:LYS:HD2 | 1:D:368:GLU:OE2 | 1.99 | 0.63 |
| 1:G:184:LEU:HD12 | 1:G:200:PRO:HB3 | 1.80 | 0.63 |
| 1:H:324:VAL:O | 1:H:328:GLN:HG3 | 1.98 | 0.63 |
| 1:E:340:ARG:HH11 | 1:E:340:ARG:CB | 2.11 | 0.63 |
| 1:J:433:LEU:C | 1:J:433:LEU:HD13 | 2.19 | 0.63 |
| 1:K:385:LYS:HA | 1:K:410:PHE:CE2 | 2.33 | 0.63 |
| 1:N:350:ILE:HG23 | 1:N:358:LEU:HD11 | 1.81 | 0.63 |
| 1:N:41:THR:HG22 | 1:N:43:GLU:N | 2.13 | 0.63 |
| 1:A:283:THR:HG23 | 1:A:284:ALA:N | 2.13 | 0.63 |
| 1:G:177:MSE:HE1 | 1:G:200:PRO:CB | 2.22 | 0.63 |
| 1:G:288:VAL:HG21 | 1:G:322:LEU:HD12 | 1.80 | 0.63 |
| 1:H:38:MSE:SE | 1:H:55:PRO:HG2 | 2.49 | 0.63 |
| 1:K:36:LYS:HG3 | 1:K:562:TYR:CD2 | 2.34 | 0.63 |
| 1:L:177:MSE:O | 1:L:181:VAL:HG23 | 1.98 | 0.63 |
| 1:O:385:LYS:HG3 | 1:O:410:PHE:CG | 2.33 | 0.63 |
| 1:A:41:THR:HG22 | 1:A:43:GLU:H | 1.64 | 0.63 |
| 1:C:92:ASN:HD22 | 1:C:92:ASN:C | 2.01 | 0.63 |
| 1:F:224:LYS:HG2 | 7:F:2038:HOH:O | 1.99 | 0.63 |
| 1:H:474:VAL:O | 1:H:478:VAL:HG23 | 1.99 | 0.63 |
| 1:J:183:LYS:HE3 | 1:J:255:GLU:CD | 2.19 | 0.63 |
| 1:O:177:MSE:HE3 | 1:O:202:MSE:HB2 | 1.79 | 0.63 |
| 1:A:407:MSE:HG2 | 1:A:416:ILE:HD11 | 1.80 | 0.63 |
| 1:H:183:LYS:HE2 | 1:H:255:GLU:OE1 | 1.99 | 0.63 |
| 1:H:79:LEU:HD21 | 1:H:125:LEU:HD12 | 1.80 | 0.63 |
| 1:J:461:TYR:CD1 | 1:J:509:GLU:HG2 | 2.34 | 0.63 |
| 1:O:104:ILE:CG1 | 1:O:108:MSE:HE3 | 2.21 | 0.63 |
| 1:A:376:ASN:O | 1:A:380:ILE:HG13 | 1.98 | 0.63 |
| 1:D:333:SER:OG | 1:D:336:GLU:HG3 | 1.99 | 0.63 |
| 1:N:378:GLU:OE2 | 1:N:402:GLN:HB3 | 1.99 | 0.63 |
| 1:M:24:LYS:NZ | 1:O:24:LYS:HD3 | 2.13 | 0.63 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:270:ARG:HG2 | 1:O:270:ARG:HH11 | 1.64 | 0.63 |
| 1:H:143:ILE:HD12 | 1:H:237:GLU:HG2 | 1.80 | 0.62 |
| 1:M:578:LYS:HZ2 | 1:M:580:LYS:CB | 2.12 | 0.62 |
| 1:A:61:GLN:HA | 1:A:64:GLN:HE21 | 1.64 | 0.62 |
| 1:F:389:LEU:HD12 | 1:F:407:MSE:HE3 | 1.80 | 0.62 |
| 1:M:276:PHE:HB3 | 1:M:486:ILE:HD12 | 1.80 | 0.62 |
| 1:O:104:ILE:HG13 | 1:O:108:MSE:CE | 2.25 | 0.62 |
| 1:B:140:ARG:HH12 | 1:B:230:ALA:CB | 2.09 | 0.62 |
| 1:F:456:SER:OG | 1:F:458:GLN:HG2 | 1.99 | 0.62 |
| 1:K:238:PHE:CE2 | 1:K:239:MSE:HE3 | 2.34 | 0.62 |
| 1:D:224:LYS:HE3 | 7:D:2018:HOH:O | 1.99 | 0.62 |
| 1:M:578:LYS:HZ2 | 1:M:580:LYS:CA | 2.12 | 0.62 |
| 1:O:38:MSE:SE | 1:O:55:PRO:HG2 | 2.50 | 0.62 |
| 1:O:492:LEU:O | 1:O:496:GLU:HG3 | 1.99 | 0.62 |
| 1:P:300:ASN:OD1 | 1:P:305:HIS:CE1 | 2.52 | 0.62 |
| 1:D:24:LYS:HG2 | 1:D:48:LEU:HA | 1.81 | 0.62 |
| 1:E:154:VAL:HG13 | 1:E:154:VAL:O | 1.98 | 0.62 |
| 1:I:41:THR:HG22 | 1:I:43:GLU:N | 2.15 | 0.62 |
| 1:N:324:VAL:O | 1:N:328:GLN:HG3 | 2.00 | 0.62 |
| 1:O:359:THR:HG23 | 1:O:362:LYS:H | 1.64 | 0.62 |
| 1:B:352:LYS:HE2 | 1:B:353:GLY:N | 2.13 | 0.62 |
| 1:E:374:MSE:HE1 | 1:E:379:ASP:HB3 | 1.82 | 0.62 |
| 1:I:164:GLU:HG3 | 1:I:225:ARG:CZ | 2.30 | 0.62 |
| 1:K:245:ARG:HG2 | 1:K:245:ARG:HH11 | 1.64 | 0.62 |
| 1:L:524:LEU:HD21 | 1:L:554:ARG:NE | 2.14 | 0.62 |
| 1:F:494:THR:HG23 | 1:F:526:ILE:HG23 | 1.81 | 0.62 |
| 1:I:104:ILE:CG1 | 1:I:108:MSE:HE3 | 2.28 | 0.62 |
| 1:M:202:MSE:HE3 | 1:M:203:LEU:O | 1.99 | 0.62 |
| 1:A:350:ILE:HG23 | 1:A:358:LEU:HD11 | 1.82 | 0.62 |
| 1:J:38:MSE:SE | 1:J:55:PRO:HG2 | 2.50 | 0.62 |
| 1:C:469:TYR:OH | 1:C:516:LEU:HD13 | 2.00 | 0.62 |
| 1:C:504:GLU:HG3 | 1:C:508:GLN:HE21 | 1.64 | 0.62 |
| 1:E:429:THR:HG22 | 1:E:430:ALA:N | 2.14 | 0.62 |
| 1:I:108:MSE:HE2 | 1:I:190:CYS:SG | 2.40 | 0.62 |
| 1:J:148:GLN:HG2 | 1:J:245:ARG:NH2 | 2.15 | 0.62 |
| 1:A:137:ILE:HB | 1:A:205:VAL:HG12 | 1.82 | 0.62 |
| 1:C:194:LYS:HD2 | 1:C:197:GLN:HE22 | 1.64 | 0.62 |
| 1:H:138:HIS:NE2 | 1:H:223:HIS:HE1 | 1.97 | 0.62 |
| 1:L:469:TYR:OH | 1:L:516:LEU:HD12 | 2.00 | 0.62 |
| 1:A:401:GLN:O | 1:A:405:GLN:HG3 | 2.00 | 0.61 |
| 1:J:239:MSE:HE1 | 1:J:252:ILE:HG21 | 1.82 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:177:MSE:HG2 | 1:L:202:MSE:HB2 | 1.80 | 0.61 |
| 1:M:243:THR:HG21 | 1:M:273:TYR:CD2 | 2.34 | 0.61 |
| 1:M:416:ILE:CB | 1:M:433:LEU:HD21 | 2.29 | 0.61 |
| 1:N:467:ASN:ND2 | 3:N:1582:OXL:O2 | 2.33 | 0.61 |
| 1:O:429:THR:H | 1:O:432:GLN:CG | 2.13 | 0.61 |
| 1:O:296:ARG:HB2 | 1:O:507:LEU:HD21 | 1.82 | 0.61 |
| 1:B:38:MSE:SE | 1:B:55:PRO:HG2 | 2.50 | 0.61 |
| 1:D:104:ILE:HD11 | 1:D:108:MSE:HE3 | 1.82 | 0.61 |
| 1:I:41:THR:HG22 | 1:I:43:GLU:H | 1.63 | 0.61 |
| 1:J:152:GLU:OE2 | 1:J:154:VAL:HG12 | 2.00 | 0.61 |
| 1:K:321:ASN:HB2 | 7:K:2024:HOH:O | 2.01 | 0.61 |
| 1:D:41:THR:HB | 1:D:44:GLU:HG3 | 1.81 | 0.61 |
| 1:M:157:ALA:HB2 | 1:M:479:ILE:HD11 | 1.81 | 0.61 |
| 1:M:454:LEU:HD12 | 1:M:454:LEU:H | 1.65 | 0.61 |
| 1:M:98:LYS:HD3 | 1:M:560:THR:CG2 | 2.31 | 0.61 |
| 1:N:324:VAL:HG12 | 1:N:328:GLN:NE2 | 2.16 | 0.61 |
| 1:A:163:GLY:HA2 | 1:A:166:ILE:HD11 | 1.82 | 0.61 |
| 1:B:296:ARG:HB2 | 1:B:507:LEU:HD21 | 1.83 | 0.61 |
| 1:G:429:THR:HG22 | 1:G:430:ALA:N | 2.15 | 0.61 |
| 1:H:77:SER:C | 1:H:81:ARG:NH1 | 2.54 | 0.61 |
| 1:K:399:PHE:HB2 | 1:K:428:CYS:HB3 | 1.82 | 0.61 |
| 1:A:429:THR:HB | 1:A:432:GLN:HG3 | 1.83 | 0.61 |
| 1:I:136:THR:HG23 | 1:I:221:LEU:HD11 | 1.81 | 0.61 |
| 1:J:297:ILE:HD11 | 1:J:507:LEU:HD12 | 1.82 | 0.61 |
| 1:A:570:TYR:OH | 1:D:139:ASP:HB3 | 2.00 | 0.61 |
| 1:H:359:THR:HG23 | 1:H:361:GLU:H | 1.64 | 0.61 |
| 1:B:42:LEU:O | 1:B:46:GLN:HG3 | 2.01 | 0.61 |
| 1:D:108:MSE:HE2 | 1:D:186:LEU:HD22 | 1.82 | 0.61 |
| 1:D:528:VAL:HG12 | 1:D:532:LYS:HE2 | 1.82 | 0.61 |
| 1:F:264:ARG:HH11 | 1:F:264:ARG:HG2 | 1.66 | 0.61 |
| 1:G:352:LYS:HA | 1:G:352:LYS:HE3 | 1.83 | 0.61 |
| 1:J:118:LEU:HD13 | 1:J:122:HIS:HD2 | 1.65 | 0.61 |
| 1:K:27:GLU:OE1 | 1:K:27:GLU:HA | 2.00 | 0.61 |
| 1:K:411:ASN:HB2 | 1:K:414:PRO:HG3 | 1.81 | 0.61 |
| 1:L:238:PHE:CD2 | 1:L:239:MSE:HE3 | 2.36 | 0.61 |
| 1:N:166:ILE:HG21 | 1:N:172:LEU:HD12 | 1.83 | 0.61 |
| 1:O:359:THR:HG22 | 1:O:362:LYS:HE2 | 1.81 | 0.61 |
| 1:B:415:ILE:HG12 | 1:B:442:ILE:HD12 | 1.83 | 0.61 |
| 1:C:288:VAL:HG21 | 1:C:322:LEU:HB3 | 1.81 | 0.61 |
| 1:I:297:ILE:HD11 | 1:I:507:LEU:HD12 | 1.83 | 0.61 |
| 1:K:91:ARG:HB2 | 1:L:129:ARG:HH12 | 1.66 | 0.61 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:137:ILE:HA | 1:H:234:LEU:HD22 | 1.82 | 0.61 |
| 1:E:533:GLU:OE1 | 1:E:536:ARG:NH1 | 2.34 | 0.60 |
| 1:G:166:ILE:HD12 | 1:G:179:ILE:HG13 | 1.83 | 0.60 |
| 1:M:113:THR:HG21 | 1:M:447:SER:OG | 2.01 | 0.60 |
| 1:C:578:LYS:HB3 | 1:C:578:LYS:NZ | 2.16 | 0.60 |
| 1:C:38:MSE:HE2 | 1:D:127:PHE:CE2 | 2.36 | 0.60 |
| 1:L:64:GLN:O | 1:L:68:ILE:HG12 | 2.01 | 0.60 |
| 1:M:315:ALA:O | 1:M:319:ILE:HG13 | 2.01 | 0.60 |
| 1:A:177:MSE:HE3 | 1:A:181:VAL:HG23 | 1.82 | 0.60 |
| 1:A:359:THR:HG23 | 1:A:362:LYS:H | 1.64 | 0.60 |
| 1:A:416:ILE:HG13 | 1:A:433:LEU:HD21 | 1.82 | 0.60 |
| 1:D:179:ILE:HB | 1:D:180:PRO:HD3 | 1.82 | 0.60 |
| 1:D:407:MSE:HG2 | 1:D:416:ILE:HD11 | 1.83 | 0.60 |
| 1:J:285:SER:HB3 | 1:J:470:VAL:HG21 | 1.82 | 0.60 |
| 1:L:500:GLN:HE21 | 1:L:500:GLN:N | 2.00 | 0.60 |
| 1:O:428:CYS:HA | 1:O:432:GLN:HE21 | 1.66 | 0.60 |
| 1:P:202:MSE:HE3 | 1:P:203:LEU:N | 2.16 | 0.60 |
| 1:A:177:MSE:HE2 | 1:A:181:VAL:HG23 | 1.82 | 0.60 |
| 1:A:72:PHE:CZ | 1:A:81:ARG:HD3 | 2.36 | 0.60 |
| 1:D:136:THR:HG22 | 1:D:139:ASP:CG | 2.21 | 0.60 |
| 1:G:359:THR:HG23 | 1:G:360:PRO:HD2 | 1.82 | 0.60 |
| 1:G:38:MSE:HB2 | 1:G:59:LEU:HD11 | 1.82 | 0.60 |
| 1:G:404:LEU:HD22 | 1:G:433:LEU:CD2 | 2.31 | 0.60 |
| 1:H:429:THR:HG22 | 1:H:430:ALA:N | 2.16 | 0.60 |
| 1:H:92:ASN:ND2 | 1:H:95:LEU:H | 1.99 | 0.60 |
| 1:I:493:THR:O | 1:I:497:VAL:HG23 | 2.01 | 0.60 |
| 1:F:299:LYS:HB3 | 1:F:299:LYS:HZ2 | 1.67 | 0.60 |
| 1:F:285:SER:HB3 | 1:F:470:VAL:HG21 | 1.84 | 0.60 |
| 1:I:184:LEU:HD12 | 1:I:200:PRO:HB3 | 1.83 | 0.60 |
| 1:E:429:THR:CG2 | 1:E:430:ALA:N | 2.65 | 0.60 |
| 1:E:502:VAL:HG12 | 1:E:507:LEU:HD22 | 1.83 | 0.60 |
| 1:F:524:LEU:O | 1:F:528:VAL:HG23 | 2.02 | 0.60 |
| 1:K:327:MSE:HE3 | 1:K:337:ALA:CB | 2.25 | 0.60 |
| 1:M:378:GLU:OE2 | 1:M:402:GLN:HB3 | 2.02 | 0.60 |
| 1:N:24:LYS:HG2 | 1:P:24:LYS:HZ1 | 1.65 | 0.60 |
| 1:P:41:THR:O | 1:P:45:ARG:HG3 | 2.02 | 0.60 |
| 1:C:340:ARG:HH11 | 1:C:340:ARG:HG2 | 1.66 | 0.60 |
| 1:P:575:GLU:O | 1:P:578:LYS:HG2 | 2.02 | 0.60 |
| 1:B:333:SER:HB3 | 1:E:536:ARG:NH1 | 2.17 | 0.60 |
| 1:I:26:TYR:HB2 | 7:I:2005:HOH:O | 2.01 | 0.60 |
| 1:K:359:THR:HG23 | 1:K:362:LYS:H | 1.67 | 0.60 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:59:LEU:HD13 | 1:P:64:GLN:HG3 | 1.83 | 0.60 |
| 1:A:41:THR:HG22 | 1:A:42:LEU:N | 2.17 | 0.60 |
| 1:C:467:ASN:HD21 | 3:C:1582:OXL:C2 | 2.14 | 0.60 |
| 1:E:221:LEU:HD13 | 1:E:223:HIS:HE1 | 1.66 | 0.60 |
| 1:G:572:TRP:O | 1:G:573:PRO:O | 2.19 | 0.60 |
| 1:I:407:MSE:HG2 | 1:I:416:ILE:HD11 | 1.84 | 0.60 |
| 1:K:417:PHE:CD1 | 1:K:444:ALA:HB3 | 2.36 | 0.60 |
| 1:K:532:LYS:HG2 | 1:K:549:LEU:HD12 | 1.84 | 0.60 |
| 1:M:38:MSE:HB2 | 1:M:59:LEU:HD11 | 1.83 | 0.60 |
| 1:O:260:ALA:HB3 | 7:O:2050:HOH:O | 2.00 | 0.60 |
| 1:P:429:THR:H | 1:P:432:GLN:NE2 | 1.99 | 0.60 |
| 1:B:41:THR:HG21 | 7:B:2003:HOH:O | 2.00 | 0.60 |
| 1:C:429:THR:HG22 | 1:C:430:ALA:N | 2.16 | 0.60 |
| 1:F:401:GLN:O | 1:F:405:GLN:HG3 | 2.02 | 0.60 |
| 1:I:502:VAL:HG22 | 1:I:514:PRO:HD3 | 1.84 | 0.60 |
| 1:M:492:LEU:O | 1:M:496:GLU:HG3 | 2.02 | 0.60 |
| 1:O:493:THR:O | 1:O:497:VAL:HG23 | 2.02 | 0.60 |
| 1:B:160:VAL:HG22 | 1:B:201:VAL:HB | 1.83 | 0.59 |
| 1:C:359:THR:HG22 | 1:C:362:LYS:H | 1.67 | 0.59 |
| 1:F:77:SER:O | 1:F:81:ARG:HG3 | 2.02 | 0.59 |
| 1:G:376:ASN:O | 1:G:380:ILE:HG13 | 2.02 | 0.59 |
| 1:I:179:ILE:HB | 1:I:180:PRO:HD3 | 1.83 | 0.59 |
| 1:N:416:ILE:HG13 | 1:N:433:LEU:CD2 | 2.31 | 0.59 |
| 1:O:85:LEU:HD12 | 1:O:110:ILE:HG21 | 1.84 | 0.59 |
| 1:A:327:MSE:HE3 | 1:A:337:ALA:CB | 2.22 | 0.59 |
| 1:E:416:ILE:HG13 | 1:E:433:LEU:CD2 | 2.32 | 0.59 |
| 1:J:184:LEU:HD12 | 1:J:200:PRO:HB3 | 1.83 | 0.59 |
| 1:M:245:ARG:HD3 | 1:M:246:TYR:CE2 | 2.37 | 0.59 |
| 1:C:223:HIS:HD2 | 1:C:224:LYS:O | 1.85 | 0.59 |
| 1:E:179:ILE:HB | 1:E:180:PRO:HD3 | 1.84 | 0.59 |
| 1:H:59:LEU:HD13 | 1:H:64:GLN:HG3 | 1.84 | 0.59 |
| 1:F:554:ARG:HG2 | 1:F:554:ARG:HH11 | 1.66 | 0.59 |
| 1:L:131:ARG:HD3 | 1:L:181:VAL:HG13 | 1.84 | 0.59 |
| 1:P:239:MSE:SE | 1:P:252:ILE:HD13 | 2.53 | 0.59 |
| 1:C:270:ARG:HG2 | 1:C:270:ARG:HH11 | 1.67 | 0.59 |
| 1:C:94:LYS:HE2 | 7:C:2003:HOH:O | 2.02 | 0.59 |
| 1:F:35:ASN:ND2 | 1:F:37:GLY:H | 1.98 | 0.59 |
| 1:J:416:ILE:HG13 | 1:J:433:LEU:CD2 | 2.30 | 0.59 |
| 1:L:227:ARG:HG3 | 1:L:227:ARG:NH1 | 2.15 | 0.59 |
| 1:N:92:ASN:HD22 | 1:N:92:ASN:C | 2.05 | 0.59 |
| 1:C:433:LEU:HG | 1:C:443:PHE:CD1 | 2.37 | 0.59 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:285:SER:HB3 | 1:H:470:VAL:HG21 | 1.85 | 0.59 |
| 1:K:261:ASN:HA | 1:K:264:ARG:NH1 | 2.17 | 0.59 |
| 1:L:59:LEU:HD13 | 1:L:64:GLN:HG2 | 1.83 | 0.59 |
| 1:O:385:LYS:HB2 | 1:O:385:LYS:HZ3 | 1.66 | 0.59 |
| 1:O:42:LEU:O | 1:O:46:GLN:HG3 | 2.02 | 0.59 |
| 1:A:136:THR:HG23 | 1:A:138:HIS:H | 1.67 | 0.59 |
| 1:C:136:THR:HG23 | 1:C:221:LEU:HD11 | 1.84 | 0.59 |
| 1:E:160:VAL:HG11 | 1:E:238:PHE:CE2 | 2.38 | 0.59 |
| 1:F:88:LEU:HD13 | 1:F:96:PHE:HA | 1.84 | 0.59 |
| 1:F:98:LYS:HD3 | 1:F:560:THR:CG2 | 2.32 | 0.59 |
| 1:G:41:THR:OG1 | 1:G:44:GLU:HG3 | 2.03 | 0.59 |
| 1:L:378:GLU:HA | 1:L:403:ILE:HD11 | 1.84 | 0.59 |
| 1:N:41:THR:HG22 | 1:N:43:GLU:H | 1.66 | 0.59 |
| 1:N:38:MSE:SE | 1:N:55:PRO:HG2 | 2.53 | 0.59 |
| 1:B:183:LYS:HE3 | 1:B:255:GLU:CD | 2.22 | 0.59 |
| 1:F:136:THR:CG2 | 1:F:221:LEU:HD11 | 2.32 | 0.59 |
| 1:K:156:LYS:HZ2 | 1:K:197:GLN:NE2 | 2.01 | 0.59 |
| 1:K:429:THR:HG22 | 1:K:430:ALA:N | 2.18 | 0.59 |
| 1:L:533:GLU:HG3 | 1:L:537:ASN:HD21 | 1.68 | 0.59 |
| 1:M:454:LEU:HD11 | 1:M:460:LEU:CG | 2.28 | 0.59 |
| 1:B:202:MSE:HE3 | 1:B:203:LEU:C | 2.23 | 0.59 |
| 1:B:158:ILE:HD12 | 1:B:242:VAL:HG11 | 1.84 | 0.59 |
| 1:C:454:LEU:HD11 | 1:C:460:LEU:HD11 | 1.85 | 0.59 |
| 1:D:494:THR:CG2 | 1:D:526:ILE:HG23 | 2.32 | 0.59 |
| 1:G:38:MSE:SE | 1:G:55:PRO:HG2 | 2.53 | 0.59 |
| 1:I:533:GLU:HG3 | 1:I:537:ASN:ND2 | 2.18 | 0.59 |
| 1:J:137:ILE:O | 1:J:140:ARG:HD2 | 2.02 | 0.59 |
| 1:J:288:VAL:HG21 | 1:J:322:LEU:HB3 | 1.84 | 0.59 |
| 1:O:164:GLU:HG2 | 1:O:258:ALA:HB2 | 1.84 | 0.59 |
| 1:C:133:LEU:HD22 | 1:C:135:ILE:CG1 | 2.32 | 0.59 |
| 1:E:297:ILE:CD1 | 1:E:507:LEU:HD12 | 2.33 | 0.59 |
| 1:I:332:VAL:HG13 | 1:I:336:GLU:HB3 | 1.83 | 0.59 |
| 1:M:502:VAL:CG1 | 1:M:507:LEU:HD13 | 2.32 | 0.59 |
| 1:N:138:HIS:NE2 | 1:N:223:HIS:HE1 | 2.01 | 0.59 |
| 1:N:327:MSE:HE3 | 1:N:337:ALA:CB | 2.24 | 0.59 |
| 1:O:165:ARG:O | 1:O:165:ARG:HD2 | 2.02 | 0.59 |
| 1:B:575:GLU:O | 1:B:578:LYS:HG3 | 2.03 | 0.58 |
| 1:C:23:LYS:HG2 | 1:C:24:LYS:N | 2.11 | 0.58 |
| 1:I:23:LYS:CE | 1:I:27:GLU:HG2 | 2.33 | 0.58 |
| 1:K:578:LYS:O | 1:K:578:LYS:HD3 | 2.03 | 0.58 |
| 1:M:578:LYS:C | 1:M:578:LYS:HD2 | 2.23 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:284:ALA:HA | 1:P:319:ILE:HG12 | 1.85 | 0.58 |
| 1:A:177:MSE:O | 1:A:180:PRO:HD2 | 2.02 | 0.58 |
| 1:A:184:LEU:HD22 | 1:A:198:CYS:HB3 | 1.85 | 0.58 |
| 1:B:132:GLY:HA2 | 1:B:200:PRO:HG2 | 1.86 | 0.58 |
| 1:G:160:VAL:CG1 | 1:G:201:VAL:HB | 2.31 | 0.58 |
| 1:J:24:LYS:NZ | 1:L:24:LYS:HD2 | 2.17 | 0.58 |
| 1:L:261:ASN:ND2 | 1:L:261:ASN:N | 2.40 | 0.58 |
| 1:M:520:GLN:HG3 | 7:M:2069:HOH:O | 2.02 | 0.58 |
| 1:P:38:MSE:SE | 1:P:55:PRO:HG2 | 2.53 | 0.58 |
| 1:A:36:LYS:HG3 | 1:A:562:TYR:CD2 | 2.38 | 0.58 |
| 1:A:429:THR:HG22 | 1:A:431:GLU:H | 1.68 | 0.58 |
| 1:D:155:ILE:HD12 | 1:D:155:ILE:N | 2.19 | 0.58 |
| 1:H:36:LYS:HG3 | 1:H:562:TYR:CD2 | 2.39 | 0.58 |
| 1:C:356:ALA:HA | 1:I:226:ILE:HD12 | 1.84 | 0.58 |
| 1:K:416:ILE:HG21 | 1:K:433:LEU:HD23 | 1.86 | 0.58 |
| 1:L:104:ILE:HG13 | 1:L:108:MSE:CE | 2.31 | 0.58 |
| 1:A:381:VAL:HG21 | 1:A:403:ILE:HG23 | 1.86 | 0.58 |
| 1:D:154:VAL:HG13 | 1:D:154:VAL:O | 2.03 | 0.58 |
| 1:D:183:LYS:HE3 | 1:D:255:GLU:CD | 2.24 | 0.58 |
| 1:E:23:LYS:HD2 | 1:E:27:GLU:HG2 | 1.84 | 0.58 |
| 1:E:300:ASN:OD1 | 1:E:305:HIS:HE1 | 1.84 | 0.58 |
| 1:I:285:SER:HB3 | 1:I:470:VAL:HG21 | 1.86 | 0.58 |
| 1:M:69:LEU:O | 1:M:73:GLU:HG3 | 2.03 | 0.58 |
| 1:P:125:LEU:HD23 | 1:P:125:LEU:O | 2.03 | 0.58 |
| 1:P:288:VAL:HG21 | 1:P:322:LEU:HB3 | 1.85 | 0.58 |
| 1:E:137:ILE:HB | 1:E:205:VAL:HG12 | 1.85 | 0.58 |
| 1:E:532:LYS:HG3 | 1:E:549:LEU:HD12 | 1.84 | 0.58 |
| 1:F:192:GLY:HA3 | 1:F:557:VAL:HG13 | 1.84 | 0.58 |
| 1:I:429:THR:HG22 | 1:I:432:GLN:CD | 2.23 | 0.58 |
| 1:K:186:LEU:HD22 | 1:K:190:CYS:SG | 2.44 | 0.58 |
| 1:L:123:TYR:HB3 | 1:L:175:TYR:CD2 | 2.39 | 0.58 |
| 1:L:223:HIS:HD2 | 1:L:224:LYS:O | 1.87 | 0.58 |
| 1:M:107:PHE:O | 1:M:111:VAL:HG12 | 2.03 | 0.58 |
| 1:M:158:ILE:HD12 | 1:M:242:VAL:HG11 | 1.85 | 0.58 |
| 1:N:354:ARG:HD2 | 1:N:356:ALA:O | 2.03 | 0.58 |
| 1:O:401:GLN:HG3 | 1:O:436:TYR:CD1 | 2.39 | 0.58 |
| 7:M:2025:HOH:O | 1:P:580:LYS:HD3 | 2.04 | 0.58 |
| 1:A:386:PRO:HG2 | 1:A:407:MSE:CE | 2.09 | 0.58 |
| 1:B:399:PHE:HB2 | 1:B:428:CYS:HB3 | 1.86 | 0.58 |
| 1:B:412:LYS:O | 1:B:413:ARG:HD2 | 2.03 | 0.58 |
| 1:F:165:ARG:HD2 | 1:F:165:ARG:O | 2.03 | 0.58 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:202:MSE:HE3 | 1:G:203:LEU:O | 2.03 | 0.58 |
| 1:H:416:ILE:CG1 | 1:H:433:LEU:HD21 | 2.30 | 0.58 |
| 1:J:202:MSE:CE | 1:J:204:ASP:HB2 | 2.33 | 0.58 |
| 1:K:239:MSE:HA | 1:K:239:MSE:CE | 2.31 | 0.58 |
| 1:K:324:VAL:O | 1:K:328:GLN:HG3 | 2.03 | 0.58 |
| 1:L:186:LEU:HD22 | 1:L:190:CYS:SG | 2.44 | 0.58 |
| 1:L:183:LYS:NZ | 1:L:467:ASN:HD22 | 2.00 | 0.58 |
| 1:M:88:LEU:HD13 | 1:M:96:PHE:HA | 1.86 | 0.58 |
| 1:N:209:ASN:OD1 | 1:N:211:THR:HB | 2.03 | 0.58 |
| 1:A:467:ASN:ND2 | 3:A:1583:OXL:O2 | 2.37 | 0.58 |
| 1:E:401:GLN:O | 1:E:405:GLN:HG3 | 2.04 | 0.58 |
| 1:K:145:THR:HA | 1:K:148:GLN:HE21 | 1.67 | 0.58 |
| 1:K:327:MSE:HE1 | 1:K:337:ALA:O | 2.04 | 0.58 |
| 1:M:359:THR:HG22 | 1:M:361:GLU:H | 1.68 | 0.58 |
| 1:A:202:MSE:HE3 | 1:A:203:LEU:O | 2.04 | 0.58 |
| 1:B:98:LYS:CD | 1:B:560:THR:HG21 | 2.29 | 0.58 |
| 1:E:136:THR:HG23 | 1:E:221:LEU:HD11 | 1.85 | 0.58 |
| 1:G:59:LEU:H | 1:G:59:LEU:HD12 | 1.69 | 0.58 |
| 1:N:354:ARG:O | 1:N:358:LEU:HD23 | 2.03 | 0.58 |
| 1:B:315:ALA:O | 1:B:319:ILE:HG13 | 2.04 | 0.58 |
| 1:H:407:MSE:HG2 | 1:H:416:ILE:HD11 | 1.85 | 0.58 |
| 1:J:381:VAL:HG21 | 1:J:403:ILE:HG23 | 1.86 | 0.58 |
| 1:K:359:THR:HG22 | 1:K:362:LYS:HD2 | 1.86 | 0.58 |
| 1:N:158:ILE:HD12 | 1:N:242:VAL:HG11 | 1.86 | 0.58 |
| 1:O:571:THR:HG23 | 1:O:572:TRP:O | 2.02 | 0.58 |
| 1:A:314:GLU:HB2 | 2:A:1581:NAP:O1N | 2.04 | 0.58 |
| 1:C:171:ASP:OD2 | 1:C:225:ARG:HD2 | 2.04 | 0.58 |
| 1:H:492:LEU:O | 1:H:496:GLU:HG3 | 2.02 | 0.58 |
| 1:K:174:CYS:HA | 1:K:202:MSE:HE3 | 1.86 | 0.58 |
| 1:L:433:LEU:HG | 1:L:443:PHE:CD1 | 2.39 | 0.58 |
| 1:P:90:ASP:OD1 | 1:P:131:ARG:NH1 | 2.36 | 0.58 |
| 1:D:38:MSE:SE | 1:D:55:PRO:HG2 | 2.53 | 0.57 |
| 1:E:349:LEU:HB2 | 1:E:380:ILE:HD13 | 1.86 | 0.57 |
| 1:E:38:MSE:SE | 1:E:55:PRO:HG2 | 2.54 | 0.57 |
| 1:H:416:ILE:HG21 | 1:H:433:LEU:HD23 | 1.85 | 0.57 |
| 1:K:136:THR:HG22 | 1:K:139:ASP:OD1 | 2.04 | 0.57 |
| 1:D:117:GLY:O | 1:D:121:GLN:HG3 | 2.04 | 0.57 |
| 1:E:407:MSE:HG2 | 1:E:416:ILE:HD11 | 1.85 | 0.57 |
| 1:G:431:GLU:OE2 | 1:G:452:VAL:HG22 | 2.04 | 0.57 |
| 1:J:112:TYR:OH | 1:J:183:LYS:NZ | 2.36 | 0.57 |
| 1:J:401:GLN:HG2 | 1:J:436:TYR:CE1 | 2.39 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:284:ALA:HA | 1:L:319:ILE:HG12 | 1.86 | 0.57 |
| 1:L:378:GLU:OE2 | 1:L:402:GLN:HB3 | 2.04 | 0.57 |
| 1:N:139:ASP:HB3 | 1:O:570:TYR:OH | 2.04 | 0.57 |
| 1:D:23:LYS:O | 1:D:24:LYS:HG3 | 2.04 | 0.57 |
| 1:E:38:MSE:HB2 | 1:E:59:LEU:HD11 | 1.86 | 0.57 |
| 1:H:580:LYS:HD3 | 1:H:580:LYS:C | 2.25 | 0.57 |
| 1:I:100:LEU:HD21 | 1:I:111:VAL:HG21 | 1.85 | 0.57 |
| 1:J:323:ILE:HG22 | 1:J:327:MSE:HE2 | 1.85 | 0.57 |
| 1:J:416:ILE:CG1 | 1:J:433:LEU:HD21 | 2.31 | 0.57 |
| 1:J:433:LEU:HG | 1:J:443:PHE:CD1 | 2.39 | 0.57 |
| 1:P:136:THR:HG23 | 1:P:221:LEU:HD11 | 1.85 | 0.57 |
| 1:A:186:LEU:HD22 | 1:A:190:CYS:SG | 2.44 | 0.57 |
| 1:E:245:ARG:HD3 | 1:E:246:TYR:CE2 | 2.39 | 0.57 |
| 1:H:238:PHE:O | 1:H:242:VAL:HG23 | 2.04 | 0.57 |
| 1:L:496:GLU:O | 1:L:500:GLN:NE2 | 2.36 | 0.57 |
| 1:N:202:MSE:CE | 1:N:204:ASP:HB2 | 2.35 | 0.57 |
| 1:O:238:PHE:CE2 | 1:O:239:MSE:HE3 | 2.39 | 0.57 |
| 1:P:223:HIS:HD2 | 1:P:224:LYS:O | 1.87 | 0.57 |
| 1:B:254:PHE:HE2 | 1:B:265:LEU:HD13 | 1.69 | 0.57 |
| 1:C:108:MSE:CE | 1:C:190:CYS:SG | 2.93 | 0.57 |
| 1:E:108:MSE:N | 1:E:109:PRO:CD | 2.67 | 0.57 |
| 1:E:24:LYS:NZ | 1:E:49:ASN:HD22 | 1.88 | 0.57 |
| 1:G:381:VAL:CG1 | 1:G:407:MSE:HE1 | 2.34 | 0.57 |
| 1:I:146:MSE:HE3 | 1:J:51:HIS:CD2 | 2.39 | 0.57 |
| 1:K:77:SER:HB2 | 1:K:80:ASP:OD2 | 2.05 | 0.57 |
| 1:L:324:VAL:O | 1:L:328:GLN:HG3 | 2.04 | 0.57 |
| 1:O:428:CYS:CA | 1:O:432:GLN:HE21 | 2.17 | 0.57 |
| 1:B:431:GLU:HG2 | 7:B:2034:HOH:O | 2.05 | 0.57 |
| 1:C:157:ALA:HB2 | 1:C:479:ILE:HD11 | 1.86 | 0.57 |
| 1:E:136:THR:HB | 1:E:139:ASP:OD2 | 2.05 | 0.57 |
| 1:G:242:VAL:HG13 | 1:G:246:TYR:HD1 | 1.69 | 0.57 |
| 1:H:505:GLU:HG3 | 7:H:2063:HOH:O | 2.05 | 0.57 |
| 1:O:327:MSE:C | 1:O:332:VAL:HG12 | 2.25 | 0.57 |
| 1:P:77:SER:O | 1:P:81:ARG:HG3 | 2.05 | 0.57 |
| 1:A:375:LYS:HD3 | 1:A:375:LYS:O | 2.04 | 0.57 |
| 1:B:575:GLU:CG | 1:B:576:ALA:N | 2.67 | 0.57 |
| 1:E:136:THR:CG2 | 1:E:138:HIS:H | 1.99 | 0.57 |
| 1:I:433:LEU:HD13 | 1:I:433:LEU:C | 2.24 | 0.57 |
| 1:K:38:MSE:SE | 1:K:55:PRO:HG2 | 2.54 | 0.57 |
| 1:L:160:VAL:HG22 | 1:L:201:VAL:HB | 1.85 | 0.57 |
| 1:L:227:ARG:HG2 | 7:L:2031:HOH:O | 2.04 | 0.57 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:N:442:ILE:HG22 | 1:N:512:LEU:HD11 | 1.86 | 0.57 |
| 1:P:358:LEU:HD23 | 1:P:363:GLU:OE1 | 2.04 | 0.57 |
| 1:B:378:GLU:HA | 1:B:403:ILE:HD13 | 1.87 | 0.57 |
| 1:B:64:GLN:NE2 | 1:B:562:TYR:OH | 2.33 | 0.57 |
| 1:F:416:ILE:CG1 | 1:F:433:LEU:HD21 | 2.34 | 0.57 |
| 1:G:327:MSE:HE1 | 1:G:340:ARG:HG3 | 1.86 | 0.57 |
| 1:L:417:PHE:CD1 | 1:L:444:ALA:HB3 | 2.40 | 0.57 |
| 1:N:413:ARG:HD2 | 7:N:2047:HOH:O | 2.05 | 0.57 |
| 1:P:466:ASN:HA | 2:P:1581:NAP:H72N | 1.69 | 0.57 |
| 1:B:428:CYS:CA | 1:B:432:GLN:HE21 | 2.18 | 0.57 |
| 1:G:429:THR:H | 1:G:432:GLN:HE21 | 1.50 | 0.57 |
| 1:G:499:ALA:HA | 7:G:2056:HOH:O | 2.05 | 0.57 |
| 1:I:72:PHE:CE1 | 1:I:81:ARG:HB3 | 2.40 | 0.57 |
| 1:K:145:THR:HA | 1:K:148:GLN:NE2 | 2.19 | 0.57 |
| 1:K:529:ARG:HG2 | 1:K:529:ARG:HH11 | 1.68 | 0.57 |
| 1:O:210:GLU:HA | 1:O:213:LEU:HD12 | 1.86 | 0.57 |
| 1:A:528:VAL:HG12 | 1:A:532:LYS:HE2 | 1.86 | 0.57 |
| 1:D:322:LEU:HD22 | 1:D:492:LEU:HD13 | 1.87 | 0.57 |
| 1:F:38:MSE:SE | 1:F:55:PRO:HG2 | 2.55 | 0.57 |
| 1:I:578:LYS:HZ1 | 1:L:222:ARG:HD3 | 1.69 | 0.57 |
| 1:J:555:SER:OG | 1:J:556:GLN:NE2 | 2.38 | 0.57 |
| 1:M:309:PHE:HB2 | 1:M:343:MSE:HG2 | 1.85 | 0.57 |
| 1:O:77:SER:O | 1:O:81:ARG:HG3 | 2.05 | 0.57 |
| 1:C:90:ASP:OD1 | 1:C:131:ARG:NH1 | 2.38 | 0.56 |
| 1:E:183:LYS:HE3 | 1:E:255:GLU:OE1 | 2.05 | 0.56 |
| 1:F:433:LEU:CD1 | 1:F:443:PHE:HB2 | 2.35 | 0.56 |
| 1:I:303:SER:HB2 | 1:I:332:VAL:HG21 | 1.87 | 0.56 |
| 1:J:359:THR:CG2 | 1:J:362:LYS:H | 2.13 | 0.56 |
| 1:J:377:LEU:O | 1:J:381:VAL:HG23 | 2.04 | 0.56 |
| 1:L:454:LEU:HD21 | 1:L:460:LEU:CD1 | 2.34 | 0.56 |
| 1:A:165:ARG:O | 1:A:165:ARG:HD2 | 2.06 | 0.56 |
| 1:A:177:MSE:HE3 | 1:A:177:MSE:O | 2.06 | 0.56 |
| 1:A:35:ASN:ND2 | 1:A:37:GLY:H | 2.04 | 0.56 |
| 1:D:210:GLU:HA | 1:D:213:LEU:HD12 | 1.86 | 0.56 |
| 1:E:243:THR:HG21 | 1:E:273:TYR:HD2 | 1.69 | 0.56 |
| 1:E:307:VAL:HG22 | 1:E:388:VAL:HB | 1.86 | 0.56 |
| 1:B:342:TRP:CH2 | 1:B:367:HIS:HB2 | 2.40 | 0.56 |
| 1:B:361:GLU:HA | 1:B:364:HIS:HD2 | 1.70 | 0.56 |
| 1:B:64:GLN:O | 1:B:68:ILE:HG12 | 2.05 | 0.56 |
| 1:F:59:LEU:HD13 | 1:F:64:GLN:HG3 | 1.87 | 0.56 |
| 1:I:433:LEU:HG | 1:I:443:PHE:CD1 | 2.40 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:K:517:VAL:HG13 | 7:K:2037:HOH:O | 2.04 | 0.56 |
| 1:M:24:LYS:HB2 | 1:M:24:LYS:HZ1 | 1.67 | 0.56 |
| 1:C:41:THR:HG22 | 1:C:43:GLU:N | 2.20 | 0.56 |
| 1:D:493:THR:O | 1:D:497:VAL:HG23 | 2.05 | 0.56 |
| 1:K:192:GLY:HA3 | 1:K:557:VAL:HG13 | 1.87 | 0.56 |
| 1:M:378:GLU:HA | 1:M:403:ILE:HD13 | 1.88 | 0.56 |
| 1:M:378:GLU:HA | 1:M:403:ILE:CD1 | 2.35 | 0.56 |
| 1:O:92:ASN:C | 1:O:92:ASN:HD22 | 2.08 | 0.56 |
| 1:P:492:LEU:O | 1:P:496:GLU:HG3 | 2.05 | 0.56 |
| 1:B:429:THR:HG22 | 1:B:431:GLU:H | 1.68 | 0.56 |
| 1:C:332:VAL:CG1 | 1:C:336:GLU:HB3 | 2.35 | 0.56 |
| 1:C:502:VAL:CG1 | 1:C:507:LEU:HD13 | 2.35 | 0.56 |
| 1:C:86:MSE:HE1 | 1:C:89:GLN:HE22 | 1.71 | 0.56 |
| 1:F:77:SER:HB3 | 1:F:80:ASP:OD2 | 2.05 | 0.56 |
| 1:G:171:ASP:OD2 | 1:G:225:ARG:HD2 | 2.06 | 0.56 |
| 1:H:429:THR:HG22 | 1:H:431:GLU:H | 1.71 | 0.56 |
| 1:J:155:ILE:HD13 | 1:J:246:TYR:CE2 | 2.40 | 0.56 |
| 1:L:407:MSE:HG3 | 1:L:414:PRO:HB3 | 1.88 | 0.56 |
| 1:N:42:LEU:O | 1:N:46:GLN:HG3 | 2.05 | 0.56 |
| 1:F:381:VAL:CG1 | 1:F:407:MSE:HE1 | 2.35 | 0.56 |
| 1:H:152:GLU:HB2 | 1:H:155:ILE:HD11 | 1.87 | 0.56 |
| 1:I:222:ARG:NH1 | 1:L:580:LYS:HE2 | 2.20 | 0.56 |
| 1:I:322:LEU:HD22 | 1:I:492:LEU:HD13 | 1.87 | 0.56 |
| 1:L:41:THR:HG22 | 1:L:42:LEU:N | 2.21 | 0.56 |
| 1:L:429:THR:H | 1:L:432:GLN:NE2 | 2.02 | 0.56 |
| 1:O:354:ARG:HE | 1:O:358:LEU:HD11 | 1.71 | 0.56 |
| 1:A:417:PHE:CD1 | 1:A:444:ALA:HB3 | 2.40 | 0.56 |
| 1:C:136:THR:CG2 | 1:C:137:ILE:N | 2.69 | 0.56 |
| 1:F:433:LEU:HD12 | 1:F:443:PHE:HB2 | 1.85 | 0.56 |
| 1:I:23:LYS:O | 1:I:24:LYS:HG3 | 2.06 | 0.56 |
| 1:J:467:ASN:ND2 | 3:J:1582:OXL:O2 | 2.39 | 0.56 |
| 1:L:154:VAL:HG23 | 1:L:154:VAL:O | 2.06 | 0.56 |
| 1:N:448:PRO:HD3 | 1:N:464:GLN:NE2 | 2.20 | 0.56 |
| 1:P:161:THR:HA | 1:P:257:PHE:CE1 | 2.41 | 0.56 |
| 1:A:429:THR:CG2 | 1:A:430:ALA:N | 2.69 | 0.56 |
| 1:F:466:ASN:HA | 2:F:1581:NAP:H72N | 1.71 | 0.56 |
| 1:G:307:VAL:CG2 | 1:G:341:ILE:HG12 | 2.36 | 0.56 |
| 1:I:104:ILE:HD11 | 1:I:108:MSE:HE3 | 1.86 | 0.56 |
| 1:K:158:ILE:HD12 | 1:K:242:VAL:HG11 | 1.88 | 0.56 |
| 1:L:334:LYS:HE3 | 1:L:338:ILE:HD11 | 1.88 | 0.56 |
| 1:L:524:LEU:HD21 | 1:L:554:ARG:HE | 1.69 | 0.56 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:N:327:MSE:HE1 | 1:N:337:ALA:O | 2.05 | 0.56 |
| 1:P:166:ILE:HD12 | 1:P:179:ILE:HG13 | 1.88 | 0.56 |
| 1:C:533:GLU:HG3 | 1:C:537:ASN:ND2 | 2.21 | 0.56 |
| 1:D:210:GLU:OE2 | 1:D:224:LYS:NZ | 2.39 | 0.56 |
| 1:D:429:THR:HG22 | 1:D:430:ALA:N | 2.21 | 0.56 |
| 1:D:466:ASN:HA | 2:D:1581:NAP:H72N | 1.71 | 0.56 |
| 1:D:547:GLU:N | 1:D:547:GLU:CD | 2.45 | 0.56 |
| 1:G:381:VAL:HG13 | 1:G:407:MSE:HE1 | 1.86 | 0.56 |
| 1:I:159:VAL:HG23 | 1:I:184:LEU:HD21 | 1.88 | 0.56 |
| 1:K:504:GLU:HG3 | 1:K:508:GLN:HE21 | 1.70 | 0.56 |
| 1:C:270:ARG:HH12 | 1:C:487:GLY:HA2 | 1.71 | 0.56 |
| 1:D:177:MSE:O | 1:D:180:PRO:HD2 | 2.06 | 0.56 |
| 1:E:26:TYR:HB2 | 7:E:2002:HOH:O | 2.06 | 0.56 |
| 1:F:104:ILE:HG13 | 1:F:108:MSE:HE3 | 1.86 | 0.56 |
| 1:H:172:LEU:O | 1:H:175:TYR:HB2 | 2.06 | 0.56 |
| 1:I:161:THR:HA | 1:I:257:PHE:CE1 | 2.41 | 0.56 |
| 1:I:265:LEU:HD22 | 1:I:269:TYR:HE1 | 1.71 | 0.56 |
| 1:K:377:LEU:O | 1:K:381:VAL:HG23 | 2.06 | 0.56 |
| 1:M:374:MSE:HE1 | 1:M:379:ASP:C | 2.26 | 0.56 |
| 1:C:194:LYS:HD2 | 1:C:197:GLN:NE2 | 2.21 | 0.56 |
| 1:C:361:GLU:O | 1:C:364:HIS:HB2 | 2.05 | 0.56 |
| 1:G:183:LYS:NZ | 1:G:467:ASN:HD22 | 2.03 | 0.56 |
| 1:K:359:THR:CG2 | 1:K:362:LYS:HG3 | 2.35 | 0.56 |
| 1:M:41:THR:OG1 | 1:M:44:GLU:HG3 | 2.06 | 0.56 |
| 1:N:520:GLN:HB2 | 5:N:1586:CL:CL | 2.43 | 0.56 |
| 1:A:229:GLN:HA | 1:A:229:GLN:NE2 | 2.21 | 0.55 |
| 1:B:72:PHE:CZ | 1:B:81:ARG:HD3 | 2.40 | 0.55 |
| 1:E:36:LYS:HD2 | 1:E:562:TYR:CG | 2.41 | 0.55 |
| 1:F:492:LEU:O | 1:F:496:GLU:HG3 | 2.07 | 0.55 |
| 1:I:317:LEU:HD23 | 1:I:343:MSE:HE1 | 1.88 | 0.55 |
| 1:J:162:ASP:O | 1:J:225:ARG:NH2 | 2.32 | 0.55 |
| 1:M:300:ASN:OD1 | 1:M:305:HIS:HE1 | 1.89 | 0.55 |
| 1:N:429:THR:HG22 | 1:N:431:GLU:N | 2.20 | 0.55 |
| 1:O:42:LEU:HD21 | 1:O:46:GLN:NE2 | 2.22 | 0.55 |
| 1:A:324:VAL:O | 1:A:328:GLN:HG3 | 2.06 | 0.55 |
| 1:B:179:ILE:HB | 1:B:180:PRO:HD3 | 1.88 | 0.55 |
| 1:C:394:ALA:HB2 | 2:C:1581:NAP:O3D | 2.06 | 0.55 |
| 1:F:186:LEU:HD22 | 1:F:190:CYS:SG | 2.45 | 0.55 |
| 1:H:401:GLN:HG3 | 1:H:436:TYR:CD1 | 2.41 | 0.55 |
| 1:P:396:GLY:O | 1:P:426:ALA:O | 2.23 | 0.55 |
| 1:E:158:ILE:HD12 | 1:E:242:VAL:HG11 | 1.87 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:243:THR:HG21 | 1:I:273:TYR:HD2 | 1.69 | 0.55 |
| 1:I:222:ARG:HD2 | 1:L:580:LYS:NZ | 2.22 | 0.55 |
| 1:B:428:CYS:HA | 1:B:432:GLN:HE21 | 1.71 | 0.55 |
| 1:C:340:ARG:NH1 | 1:C:340:ARG:HG2 | 2.21 | 0.55 |
| 1:D:323:ILE:HG22 | 1:D:327:MSE:HE2 | 1.87 | 0.55 |
| 1:E:239:MSE:HE1 | 1:E:252:ILE:HG21 | 1.86 | 0.55 |
| 1:F:212:LEU:HD13 | 1:F:218:TYR:HE1 | 1.72 | 0.55 |
| 1:J:165:ARG:HD2 | 1:J:165:ARG:O | 2.07 | 0.55 |
| 1:L:163:GLY:HA2 | 1:L:166:ILE:HD11 | 1.87 | 0.55 |
| 1:L:416:ILE:HG13 | 1:L:433:LEU:CD2 | 2.30 | 0.55 |
| 1:M:529:ARG:HH11 | 1:M:529:ARG:HG2 | 1.71 | 0.55 |
| 1:P:227:ARG:HG3 | 1:P:227:ARG:HH11 | 1.72 | 0.55 |
| 1:G:483:LEU:HD23 | 1:G:486:ILE:HG12 | 1.88 | 0.55 |
| 1:G:543:TYR:HA | 1:G:544:PRO:C | 2.26 | 0.55 |
| 1:H:158:ILE:HG22 | 1:H:160:VAL:HG23 | 1.88 | 0.55 |
| 1:J:378:GLU:OE2 | 1:J:402:GLN:HB3 | 2.06 | 0.55 |
| 1:L:179:ILE:HB | 1:L:180:PRO:HD3 | 1.88 | 0.55 |
| 1:N:36:LYS:HG3 | 1:N:562:TYR:CD2 | 2.42 | 0.55 |
| 1:N:536:ARG:HG3 | 1:N:536:ARG:HH11 | 1.72 | 0.55 |
| 1:O:239:MSE:HE1 | 1:O:252:ILE:HG12 | 1.89 | 0.55 |
| 1:C:467:ASN:ND2 | 3:C:1582:OXL:O2 | 2.40 | 0.55 |
| 1:J:92:ASN:C | 1:J:92:ASN:HD22 | 2.09 | 0.55 |
| 1:N:374:MSE:CE | 1:N:379:ASP:HB3 | 2.37 | 0.55 |
| 1:P:150:TRP:CE2 | 1:P:199:LEU:HD13 | 2.41 | 0.55 |
| 1:P:399:PHE:HB2 | 1:P:428:CYS:HB3 | 1.88 | 0.55 |
| 1:C:312:ALA:HB3 | 1:C:362:LYS:HE2 | 1.89 | 0.55 |
| 1:C:86:MSE:HE1 | 1:C:89:GLN:NE2 | 2.21 | 0.55 |
| 1:E:24:LYS:NZ | 1:E:49:ASN:ND2 | 2.47 | 0.55 |
| 1:F:41:THR:HG22 | 1:F:43:GLU:N | 2.22 | 0.55 |
| 1:I:327:MSE:HE1 | 1:I:337:ALA:O | 2.07 | 0.55 |
| 1:J:329:LYS:HE2 | 1:J:496:GLU:OE2 | 2.06 | 0.55 |
| 1:K:29:LEU:HA | 1:K:35:ASN:HD22 | 1.71 | 0.55 |
| 1:O:431:GLU:HB2 | 7:O:2063:HOH:O | 2.05 | 0.55 |
| 1:O:433:LEU:HG | 1:O:443:PHE:CD1 | 2.42 | 0.55 |
| 1:O:90:ASP:OD1 | 1:O:131:ARG:NH1 | 2.40 | 0.55 |
| 1:A:24:LYS:O | 1:A:24:LYS:HD3 | 2.07 | 0.55 |
| 1:A:528:VAL:CG1 | 1:A:532:LYS:HE2 | 2.37 | 0.55 |
| 1:D:389:LEU:CD1 | 1:D:407:MSE:HE3 | 2.37 | 0.55 |
| 1:F:162:ASP:O | 1:F:225:ARG:NH2 | 2.39 | 0.55 |
| 1:I:158:ILE:HD12 | 1:I:242:VAL:HG11 | 1.88 | 0.55 |
| 1:L:140:ARG:HD3 | 7:L:2032:HOH:O | 2.06 | 0.55 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:357:SER:O | 1:O:358:LEU:HD12 | 2.06 | 0.55 |
| 1:B:125:LEU:HD13 | 1:B:125:LEU:O | 2.07 | 0.55 |
| 1:A:27:GLU:OE1 | 1:B:27:GLU:HG3 | 2.06 | 0.55 |
| 1:L:418:ALA:O | 1:L:445:SER:HA | 2.07 | 0.55 |
| 1:D:61:GLN:O | 1:D:65:VAL:HG23 | 2.07 | 0.55 |
| 1:F:402:GLN:CD | 1:F:402:GLN:H | 2.11 | 0.55 |
| 1:G:475:ALA:O | 1:G:479:ILE:HG13 | 2.07 | 0.55 |
| 1:I:354:ARG:HB3 | 1:I:358:LEU:HD21 | 1.88 | 0.55 |
| 1:L:429:THR:HG22 | 1:L:430:ALA:N | 2.21 | 0.55 |
| 1:P:416:ILE:HG13 | 1:P:433:LEU:CD2 | 2.29 | 0.55 |
| 1:B:284:ALA:HA | 1:B:319:ILE:HG12 | 1.89 | 0.54 |
| 1:C:177:MSE:HG2 | 1:C:202:MSE:HG3 | 1.89 | 0.54 |
| 1:D:322:LEU:HD21 | 1:D:492:LEU:HB2 | 1.88 | 0.54 |
| 1:F:401:GLN:HG2 | 1:F:436:TYR:CE2 | 2.41 | 0.54 |
| 1:O:177:MSE:HA | 1:O:177:MSE:HE3 | 1.86 | 0.54 |
| 1:P:41:THR:HG21 | 7:P:2006:HOH:O | 2.05 | 0.54 |
| 1:A:132:GLY:HA2 | 1:A:200:PRO:HG2 | 1.89 | 0.54 |
| 1:B:529:ARG:HG2 | 1:B:529:ARG:HH11 | 1.71 | 0.54 |
| 1:C:141:GLY:H | 1:C:237:GLU:CD | 2.10 | 0.54 |
| 1:D:388:VAL:HG22 | 1:D:415:ILE:HB | 1.89 | 0.54 |
| 1:L:288:VAL:HG21 | 1:L:322:LEU:HB3 | 1.89 | 0.54 |
| 1:B:156:LYS:HD3 | 1:B:479:ILE:HG23 | 1.88 | 0.54 |
| 1:B:314:GLU:HB2 | 2:B:1581:NAP:O1N | 2.07 | 0.54 |
| 1:B:66:TYR:CZ | 1:B:70:LYS:HD3 | 2.42 | 0.54 |
| 1:E:183:LYS:HE2 | 5:E:1586:CL:CL | 2.44 | 0.54 |
| 1:J:303:SER:HB2 | 1:J:332:VAL:HG21 | 1.89 | 0.54 |
| 1:J:351:VAL:O | 1:J:354:ARG:HB2 | 2.08 | 0.54 |
| 1:K:171:ASP:OD2 | 1:K:225:ARG:HD2 | 2.07 | 0.54 |
| 1:A:433:LEU:HD12 | 1:A:443:PHE:HB2 | 1.90 | 0.54 |
| 1:B:575:GLU:HG3 | 1:B:576:ALA:N | 2.23 | 0.54 |
| 1:D:433:LEU:HD12 | 1:D:443:PHE:HB2 | 1.90 | 0.54 |
| 1:F:136:THR:CG2 | 1:F:137:ILE:N | 2.71 | 0.54 |
| 1:F:24:LYS:HD3 | 1:H:24:LYS:HD2 | 1.89 | 0.54 |
| 1:G:239:MSE:HE3 | 1:G:254:PHE:CZ | 2.42 | 0.54 |
| 1:K:252:ILE:N | 1:K:252:ILE:HD12 | 2.23 | 0.54 |
| 1:M:429:THR:HB | 1:M:432:GLN:CG | 2.23 | 0.54 |
| 1:M:64:GLN:O | 1:M:68:ILE:HG12 | 2.07 | 0.54 |
| 1:A:104:ILE:HD11 | 1:A:108:MSE:HE3 | 1.88 | 0.54 |
| 1:A:118:LEU:HD22 | 1:A:122:HIS:HD2 | 1.72 | 0.54 |
| 1:C:391:GLY:HA3 | 1:C:427:GLU:HG2 | 1.89 | 0.54 |
| 1:C:502:VAL:HG11 | 1:C:507:LEU:HD13 | 1.90 | 0.54 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:317:LEU:HD23 | 1:H:343:MSE:HE1 | 1.89 | 0.54 |
| 1:K:117:GLY:O | 1:K:121:GLN:HG3 | 2.08 | 0.54 |
| 1:K:378:GLU:HA | 1:K:403:ILE:HD13 | 1.89 | 0.54 |
| 1:M:396:GLY:O | 1:M:426:ALA:O | 2.24 | 0.54 |
| 1:A:108:MSE:N | 1:A:109:PRO:CD | 2.70 | 0.54 |
| 1:A:254:PHE:CE2 | 1:A:265:LEU:HD13 | 2.43 | 0.54 |
| 1:E:51:HIS:CD2 | 1:F:146:MSE:HE3 | 2.42 | 0.54 |
| 1:F:61:GLN:HA | 1:F:64:GLN:HE21 | 1.73 | 0.54 |
| 1:H:179:ILE:HB | 1:H:180:PRO:HD3 | 1.89 | 0.54 |
| 1:H:156:LYS:HD3 | 1:H:479:ILE:HG23 | 1.90 | 0.54 |
| 1:I:416:ILE:HG13 | 1:I:433:LEU:CD2 | 2.37 | 0.54 |
| 1:J:148:GLN:HG2 | 1:J:245:ARG:HH21 | 1.72 | 0.54 |
| 1:N:143:ILE:HD12 | 1:N:237:GLU:HG2 | 1.90 | 0.54 |
| 1:C:533:GLU:HA | 1:C:536:ARG:NH1 | 2.23 | 0.54 |
| 1:D:108:MSE:N | 1:D:109:PRO:CD | 2.71 | 0.54 |
| 1:D:433:LEU:HG | 1:D:443:PHE:CD1 | 2.43 | 0.54 |
| 1:D:47:GLN:HE22 | 1:D:566:VAL:HG13 | 1.73 | 0.54 |
| 1:G:343:MSE:O | 1:G:349:LEU:HD12 | 2.08 | 0.54 |
| 1:I:38:MSE:SE | 1:I:55:PRO:HG2 | 2.58 | 0.54 |
| 1:A:136:THR:HB | 1:A:139:ASP:OD2 | 2.07 | 0.54 |
| 1:A:162:ASP:O | 1:A:225:ARG:NH2 | 2.41 | 0.54 |
| 1:E:202:MSE:HE3 | 1:E:203:LEU:N | 2.23 | 0.54 |
| 1:I:108:MSE:HB3 | 1:I:109:PRO:HD3 | 1.89 | 0.54 |
| 1:J:270:ARG:HH11 | 1:J:270:ARG:CG | 2.19 | 0.54 |
| 1:N:251:LEU:HD23 | 1:N:478:VAL:HG11 | 1.88 | 0.54 |
| 1:O:41:THR:HG22 | 1:O:43:GLU:N | 2.23 | 0.54 |
| 1:A:92:ASN:ND2 | 1:A:92:ASN:C | 2.62 | 0.54 |
| 1:B:90:ASP:OD2 | 1:B:131:ARG:NH1 | 2.30 | 0.54 |
| 1:I:171:ASP:OD2 | 1:I:225:ARG:HD2 | 2.07 | 0.54 |
| 1:I:396:GLY:O | 1:I:426:ALA:O | 2.26 | 0.54 |
| 1:I:505:GLU:HG3 | 7:I:2059:HOH:O | 2.08 | 0.54 |
| 1:K:41:THR:OG1 | 1:K:44:GLU:HG3 | 2.08 | 0.54 |
| 1:L:332:VAL:HG22 | 1:L:336:GLU:HB2 | 1.89 | 0.54 |
| 1:N:23:LYS:O | 1:N:28:VAL:HG22 | 2.07 | 0.54 |
| 1:N:192:GLY:HA3 | 1:N:557:VAL:HG13 | 1.90 | 0.54 |
| 1:F:94:LYS:HE2 | 1:F:559:SER:O | 2.07 | 0.54 |
| 1:I:502:VAL:HG12 | 1:I:507:LEU:CD2 | 2.38 | 0.54 |
| 1:A:162:ASP:O | 1:A:202:MSE:HE1 | 2.07 | 0.53 |
| 1:A:98:LYS:CD | 1:A:560:THR:HG21 | 2.35 | 0.53 |
| 1:B:184:LEU:HD22 | 1:B:198:CYS:HB3 | 1.90 | 0.53 |
| 1:L:177:MSE:O | 1:L:180:PRO:HD2 | 2.08 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:L:352:LYS:NZ | 1:L:352:LYS:HB3 | 2.23 | 0.53 |
| 1:N:429:THR:CG2 | 1:N:430:ALA:N | 2.70 | 0.53 |
| 1:N:77:SER:O | 1:N:81:ARG:HG3 | 2.08 | 0.53 |
| 1:P:171:ASP:OD2 | 1:P:225:ARG:HD2 | 2.08 | 0.53 |
| 1:P:179:ILE:HB | 1:P:180:PRO:HD3 | 1.90 | 0.53 |
| 1:B:405:GLN:NE2 | 1:B:436:TYR:O | 2.39 | 0.53 |
| 1:B:77:SER:HB3 | 1:B:80:ASP:OD2 | 2.08 | 0.53 |
| 1:C:158:ILE:HD12 | 1:C:242:VAL:HG11 | 1.90 | 0.53 |
| 1:C:183:LYS:HE3 | 1:C:255:GLU:CD | 2.29 | 0.53 |
| 1:F:157:ALA:HB2 | 1:F:479:ILE:HD11 | 1.89 | 0.53 |
| 1:F:239:MSE:CE | 1:F:252:ILE:HD13 | 2.37 | 0.53 |
| 1:J:276:PHE:HB3 | 1:J:486:ILE:HD12 | 1.90 | 0.53 |
| 1:J:33:HIS:CD2 | 1:J:93:GLU:OE1 | 2.61 | 0.53 |
| 1:L:92:ASN:C | 1:L:92:ASN:ND2 | 2.60 | 0.53 |
| 1:M:137:ILE:HA | 1:M:234:LEU:HD22 | 1.90 | 0.53 |
| 1:O:136:THR:CG2 | 1:O:221:LEU:HD11 | 2.35 | 0.53 |
| 1:O:44:GLU:O | 1:O:48:LEU:HD13 | 2.08 | 0.53 |
| 1:B:61:GLN:HE22 | 1:B:560:THR:CG2 | 2.21 | 0.53 |
| 1:C:132:GLY:HA3 | 1:C:177:MSE:CE | 2.37 | 0.53 |
| 1:E:327:MSE:O | 1:E:332:VAL:HG12 | 2.08 | 0.53 |
| 1:E:502:VAL:HG22 | 1:E:514:PRO:HD3 | 1.90 | 0.53 |
| 1:G:270:ARG:HH11 | 1:G:270:ARG:HG2 | 1.73 | 0.53 |
| 1:I:133:LEU:HD23 | 1:I:134:PHE:N | 2.23 | 0.53 |
| 1:J:359:THR:HG22 | 1:J:362:LYS:CG | 2.38 | 0.53 |
| 1:J:24:LYS:HG2 | 1:J:48:LEU:HA | 1.89 | 0.53 |
| 1:M:172:LEU:O | 1:M:175:TYR:HB2 | 2.09 | 0.53 |
| 1:N:543:TYR:HA | 1:N:544:PRO:C | 2.29 | 0.53 |
| 1:N:90:ASP:OD1 | 1:N:131:ARG:NH1 | 2.28 | 0.53 |
| 1:C:132:GLY:HA3 | 1:C:177:MSE:HE1 | 1.91 | 0.53 |
| 1:F:407:MSE:HG2 | 1:F:416:ILE:HD11 | 1.90 | 0.53 |
| 1:H:315:ALA:O | 1:H:319:ILE:HG13 | 2.09 | 0.53 |
| 1:L:381:VAL:HG11 | 1:L:407:MSE:CE | 2.39 | 0.53 |
| 1:O:156:LYS:HE2 | 1:O:197:GLN:NE2 | 2.24 | 0.53 |
| 1:O:354:ARG:NE | 1:O:358:LEU:HD11 | 2.23 | 0.53 |
| 1:B:36:LYS:HD3 | 1:B:562:TYR:HB3 | 1.89 | 0.53 |
| 1:B:428:CYS:HB2 | 1:B:432:GLN:HE21 | 1.73 | 0.53 |
| 1:E:30:ARG:O | 1:F:30:ARG:HD2 | 2.09 | 0.53 |
| 1:H:529:ARG:HG2 | 1:H:529:ARG:HH11 | 1.74 | 0.53 |
| 1:I:467:ASN:H | 2:I:1581:NAP:H72N | 1.54 | 0.53 |
| 1:J:389:LEU:CD1 | 1:J:407:MSE:HE3 | 2.38 | 0.53 |
| 1:J:64:GLN:NE2 | 1:J:562:TYR:OH | 2.41 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:N:413:ARG:CD | 7:N:2047:HOH:O | 2.55 | 0.53 |
| 1:O:359:THR:CG2 | 1:O:362:LYS:HG3 | 2.38 | 0.53 |
| 1:C:536:ARG:NE | 1:H:333:SER:HB3 | 2.24 | 0.53 |
| 1:N:85:LEU:HD12 | 1:N:110:ILE:HG21 | 1.90 | 0.53 |
| 1:B:302:LEU:O | 1:B:327:MSE:HE2 | 2.09 | 0.53 |
| 1:C:164:GLU:HG2 | 1:C:258:ALA:HB2 | 1.90 | 0.53 |
| 1:C:77:SER:O | 1:C:81:ARG:HG3 | 2.07 | 0.53 |
| 1:E:24:LYS:CG | 1:E:25:GLY:N | 2.60 | 0.53 |
| 1:F:227:ARG:NH1 | 1:F:227:ARG:HG3 | 2.23 | 0.53 |
| 1:G:184:LEU:HD22 | 1:G:198:CYS:HB3 | 1.90 | 0.53 |
| 1:G:319:ILE:O | 1:G:323:ILE:HG13 | 2.09 | 0.53 |
| 1:J:177:MSE:HE2 | 1:J:202:MSE:HB2 | 1.90 | 0.53 |
| 1:J:24:LYS:HZ2 | 1:L:24:LYS:CD | 2.21 | 0.53 |
| 1:M:342:TRP:HA | 7:M:2041:HOH:O | 2.08 | 0.53 |
| 1:M:454:LEU:CD1 | 1:M:460:LEU:HG | 2.31 | 0.53 |
| 1:O:123:TYR:HB3 | 1:O:175:TYR:CD2 | 2.44 | 0.53 |
| 1:C:245:ARG:HD3 | 1:C:246:TYR:CE2 | 2.44 | 0.53 |
| 1:C:381:VAL:HG13 | 1:C:407:MSE:HE1 | 1.90 | 0.53 |
| 1:D:136:THR:OG1 | 1:D:221:LEU:HD11 | 2.08 | 0.53 |
| 1:E:162:ASP:C | 1:E:202:MSE:HE1 | 2.29 | 0.53 |
| 1:G:431:GLU:OE2 | 1:G:452:VAL:HG13 | 2.09 | 0.53 |
| 1:I:91:ARG:NH2 | 7:I:2015:HOH:O | 2.40 | 0.53 |
| 1:J:154:VAL:O | 1:J:154:VAL:HG13 | 2.08 | 0.53 |
| 1:J:429:THR:HG22 | 1:J:430:ALA:N | 2.23 | 0.53 |
| 1:J:543:TYR:HA | 1:J:544:PRO:C | 2.30 | 0.53 |
| 1:L:41:THR:HG22 | 1:L:43:GLU:H | 1.74 | 0.53 |
| 1:N:492:LEU:O | 1:N:496:GLU:HG3 | 2.09 | 0.53 |
| 1:A:179:ILE:HB | 1:A:180:PRO:HD3 | 1.90 | 0.53 |
| 1:A:493:THR:O | 1:A:497:VAL:HG23 | 2.08 | 0.53 |
| 1:B:300:ASN:ND2 | 1:B:305:HIS:CE1 | 2.77 | 0.53 |
| 1:E:570:TYR:H | 1:G:46:GLN:HE22 | 1.55 | 0.53 |
| 1:J:24:LYS:HD2 | 1:L:24:LYS:HD2 | 1.91 | 0.53 |
| 1:J:359:THR:HG22 | 1:J:362:LYS:HB2 | 1.91 | 0.53 |
| 1:K:467:ASN:H | 2:K:1581:NAP:H72N | 1.57 | 0.53 |
| 1:L:156:LYS:HD3 | 1:L:479:ILE:HG23 | 1.90 | 0.53 |
| 1:M:24:LYS:HE2 | 1:O:24:LYS:HZ3 | 1.73 | 0.53 |
| 1:O:412:LYS:HB2 | 1:O:412:LYS:HZ2 | 1.69 | 0.53 |
| 1:D:160:VAL:HG11 | 1:D:238:PHE:CE2 | 2.43 | 0.53 |
| 1:D:359:THR:HG21 | 7:D:2029:HOH:O | 2.08 | 0.53 |
| 1:I:404:LEU:HD13 | 1:I:433:LEU:HA | 1.89 | 0.53 |
| 1:I:554:ARG:HH11 | 1:I:554:ARG:HG2 | 1.74 | 0.53 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:402:GLN:H | 1:K:402:GLN:NE2 | 2.06 | 0.53 |
| 1:A:104:ILE:CD1 | 1:A:108:MSE:HE3 | 2.39 | 0.52 |
| 1:A:521:GLN:O | 1:A:525:LYS:HG3 | 2.09 | 0.52 |
| 1:B:38:MSE:HB2 | 1:B:59:LEU:HD11 | 1.91 | 0.52 |
| 1:F:429:THR:HG22 | 1:F:430:ALA:N | 2.24 | 0.52 |
| 1:F:469:TYR:OH | 1:F:516:LEU:HD13 | 2.09 | 0.52 |
| 1:N:252:ILE:HD12 | 1:N:252:ILE:N | 2.24 | 0.52 |
| 1:P:401:GLN:HG3 | 1:P:402:GLN:NE2 | 2.25 | 0.52 |
| 1:A:137:ILE:HA | 1:A:234:LEU:HD22 | 1.92 | 0.52 |
| 1:A:38:MSE:SE | 1:A:55:PRO:HG2 | 2.59 | 0.52 |
| 1:B:474:VAL:O | 1:B:478:VAL:HG23 | 2.10 | 0.52 |
| 1:C:108:MSE:HE1 | 1:C:190:CYS:SG | 2.49 | 0.52 |
| 1:D:245:ARG:HG2 | 1:D:246:TYR:CE2 | 2.44 | 0.52 |
| 1:E:270:ARG:HH12 | 1:E:487:GLY:HA2 | 1.74 | 0.52 |
| 1:E:243:THR:HG21 | 1:E:273:TYR:CD2 | 2.43 | 0.52 |
| 1:K:429:THR:HG22 | 1:K:431:GLU:H | 1.74 | 0.52 |
| 1:O:156:LYS:HE2 | 1:O:197:GLN:CD | 2.30 | 0.52 |
| 1:O:239:MSE:HA | 1:O:239:MSE:CE | 2.37 | 0.52 |
| 1:O:324:VAL:HG12 | 1:O:328:GLN:HE21 | 1.73 | 0.52 |
| 1:B:41:THR:CG2 | 1:B:43:GLU:H | 2.19 | 0.52 |
| 1:D:429:THR:HG22 | 1:D:431:GLU:H | 1.73 | 0.52 |
| 1:G:528:VAL:O | 1:G:532:LYS:HG3 | 2.09 | 0.52 |
| 1:J:202:MSE:HE1 | 1:J:204:ASP:CA | 2.39 | 0.52 |
| 1:J:284:ALA:HA | 1:J:319:ILE:HG12 | 1.91 | 0.52 |
| 1:L:192:GLY:HA3 | 1:L:557:VAL:HG22 | 1.92 | 0.52 |
| 1:N:433:LEU:HG | 1:N:443:PHE:CD1 | 2.45 | 0.52 |
| 1:P:98:LYS:HD3 | 1:P:560:THR:HG21 | 1.90 | 0.52 |
| 1:A:88:LEU:HD13 | 1:A:96:PHE:HA | 1.90 | 0.52 |
| 1:C:108:MSE:HE2 | 1:C:186:LEU:CD1 | 2.40 | 0.52 |
| 1:C:288:VAL:HG12 | 1:C:292:LEU:HD22 | 1.92 | 0.52 |
| 1:C:504:GLU:HG3 | 1:C:508:GLN:NE2 | 2.23 | 0.52 |
| 1:G:223:HIS:HD2 | 1:G:224:LYS:O | 1.92 | 0.52 |
| 1:G:433:LEU:HD12 | 1:G:443:PHE:HB2 | 1.92 | 0.52 |
| 1:G:61:GLN:HE22 | 1:G:98:LYS:HD3 | 1.74 | 0.52 |
| 1:H:329:LYS:NZ | 1:H:496:GLU:OE2 | 2.40 | 0.52 |
| 1:I:29:LEU:HD23 | 1:I:35:ASN:HD22 | 1.73 | 0.52 |
| 1:L:82:TYR:CE2 | 1:L:86:MSE:HG3 | 2.44 | 0.52 |
| 1:N:154:VAL:O | 1:N:154:VAL:HG13 | 2.10 | 0.52 |
| 1:N:343:MSE:O | 1:N:349:LEU:HD12 | 2.10 | 0.52 |
| 1:N:41:THR:HB | 1:N:44:GLU:HG3 | 1.91 | 0.52 |
| 1:O:401:GLN:O | 1:O:405:GLN:HG3 | 2.09 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:528:VAL:HG22 | 1:E:553:ILE:HD12 | 1.90 | 0.52 |
| 1:J:86:MSE:HE1 | 1:J:131:ARG:HH11 | 1.75 | 0.52 |
| 1:J:120:CYS:O | 1:J:175:TYR:HB3 | 2.09 | 0.52 |
| 1:J:429:THR:H | 1:J:432:GLN:CG | 2.23 | 0.52 |
| 1:M:556:GLN:CA | 1:M:556:GLN:HE21 | 2.22 | 0.52 |
| 1:N:160:VAL:HG21 | 1:N:238:PHE:CE2 | 2.44 | 0.52 |
| 1:N:352:LYS:O | 1:N:352:LYS:HG2 | 2.07 | 0.52 |
| 1:P:332:VAL:HG22 | 1:P:336:GLU:HB3 | 1.91 | 0.52 |
| 1:E:209:ASN:OD1 | 1:E:211:THR:HB | 2.09 | 0.52 |
| 1:F:125:LEU:HD13 | 1:F:125:LEU:O | 2.09 | 0.52 |
| 1:F:166:ILE:HG21 | 1:F:172:LEU:HD12 | 1.91 | 0.52 |
| 1:L:327:MSE:HE3 | 1:L:337:ALA:CB | 2.27 | 0.52 |
| 1:L:398:ALA:HB3 | 1:L:427:GLU:HG3 | 1.90 | 0.52 |
| 1:O:207:THR:HA | 1:O:225:ARG:HG2 | 1.92 | 0.52 |
| 1:O:238:PHE:HD2 | 1:O:239:MSE:HE3 | 1.73 | 0.52 |
| 1:A:433:LEU:HD12 | 1:A:434:TYR:CD2 | 2.44 | 0.52 |
| 1:B:108:MSE:N | 1:B:109:PRO:CD | 2.73 | 0.52 |
| 1:B:312:ALA:HB2 | 1:B:343:MSE:HG2 | 1.91 | 0.52 |
| 1:D:108:MSE:CE | 1:D:190:CYS:SG | 2.97 | 0.52 |
| 1:F:319:ILE:O | 1:F:323:ILE:HG13 | 2.10 | 0.52 |
| 1:H:161:THR:HA | 1:H:257:PHE:CE1 | 2.45 | 0.52 |
| 1:H:529:ARG:HG2 | 1:H:529:ARG:NH1 | 2.25 | 0.52 |
| 1:E:324:VAL:O | 1:E:328:GLN:HG3 | 2.10 | 0.52 |
| 1:E:492:LEU:O | 1:E:496:GLU:HG3 | 2.09 | 0.52 |
| 1:G:270:ARG:HH12 | 1:G:487:GLY:HA2 | 1.73 | 0.52 |
| 1:M:243:THR:HG21 | 1:M:273:TYR:HD2 | 1.75 | 0.52 |
| 1:K:330:GLU:O | 1:O:300:ASN:HA | 2.10 | 0.52 |
| 1:O:428:CYS:HA | 1:O:432:GLN:NE2 | 2.25 | 0.52 |
| 1:P:158:ILE:HG23 | 1:P:199:LEU:O | 2.10 | 0.52 |
| 1:B:332:VAL:CG1 | 1:B:336:GLU:HB3 | 2.40 | 0.52 |
| 1:G:288:VAL:CG2 | 1:G:322:LEU:HD12 | 2.40 | 0.52 |
| 1:G:394:ALA:HB2 | 2:G:1581:NAP:O3D | 2.10 | 0.52 |
| 1:H:141:GLY:H | 1:H:237:GLU:CD | 2.13 | 0.52 |
| 1:H:571:THR:HG23 | 7:H:2075:HOH:O | 2.09 | 0.52 |
| 1:I:238:PHE:CE2 | 1:I:239:MSE:HE3 | 2.45 | 0.52 |
| 1:I:536:ARG:HD2 | 7:I:2069:HOH:O | 2.09 | 0.52 |
| 1:J:41:THR:HG22 | 1:J:43:GLU:N | 2.24 | 0.52 |
| 1:N:352:LYS:O | 1:N:352:LYS:CG | 2.58 | 0.52 |
| 1:N:72:PHE:CE2 | 1:N:81:ARG:HD3 | 2.45 | 0.52 |
| 1:O:166:ILE:HD12 | 1:O:179:ILE:HG13 | 1.91 | 0.52 |
| 1:A:284:ALA:HA | 1:A:319:ILE:HG12 | 1.92 | 0.52 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:59:LEU:H | 1:B:59:LEU:HD12 | 1.74 | 0.52 |
| 1:I:284:ALA:HA | 1:I:319:ILE:HG12 | 1.91 | 0.52 |
| 1:I:38:MSE:HB2 | 1:I:59:LEU:HD11 | 1.92 | 0.52 |
| 1:J:317:LEU:HD23 | 1:J:343:MSE:HE1 | 1.92 | 0.52 |
| 1:K:136:THR:HG22 | 1:K:139:ASP:CG | 2.30 | 0.52 |
| 1:M:138:HIS:NE2 | 1:M:223:HIS:HE1 | 2.08 | 0.52 |
| 1:M:35:ASN:ND2 | 1:M:37:GLY:H | 2.07 | 0.52 |
| 1:O:407:MSE:HG2 | 1:O:416:ILE:HD11 | 1.91 | 0.52 |
| 1:C:35:ASN:ND2 | 1:C:37:GLY:H | 2.08 | 0.51 |
| 1:H:429:THR:H | 1:H:432:GLN:NE2 | 2.07 | 0.51 |
| 1:I:320:ALA:O | 1:I:324:VAL:HG23 | 2.10 | 0.51 |
| 1:I:467:ASN:N | 2:I:1581:NAP:H72N | 2.09 | 0.51 |
| 1:J:245:ARG:HG2 | 1:J:246:TYR:CD2 | 2.45 | 0.51 |
| 1:I:222:ARG:HD2 | 1:L:580:LYS:HE2 | 1.92 | 0.51 |
| 1:M:468:SER:HA | 1:M:471:PHE:CE2 | 2.45 | 0.51 |
| 1:N:112:TYR:CE2 | 1:N:468:SER:OG | 2.63 | 0.51 |
| 1:O:41:THR:HG22 | 1:O:42:LEU:N | 2.25 | 0.51 |
| 1:O:429:THR:HG22 | 1:O:430:ALA:N | 2.25 | 0.51 |
| 1:P:155:ILE:HB | 1:P:246:TYR:CD2 | 2.46 | 0.51 |
| 1:A:416:ILE:HG13 | 1:A:433:LEU:CD2 | 2.39 | 0.51 |
| 1:B:145:THR:O | 1:B:148:GLN:HG2 | 2.10 | 0.51 |
| 1:B:352:LYS:CE | 1:B:353:GLY:H | 2.20 | 0.51 |
| 1:C:152:GLU:HB3 | 1:C:155:ILE:CD1 | 2.40 | 0.51 |
| 1:F:75:LEU:HD11 | 1:F:84:LEU:HD22 | 1.92 | 0.51 |
| 1:G:92:ASN:C | 1:G:92:ASN:HD22 | 2.12 | 0.51 |
| 1:H:529:ARG:HD3 | 7:H:2068:HOH:O | 2.09 | 0.51 |
| 1:I:377:LEU:O | 1:I:381:VAL:HG23 | 2.11 | 0.51 |
| 1:J:461:TYR:HD1 | 1:J:509:GLU:HG2 | 1.75 | 0.51 |
| 1:K:381:VAL:HG11 | 1:K:407:MSE:CE | 2.41 | 0.51 |
| 1:N:162:ASP:O | 1:N:225:ARG:NH2 | 2.33 | 0.51 |
| 1:B:429:THR:H | 1:B:432:GLN:CG | 2.23 | 0.51 |
| 1:F:416:ILE:HG13 | 1:F:433:LEU:CD2 | 2.36 | 0.51 |
| 1:F:431:GLU:OE2 | 1:F:452:VAL:HG22 | 2.10 | 0.51 |
| 1:H:284:ALA:HA | 1:H:319:ILE:HG12 | 1.92 | 0.51 |
| 1:J:96:PHE:CZ | 1:J:100:LEU:HD11 | 2.44 | 0.51 |
| 1:J:556:GLN:NE2 | 1:J:556:GLN:N | 2.57 | 0.51 |
| 1:O:158:ILE:HG22 | 1:O:160:VAL:HG23 | 1.91 | 0.51 |
| 1:O:65:VAL:HG13 | 1:O:99:VAL:HG22 | 1.91 | 0.51 |
| 1:C:251:LEU:C | 1:C:252:ILE:HD12 | 2.31 | 0.51 |
| 1:C:401:GLN:NE2 | 1:C:436:TYR:CE1 | 2.78 | 0.51 |
| 1:C:533:GLU:HA | 1:C:536:ARG:HH11 | 1.74 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:381:VAL:HG13 | 1:F:407:MSE:HE1 | 1.92 | 0.51 |
| 1:I:300:ASN:OD1 | 1:I:305:HIS:HE1 | 1.92 | 0.51 |
| 1:J:303:SER:CB | 1:J:332:VAL:HG21 | 2.41 | 0.51 |
| 1:K:454:LEU:HB3 | 1:K:455:PRO:HD2 | 1.90 | 0.51 |
| 1:L:136:THR:CG2 | 1:L:137:ILE:N | 2.73 | 0.51 |
| 1:M:429:THR:HG22 | 1:M:430:ALA:N | 2.25 | 0.51 |
| 1:M:98:LYS:HD3 | 1:M:560:THR:HG23 | 1.91 | 0.51 |
| 1:N:215:ASP:O | 1:N:222:ARG:NH2 | 2.43 | 0.51 |
| 1:B:354:ARG:HD2 | 1:B:356:ALA:O | 2.10 | 0.51 |
| 1:C:543:TYR:HA | 1:C:544:PRO:C | 2.31 | 0.51 |
| 1:G:433:LEU:O | 1:G:437:THR:HG23 | 2.10 | 0.51 |
| 1:H:361:GLU:O | 1:H:364:HIS:HB2 | 2.11 | 0.51 |
| 1:I:288:VAL:HG21 | 1:I:322:LEU:HB3 | 1.93 | 0.51 |
| 1:J:388:VAL:HG22 | 1:J:415:ILE:HB | 1.93 | 0.51 |
| 1:K:136:THR:OG1 | 1:K:221:LEU:HD11 | 2.10 | 0.51 |
| 1:M:125:LEU:N | 5:M:1591:CL:CL | 2.81 | 0.51 |
| 1:M:179:ILE:HB | 1:M:180:PRO:HD3 | 1.92 | 0.51 |
| 1:O:42:LEU:C | 1:O:42:LEU:HD23 | 2.30 | 0.51 |
| 1:A:350:ILE:CD1 | 1:A:362:LYS:HD2 | 2.41 | 0.51 |
| 1:B:238:PHE:O | 1:B:242:VAL:HG23 | 2.11 | 0.51 |
| 1:C:431:GLU:HG3 | 7:C:2052:HOH:O | 2.11 | 0.51 |
| 1:D:141:GLY:H | 1:D:237:GLU:CD | 2.13 | 0.51 |
| 1:D:150:TRP:CE2 | 1:D:199:LEU:HD13 | 2.46 | 0.51 |
| 1:E:133:LEU:HB2 | 1:E:199:LEU:HD11 | 1.92 | 0.51 |
| 1:E:44:GLU:O | 1:E:48:LEU:HB2 | 2.11 | 0.51 |
| 1:E:92:ASN:C | 1:E:92:ASN:HD22 | 2.13 | 0.51 |
| 1:F:401:GLN:HG2 | 1:F:436:TYR:CE1 | 2.45 | 0.51 |
| 1:G:136:THR:HB | 1:G:139:ASP:OD2 | 2.10 | 0.51 |
| 1:I:92:ASN:C | 1:I:92:ASN:ND2 | 2.62 | 0.51 |
| 1:J:529:ARG:HG2 | 1:J:529:ARG:HH11 | 1.76 | 0.51 |
| 1:L:174:CYS:HA | 1:L:202:MSE:HE3 | 1.91 | 0.51 |
| 1:L:140:ARG:NH2 | 1:L:230:ALA:HA | 2.25 | 0.51 |
| 1:L:301:ARG:HB3 | 1:L:330:GLU:OE1 | 2.11 | 0.51 |
| 1:M:454:LEU:HB3 | 1:M:455:PRO:HD2 | 1.93 | 0.51 |
| 1:B:113:THR:HG22 | 1:B:114:PRO:HA | 1.92 | 0.51 |
| 1:D:171:ASP:OD2 | 1:D:225:ARG:HD2 | 2.11 | 0.51 |
| 1:D:319:ILE:O | 1:D:323:ILE:HG13 | 2.10 | 0.51 |
| 1:E:160:VAL:HG12 | 1:E:201:VAL:CB | 2.39 | 0.51 |
| 1:F:223:HIS:HD2 | 1:F:224:LYS:O | 1.93 | 0.51 |
| 1:F:322:LEU:HD11 | 1:F:492:LEU:HA | 1.93 | 0.51 |
| 1:L:190:CYS:HB3 | 1:L:519:ILE:HD13 | 1.93 | 0.51 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:140:ARG:HH11 | 1:N:140:ARG:HB3 | 1.74 | 0.51 |
| 1:N:136:THR:CG2 | 1:N:221:LEU:HD11 | 2.36 | 0.51 |
| 1:N:88:LEU:HD22 | 1:N:96:PHE:HB2 | 1.93 | 0.51 |
| 1:A:319:ILE:O | 1:A:323:ILE:HG13 | 2.11 | 0.51 |
| 1:B:117:GLY:O | 1:B:121:GLN:HG3 | 2.11 | 0.51 |
| 1:B:429:THR:HG22 | 1:B:430:ALA:N | 2.26 | 0.51 |
| 1:D:554:ARG:HH11 | 1:D:554:ARG:HG2 | 1.76 | 0.51 |
| 1:D:92:ASN:ND2 | 1:D:95:LEU:H | 2.08 | 0.51 |
| 1:E:399:PHE:HB2 | 1:E:428:CYS:HB3 | 1.93 | 0.51 |
| 1:H:78:ASP:N | 1:H:81:ARG:NH1 | 2.58 | 0.51 |
| 1:I:536:ARG:CD | 7:I:2069:HOH:O | 2.58 | 0.51 |
| 1:L:166:ILE:HG21 | 1:L:172:LEU:HD12 | 1.93 | 0.51 |
| 1:P:160:VAL:HG12 | 1:P:161:THR:N | 2.26 | 0.51 |
| 1:E:132:GLY:HA2 | 1:E:200:PRO:HG2 | 1.93 | 0.51 |
| 1:E:270:ARG:NH2 | 1:E:281:GLN:NE2 | 2.59 | 0.51 |
| 1:F:166:ILE:HD12 | 1:F:179:ILE:CG1 | 2.40 | 0.51 |
| 1:F:429:THR:H | 1:F:432:GLN:HE21 | 1.56 | 0.51 |
| 1:G:42:LEU:O | 1:G:46:GLN:HG3 | 2.10 | 0.51 |
| 1:H:214:LYS:NZ | 1:H:214:LYS:HB2 | 2.26 | 0.51 |
| 1:H:270:ARG:HH12 | 1:H:487:GLY:HA2 | 1.76 | 0.51 |
| 1:I:36:LYS:HD2 | 1:I:562:TYR:CG | 2.46 | 0.51 |
| 1:P:476:LEU:HB3 | 1:P:527:ALA:HB2 | 1.93 | 0.51 |
| 1:P:36:LYS:HE2 | 1:P:562:TYR:HB3 | 1.93 | 0.51 |
| 1:A:207:THR:HA | 1:A:225:ARG:HH11 | 1.76 | 0.51 |
| 1:A:31:ASP:HA | 1:B:30:ARG:NH1 | 2.26 | 0.51 |
| 1:A:391:GLY:HA3 | 1:A:427:GLU:HG2 | 1.92 | 0.51 |
| 1:D:166:ILE:HD12 | 1:D:179:ILE:HG13 | 1.93 | 0.51 |
| 1:D:431:GLU:OE2 | 1:D:452:VAL:HG13 | 2.10 | 0.51 |
| 1:G:314:GLU:HB2 | 2:G:1581:NAP:O1N | 2.10 | 0.51 |
| 1:G:476:LEU:HB3 | 1:G:527:ALA:HB2 | 1.93 | 0.51 |
| 1:I:136:THR:HB | 1:I:139:ASP:OD2 | 2.11 | 0.51 |
| 1:J:502:VAL:HG12 | 1:J:507:LEU:CD2 | 2.39 | 0.51 |
| 1:K:41:THR:O | 1:K:45:ARG:HG3 | 2.11 | 0.51 |
| 1:L:454:LEU:HD21 | 1:L:460:LEU:CG | 2.41 | 0.51 |
| 1:N:401:GLN:HG2 | 1:N:436:TYR:CE2 | 2.46 | 0.51 |
| 1:N:59:LEU:C | 1:N:59:LEU:HD12 | 2.32 | 0.51 |
| 1:C:433:LEU:HG | 1:C:443:PHE:HD1 | 1.76 | 0.50 |
| 1:E:404:LEU:HD13 | 1:E:433:LEU:HA | 1.93 | 0.50 |
| 1:H:140:ARG:NH1 | 1:H:230:ALA:HA | 2.26 | 0.50 |
| 1:K:342:TRP:CH2 | 1:K:367:HIS:HB2 | 2.46 | 0.50 |
| 1:A:401:GLN:HG2 | 1:A:436:TYR:CE1 | 2.46 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:416:ILE:CG1 | 1:A:433:LEU:HD21 | 2.40 | 0.50 |
| 1:C:467:ASN:H | 2:C:1581:NAP:H72N | 1.59 | 0.50 |
| 1:C:556:GLN:HE21 | 1:C:556:GLN:N | 2.09 | 0.50 |
| 1:C:61:GLN:NE2 | 1:C:98:LYS:HD2 | 2.27 | 0.50 |
| 1:F:238:PHE:CE2 | 1:F:239:MSE:HE3 | 2.45 | 0.50 |
| 1:F:553:ILE:O | 1:F:557:VAL:HG23 | 2.11 | 0.50 |
| 1:I:270:ARG:NH1 | 5:I:1588:CL:CL | 2.81 | 0.50 |
| 1:I:543:TYR:HA | 1:I:544:PRO:C | 2.32 | 0.50 |
| 1:J:270:ARG:HG2 | 1:J:270:ARG:NH1 | 2.25 | 0.50 |
| 1:J:378:GLU:HA | 1:J:403:ILE:HD13 | 1.92 | 0.50 |
| 1:N:210:GLU:OE2 | 1:N:224:LYS:HE2 | 2.12 | 0.50 |
| 1:N:288:VAL:O | 1:N:292:LEU:HD13 | 2.12 | 0.50 |
| 1:N:86:MSE:HE2 | 7:N:2024:HOH:O | 2.11 | 0.50 |
| 1:P:162:ASP:C | 1:P:202:MSE:HE1 | 2.31 | 0.50 |
| 1:P:327:MSE:HE1 | 1:P:337:ALA:O | 2.11 | 0.50 |
| 1:A:108:MSE:HE2 | 1:A:190:CYS:SG | 2.51 | 0.50 |
| 1:A:90:ASP:OD1 | 1:A:131:ARG:NH1 | 2.44 | 0.50 |
| 1:A:283:THR:CG2 | 1:A:284:ALA:N | 2.74 | 0.50 |
| 1:C:41:THR:HB | 1:C:44:GLU:HG3 | 1.92 | 0.50 |
| 1:D:314:GLU:HB2 | 2:D:1581:NAP:O1N | 2.11 | 0.50 |
| 1:D:378:GLU:OE1 | 1:D:382:LYS:HE3 | 2.11 | 0.50 |
| 1:F:166:ILE:HD12 | 1:F:179:ILE:HG13 | 1.93 | 0.50 |
| 1:H:351:VAL:CG1 | 1:H:369:HIS:HB3 | 2.41 | 0.50 |
| 1:I:104:ILE:HG13 | 1:I:108:MSE:HE3 | 1.93 | 0.50 |
| 1:I:389:LEU:HD12 | 1:I:407:MSE:HE3 | 1.93 | 0.50 |
| 1:K:264:ARG:HH11 | 1:K:264:ARG:HG2 | 1.76 | 0.50 |
| 1:M:140:ARG:HG3 | 1:M:234:LEU:HD13 | 1.92 | 0.50 |
| 1:O:243:THR:HG21 | 1:O:273:TYR:CD2 | 2.46 | 0.50 |
| 1:O:429:THR:H | 1:O:432:GLN:NE2 | 2.10 | 0.50 |
| 1:C:38:MSE:CB | 1:C:59:LEU:HD11 | 2.39 | 0.50 |
| 1:H:467:ASN:HB3 | 1:H:471:PHE:HD2 | 1.76 | 0.50 |
| 1:I:152:GLU:CD | 1:I:196:HIS:NE2 | 2.65 | 0.50 |
| 1:L:127:PHE:O | 1:L:128:ARG:NH1 | 2.42 | 0.50 |
| 1:L:354:ARG:HH21 | 1:L:358:LEU:HD22 | 1.77 | 0.50 |
| 1:M:61:GLN:HA | 1:M:64:GLN:HE21 | 1.75 | 0.50 |
| 1:N:188:THR:HG21 | 1:N:195:PRO:HG3 | 1.92 | 0.50 |
| 1:N:347:LYS:HD3 | 1:N:357:SER:HB2 | 1.93 | 0.50 |
| 1:P:120:CYS:O | 1:P:175:TYR:HB3 | 2.10 | 0.50 |
| 1:P:364:HIS:HB2 | 7:P:2053:HOH:O | 2.11 | 0.50 |
| 1:P:41:THR:HB | 1:P:44:GLU:HG3 | 1.94 | 0.50 |
| 1:A:324:VAL:HG12 | 1:A:328:GLN:NE2 | 2.25 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:429:THR:H | 1:B:432:GLN:NE2 | 2.09 | 0.50 |
| 1:C:536:ARG:NE | 1:H:333:SER:CB | 2.74 | 0.50 |
| 1:D:61:GLN:HA | 1:D:64:GLN:HE21 | 1.76 | 0.50 |
| 1:E:24:LYS:HG2 | 1:E:25:GLY:H | 1.68 | 0.50 |
| 1:E:502:VAL:CG1 | 1:E:507:LEU:HD22 | 2.41 | 0.50 |
| 1:G:108:MSE:N | 1:G:109:PRO:CD | 2.75 | 0.50 |
| 1:K:492:LEU:O | 1:K:496:GLU:HG3 | 2.11 | 0.50 |
| 1:M:133:LEU:HB2 | 1:M:199:LEU:HD11 | 1.93 | 0.50 |
| 1:M:572:TRP:HA | 7:M:2077:HOH:O | 2.11 | 0.50 |
| 1:A:133:LEU:HD22 | 1:A:135:ILE:HG13 | 1.93 | 0.50 |
| 1:A:386:PRO:O | 1:A:407:MSE:HE3 | 2.12 | 0.50 |
| 1:E:168:GLY:O | 1:E:425:LYS:HE2 | 2.12 | 0.50 |
| 1:H:92:ASN:C | 1:H:92:ASN:ND2 | 2.58 | 0.50 |
| 1:J:466:ASN:HA | 2:J:1581:NAP:N7N | 2.17 | 0.50 |
| 1:K:352:LYS:NZ | 1:K:352:LYS:HB3 | 2.27 | 0.50 |
| 1:O:332:VAL:HG22 | 1:O:336:GLU:HB2 | 1.93 | 0.50 |
| 1:B:205:VAL:HG22 | 7:B:2016:HOH:O | 2.10 | 0.50 |
| 1:B:288:VAL:HG12 | 1:B:292:LEU:HD22 | 1.94 | 0.50 |
| 1:D:359:THR:HG22 | 1:D:361:GLU:N | 2.21 | 0.50 |
| 1:D:399:PHE:HB2 | 1:D:428:CYS:HB3 | 1.92 | 0.50 |
| 1:E:71:ASN:HB3 | 1:E:84:LEU:HD11 | 1.93 | 0.50 |
| 1:G:227:ARG:NH1 | 1:G:227:ARG:HG3 | 2.25 | 0.50 |
| 1:G:359:THR:HG22 | 1:G:361:GLU:N | 2.23 | 0.50 |
| 1:H:137:ILE:HD13 | 1:H:226:ILE:HB | 1.93 | 0.50 |
| 1:I:61:GLN:O | 1:I:65:VAL:HG23 | 2.12 | 0.50 |
| 1:K:406:ASP:O | 1:K:409:ALA:HB3 | 2.11 | 0.50 |
| 1:M:502:VAL:HG11 | 1:M:507:LEU:HD13 | 1.93 | 0.50 |
| 1:M:532:LYS:HG2 | 1:M:549:LEU:HD12 | 1.93 | 0.50 |
| 1:P:58:PHE:N | 5:P:1591:CL:CL | 2.65 | 0.50 |
| 1:A:543:TYR:HA | 1:A:544:PRO:C | 2.32 | 0.50 |
| 1:B:285:SER:HB3 | 1:B:470:VAL:HG21 | 1.92 | 0.50 |
| 1:D:165:ARG:HD2 | 1:D:165:ARG:O | 2.10 | 0.50 |
| 1:E:177:MSE:O | 1:E:180:PRO:HD2 | 2.12 | 0.50 |
| 1:F:270:ARG:HH11 | 1:F:270:ARG:HG2 | 1.77 | 0.50 |
| 1:H:140:ARG:HH12 | 1:H:230:ALA:CB | 2.25 | 0.50 |
| 1:H:429:THR:CG2 | 1:H:430:ALA:N | 2.75 | 0.50 |
| 1:J:261:ASN:HA | 1:J:264:ARG:NH1 | 2.27 | 0.50 |
| 1:K:64:GLN:NE2 | 1:K:562:TYR:OH | 2.42 | 0.50 |
| 1:K:92:ASN:C | 1:K:92:ASN:HD22 | 2.15 | 0.50 |
| 1:L:504:GLU:O | 1:L:508:GLN:HG3 | 2.12 | 0.50 |
| 1:P:92:ASN:ND2 | 1:P:92:ASN:C | 2.61 | 0.50 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:533:GLU:HG3 | 1:B:537:ASN:HD21 | 1.77 | 0.50 |
| 1:D:137:ILE:HA | 1:D:234:LEU:HD22 | 1.93 | 0.50 |
| 1:E:183:LYS:HE3 | 1:E:255:GLU:CD | 2.32 | 0.50 |
| 1:F:132:GLY:HA2 | 1:F:200:PRO:HG2 | 1.94 | 0.50 |
| 1:F:136:THR:HG22 | 1:F:137:ILE:N | 2.27 | 0.50 |
| 1:F:575:GLU:O | 1:F:578:LYS:HG2 | 2.11 | 0.50 |
| 1:I:502:VAL:CG2 | 1:I:514:PRO:HD3 | 2.42 | 0.50 |
| 1:I:533:GLU:CD | 1:I:536:ARG:NH1 | 2.65 | 0.50 |
| 1:M:98:LYS:HD3 | 1:M:560:THR:HG21 | 1.93 | 0.50 |
| 1:N:260:ALA:O | 1:N:264:ARG:HG2 | 2.12 | 0.50 |
| 1:P:350:ILE:HD13 | 1:P:362:LYS:HB3 | 1.94 | 0.50 |
| 1:C:138:HIS:NE2 | 1:C:223:HIS:HE1 | 2.10 | 0.49 |
| 1:C:433:LEU:HD12 | 1:C:443:PHE:HB2 | 1.93 | 0.49 |
| 1:C:322:LEU:HD22 | 1:C:492:LEU:HD13 | 1.93 | 0.49 |
| 1:D:136:THR:O | 1:D:139:ASP:OD2 | 2.29 | 0.49 |
| 1:D:61:GLN:HE21 | 1:D:98:LYS:HE2 | 1.77 | 0.49 |
| 1:K:303:SER:HB3 | 1:K:332:VAL:HG21 | 1.94 | 0.49 |
| 1:P:243:THR:HG21 | 1:P:273:TYR:CD2 | 2.47 | 0.49 |
| 1:P:381:VAL:CG1 | 1:P:407:MSE:HE1 | 2.42 | 0.49 |
| 1:B:131:ARG:HD3 | 1:B:181:VAL:HG13 | 1.94 | 0.49 |
| 1:C:328:GLN:HA | 1:C:332:VAL:O | 2.12 | 0.49 |
| 1:H:184:LEU:HD22 | 1:H:198:CYS:HB3 | 1.92 | 0.49 |
| 1:I:319:ILE:O | 1:I:323:ILE:HG13 | 2.11 | 0.49 |
| 1:J:24:LYS:NZ | 1:L:24:LYS:CD | 2.75 | 0.49 |
| 1:L:160:VAL:HG21 | 1:L:238:PHE:CE2 | 2.47 | 0.49 |
| 1:L:90:ASP:OD1 | 1:L:131:ARG:NH1 | 2.45 | 0.49 |
| 1:M:351:VAL:O | 1:M:354:ARG:HB2 | 2.12 | 0.49 |
| 1:N:24:LYS:HD2 | 1:N:24:LYS:N | 2.27 | 0.49 |
| 1:N:376:ASN:O | 1:N:380:ILE:HG13 | 2.11 | 0.49 |
| 1:P:108:MSE:HB3 | 1:P:109:PRO:HD3 | 1.94 | 0.49 |
| 1:A:378:GLU:HA | 1:A:403:ILE:CD1 | 2.42 | 0.49 |
| 1:A:389:LEU:HD22 | 1:A:399:PHE:CZ | 2.48 | 0.49 |
| 1:D:301:ARG:HB3 | 1:D:330:GLU:OE1 | 2.13 | 0.49 |
| 1:E:429:THR:HB | 1:E:432:GLN:HG3 | 1.94 | 0.49 |
| 1:H:222:ARG:NH1 | 1:H:222:ARG:HG3 | 2.26 | 0.49 |
| 1:H:323:ILE:HG22 | 1:H:327:MSE:HE2 | 1.94 | 0.49 |
| 1:J:77:SER:O | 1:J:81:ARG:HG3 | 2.12 | 0.49 |
| 1:L:183:LYS:HE3 | 1:L:255:GLU:CD | 2.32 | 0.49 |
| 1:M:148:GLN:CG | 1:M:245:ARG:HH21 | 2.22 | 0.49 |
| 1:M:242:VAL:HG13 | 1:M:246:TYR:HD1 | 1.78 | 0.49 |
| 1:M:578:LYS:HZ2 | 1:M:580:LYS:N | 2.10 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:381:VAL:CG1 | 1:O:407:MSE:HE1 | 2.40 | 0.49 |
| 1:B:428:CYS:HA | 1:B:432:GLN:NE2 | 2.27 | 0.49 |
| 1:C:533:GLU:CD | 1:C:536:ARG:NH1 | 2.66 | 0.49 |
| 1:E:165:ARG:HD2 | 1:E:165:ARG:O | 2.11 | 0.49 |
| 1:I:136:THR:CG2 | 1:I:137:ILE:N | 2.75 | 0.49 |
| 1:K:131:ARG:NH1 | 7:K:2013:HOH:O | 2.45 | 0.49 |
| 1:P:164:GLU:HG2 | 1:P:258:ALA:HB2 | 1.94 | 0.49 |
| 1:P:202:MSE:CE | 1:P:203:LEU:C | 2.81 | 0.49 |
| 1:P:500:GLN:HE21 | 1:P:500:GLN:CA | 2.25 | 0.49 |
| 1:A:279:ASP:O | 1:A:283:THR:HG21 | 2.13 | 0.49 |
| 1:C:72:PHE:CZ | 1:C:81:ARG:HD3 | 2.47 | 0.49 |
| 1:D:467:ASN:ND2 | 3:D:1582:OXL:O2 | 2.46 | 0.49 |
| 1:F:238:PHE:O | 1:F:242:VAL:HG22 | 2.13 | 0.49 |
| 1:F:429:THR:HG22 | 1:F:431:GLU:H | 1.77 | 0.49 |
| 1:I:274:CYS:SG | 1:I:478:VAL:HG11 | 2.53 | 0.49 |
| 1:O:302:LEU:HD22 | 1:O:327:MSE:HG3 | 1.93 | 0.49 |
| 1:O:340:ARG:HH11 | 1:O:340:ARG:HG2 | 1.77 | 0.49 |
| 1:P:202:MSE:CE | 1:P:203:LEU:O | 2.59 | 0.49 |
| 1:A:184:LEU:O | 1:A:187:TYR:HB2 | 2.13 | 0.49 |
| 1:D:61:GLN:HE21 | 1:D:98:LYS:CE | 2.25 | 0.49 |
| 1:E:177:MSE:HE2 | 1:E:202:MSE:HB3 | 1.93 | 0.49 |
| 1:H:152:GLU:OE1 | 1:H:196:HIS:O | 2.31 | 0.49 |
| 1:H:260:ALA:O | 1:H:264:ARG:HG2 | 2.12 | 0.49 |
| 1:I:141:GLY:H | 1:I:237:GLU:CD | 2.16 | 0.49 |
| 1:I:61:GLN:HE22 | 1:I:560:THR:HG23 | 1.78 | 0.49 |
| 1:K:154:VAL:CG1 | 1:K:154:VAL:O | 2.60 | 0.49 |
| 1:K:578:LYS:HE2 | 1:K:580:LYS:HB2 | 1.95 | 0.49 |
| 1:L:140:ARG:CD | 7:L:2032:HOH:O | 2.59 | 0.49 |
| 1:N:317:LEU:HD23 | 1:N:343:MSE:HE1 | 1.94 | 0.49 |
| 1:O:572:TRP:O | 1:O:573:PRO:O | 2.31 | 0.49 |
| 1:A:359:THR:CG2 | 1:A:362:LYS:HE2 | 2.37 | 0.49 |
| 1:B:64:GLN:HB3 | 1:B:95:LEU:HD21 | 1.93 | 0.49 |
| 1:C:429:THR:CG2 | 1:C:430:ALA:N | 2.74 | 0.49 |
| 1:F:222:ARG:HD2 | 1:G:578:LYS:NZ | 2.28 | 0.49 |
| 1:F:299:LYS:HZ3 | 1:F:299:LYS:HB3 | 1.73 | 0.49 |
| 1:G:164:GLU:CG | 1:G:258:ALA:HB2 | 2.33 | 0.49 |
| 1:J:147:LEU:HB3 | 1:J:245:ARG:HD2 | 1.95 | 0.49 |
| 1:B:223:HIS:HD2 | 1:B:224:LYS:O | 1.95 | 0.49 |
| 1:B:350:ILE:HD13 | 1:B:362:LYS:HB3 | 1.95 | 0.49 |
| 1:E:358:LEU:HD23 | 1:E:363:GLU:HG2 | 1.94 | 0.49 |
| 1:F:442:ILE:CG2 | 1:F:512:LEU:HD21 | 2.42 | 0.49 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:404:LEU:HD22 | 1:G:433:LEU:HD23 | 1.94 | 0.49 |
| 1:J:125:LEU:C | 1:J:125:LEU:HD23 | 2.32 | 0.49 |
| 1:K:433:LEU:C | 1:K:433:LEU:HD13 | 2.33 | 0.49 |
| 1:L:352:LYS:HG2 | 1:L:366:ALA:O | 2.12 | 0.49 |
| 1:N:250:CYS:O | 1:N:252:ILE:HD12 | 2.12 | 0.49 |
| 1:O:300:ASN:HB2 | 1:O:304:ASP:OD2 | 2.12 | 0.49 |
| 1:P:270:ARG:HH12 | 1:P:487:GLY:HA2 | 1.77 | 0.49 |
| 1:D:152:GLU:OE1 | 1:D:196:HIS:CE1 | 2.66 | 0.49 |
| 1:D:160:VAL:CG1 | 1:D:201:VAL:HB | 2.22 | 0.49 |
| 1:H:132:GLY:HA2 | 1:H:200:PRO:HG2 | 1.95 | 0.49 |
| 1:H:133:LEU:HB2 | 1:H:199:LEU:HD11 | 1.95 | 0.49 |
| 1:H:361:GLU:N | 1:H:361:GLU:OE1 | 2.45 | 0.49 |
| 1:I:406:ASP:HB3 | 1:I:410:PHE:CZ | 2.47 | 0.49 |
| 1:J:108:MSE:HB3 | 1:J:109:PRO:HD3 | 1.95 | 0.49 |
| 1:J:166:ILE:HG21 | 1:J:172:LEU:HD12 | 1.95 | 0.49 |
| 1:J:354:ARG:HB3 | 1:J:358:LEU:CD2 | 2.40 | 0.49 |
| 1:M:470:VAL:HG13 | 1:M:494:THR:HG21 | 1.95 | 0.49 |
| 1:N:207:THR:HA | 1:N:225:ARG:HG2 | 1.94 | 0.49 |
| 1:B:154:VAL:O | 1:B:154:VAL:HG13 | 2.12 | 0.49 |
| 1:B:413:ARG:HH11 | 1:B:413:ARG:HG3 | 1.78 | 0.49 |
| 1:D:107:PHE:O | 1:D:111:VAL:HG12 | 2.13 | 0.49 |
| 1:D:361:GLU:O | 1:D:364:HIS:HB2 | 2.13 | 0.49 |
| 1:G:254:PHE:CE2 | 1:G:265:LEU:HD13 | 2.48 | 0.49 |
| 1:I:359:THR:HG22 | 1:I:362:LYS:CG | 2.43 | 0.49 |
| 1:I:492:LEU:O | 1:I:496:GLU:HG3 | 2.12 | 0.49 |
| 1:K:575:GLU:HG2 | 1:K:576:ALA:N | 2.28 | 0.49 |
| 1:L:543:TYR:HA | 1:L:544:PRO:C | 2.33 | 0.49 |
| 1:M:165:ARG:O | 1:M:165:ARG:HD2 | 2.13 | 0.49 |
| 1:N:61:GLN:HG2 | 1:N:562:TYR:CE1 | 2.47 | 0.49 |
| 1:N:61:GLN:HE21 | 1:N:98:LYS:HE2 | 1.76 | 0.49 |
| 1:P:319:ILE:O | 1:P:323:ILE:HG13 | 2.13 | 0.49 |
| 1:A:92:ASN:OD1 | 1:A:95:LEU:HB2 | 2.12 | 0.48 |
| 1:B:92:ASN:C | 1:B:92:ASN:HD22 | 2.15 | 0.48 |
| 1:D:172:LEU:O | 1:D:175:TYR:HB2 | 2.13 | 0.48 |
| 1:E:401:GLN:HG2 | 1:E:436:TYR:CE2 | 2.48 | 0.48 |
| 1:F:239:MSE:HE1 | 1:F:252:ILE:HG21 | 1.94 | 0.48 |
| 1:G:232:ASP:OD1 | 1:G:264:ARG:NH2 | 2.40 | 0.48 |
| 1:G:243:THR:CG2 | 1:G:248:MSE:HA | 2.42 | 0.48 |
| 1:H:416:ILE:HG13 | 1:H:433:LEU:CD2 | 2.37 | 0.48 |
| 1:G:220:GLY:HA2 | 1:H:56:PRO:HG2 | 1.95 | 0.48 |
| 1:I:533:GLU:OE2 | 1:I:536:ARG:NH1 | 2.46 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:172:LEU:O | 1:J:175:TYR:HB2 | 2.13 | 0.48 |
| 1:K:467:ASN:ND2 | 3:K:1582:OXL:O2 | 2.46 | 0.48 |
| 1:L:327:MSE:HE1 | 1:L:337:ALA:O | 2.12 | 0.48 |
| 1:O:250:CYS:O | 1:O:252:ILE:HD12 | 2.13 | 0.48 |
| 1:O:48:LEU:HD11 | 1:O:565:PHE:HB3 | 1.95 | 0.48 |
| 1:P:284:ALA:HB1 | 1:P:322:LEU:HB2 | 1.95 | 0.48 |
| 1:P:428:CYS:HB2 | 1:P:432:GLN:HE21 | 1.77 | 0.48 |
| 1:C:59:LEU:HD12 | 1:C:59:LEU:H | 1.77 | 0.48 |
| 1:F:575:GLU:HG3 | 1:F:575:GLU:H | 1.42 | 0.48 |
| 1:G:408:ALA:HB1 | 1:G:440:ARG:NH2 | 2.28 | 0.48 |
| 1:H:171:ASP:OD2 | 1:H:225:ARG:NH1 | 2.45 | 0.48 |
| 1:H:467:ASN:HB3 | 1:H:471:PHE:CD2 | 2.47 | 0.48 |
| 1:I:166:ILE:HA | 1:I:256:ASP:OD1 | 2.13 | 0.48 |
| 1:J:150:TRP:CE2 | 1:J:199:LEU:HD13 | 2.48 | 0.48 |
| 1:J:429:THR:H | 1:J:432:GLN:HG3 | 1.78 | 0.48 |
| 1:J:66:TYR:O | 1:J:70:LYS:HG2 | 2.13 | 0.48 |
| 1:L:251:LEU:C | 1:L:252:ILE:HD12 | 2.34 | 0.48 |
| 1:M:163:GLY:HA2 | 1:M:166:ILE:HD11 | 1.96 | 0.48 |
| 1:M:324:VAL:O | 1:M:328:GLN:HG3 | 2.12 | 0.48 |
| 1:N:349:LEU:HB2 | 1:N:380:ILE:HD13 | 1.94 | 0.48 |
| 1:O:158:ILE:HD12 | 1:O:242:VAL:HG11 | 1.94 | 0.48 |
| 1:A:161:THR:HA | 1:A:257:PHE:CE1 | 2.48 | 0.48 |
| 1:A:165:ARG:HD2 | 1:A:165:ARG:C | 2.34 | 0.48 |
| 1:C:207:THR:HA | 1:C:225:ARG:HG2 | 1.95 | 0.48 |
| 1:D:158:ILE:HD12 | 1:D:242:VAL:HG11 | 1.95 | 0.48 |
| 1:E:221:LEU:HD13 | 1:E:223:HIS:CE1 | 2.48 | 0.48 |
| 1:E:36:LYS:HD2 | 1:E:562:TYR:HB3 | 1.96 | 0.48 |
| 1:G:548:ASP:OD2 | 1:G:551:ALA:CB | 2.60 | 0.48 |
| 1:H:167:LEU:HD23 | 1:H:422:PRO:HD3 | 1.94 | 0.48 |
| 1:I:23:LYS:HE2 | 1:I:27:GLU:HG2 | 1.95 | 0.48 |
| 1:I:570:TYR:H | 1:K:46:GLN:HE22 | 1.61 | 0.48 |
| 1:K:152:GLU:OE1 | 1:K:196:HIS:CE1 | 2.66 | 0.48 |
| 1:K:471:PHE:CG | 1:K:472:PRO:HD3 | 2.49 | 0.48 |
| 1:L:104:ILE:CG1 | 1:L:108:MSE:HE3 | 2.37 | 0.48 |
| 1:M:24:LYS:HZ3 | 1:O:24:LYS:HE2 | 1.79 | 0.48 |
| 1:O:328:GLN:HE22 | 1:O:334:LYS:NZ | 2.11 | 0.48 |
| 1:A:399:PHE:HB2 | 1:A:428:CYS:HB3 | 1.95 | 0.48 |
| 1:F:543:TYR:HA | 1:F:544:PRO:C | 2.34 | 0.48 |
| 1:G:100:LEU:HD21 | 1:G:111:VAL:HG21 | 1.96 | 0.48 |
| 1:G:227:ARG:HH11 | 1:G:227:ARG:CG | 2.24 | 0.48 |
| 1:I:578:LYS:O | 1:I:578:LYS:HD2 | 2.12 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:94:LYS:HD2 | 1:J:560:THR:O | 2.12 | 0.48 |
| 1:K:239:MSE:HE1 | 1:K:252:ILE:HG21 | 1.95 | 0.48 |
| 1:L:243:THR:HG21 | 1:L:273:TYR:CD2 | 2.49 | 0.48 |
| 1:O:85:LEU:HD12 | 1:O:110:ILE:CG2 | 2.42 | 0.48 |
| 1:P:404:LEU:HD22 | 1:P:433:LEU:CD2 | 2.44 | 0.48 |
| 1:A:41:THR:CG2 | 1:A:42:LEU:N | 2.77 | 0.48 |
| 1:B:254:PHE:CE2 | 1:B:265:LEU:HD13 | 2.47 | 0.48 |
| 1:C:263:PHE:CZ | 1:C:317:LEU:HD12 | 2.49 | 0.48 |
| 1:D:572:TRP:O | 1:D:577:MSE:HE2 | 2.13 | 0.48 |
| 1:E:238:PHE:CE2 | 1:E:239:MSE:HE3 | 2.48 | 0.48 |
| 1:F:350:ILE:HD13 | 1:F:362:LYS:HB3 | 1.94 | 0.48 |
| 1:G:474:VAL:O | 1:G:478:VAL:HG23 | 2.14 | 0.48 |
| 1:H:136:THR:CG2 | 1:H:137:ILE:N | 2.76 | 0.48 |
| 1:J:202:MSE:HE1 | 1:J:204:ASP:HA | 1.94 | 0.48 |
| 1:J:556:GLN:NE2 | 1:J:556:GLN:CA | 2.75 | 0.48 |
| 1:L:245:ARG:HD3 | 1:L:246:TYR:CE2 | 2.48 | 0.48 |
| 1:N:433:LEU:HG | 1:N:443:PHE:HB2 | 1.94 | 0.48 |
| 1:O:125:LEU:N | 5:O:1591:CL:CL | 2.79 | 0.48 |
| 1:O:579:VAL:HG23 | 1:O:579:VAL:O | 2.14 | 0.48 |
| 1:A:215:ASP:O | 1:A:222:ARG:NH2 | 2.47 | 0.48 |
| 1:A:42:LEU:O | 1:A:46:GLN:HG3 | 2.13 | 0.48 |
| 1:B:374:MSE:CE | 1:B:379:ASP:HB3 | 2.43 | 0.48 |
| 1:B:41:THR:O | 1:B:45:ARG:HG3 | 2.13 | 0.48 |
| 1:C:270:ARG:CG | 1:C:270:ARG:HH11 | 2.27 | 0.48 |
| 1:C:323:ILE:CG2 | 1:C:327:MSE:HE2 | 2.25 | 0.48 |
| 1:C:381:VAL:CG1 | 1:C:407:MSE:HE1 | 2.44 | 0.48 |
| 1:C:536:ARG:HE | 1:H:333:SER:HB2 | 1.79 | 0.48 |
| 1:E:250:CYS:O | 1:E:252:ILE:HD12 | 2.14 | 0.48 |
| 1:E:349:LEU:HB2 | 1:E:380:ILE:CD1 | 2.43 | 0.48 |
| 1:F:240:GLU:O | 1:F:244:SER:HB2 | 2.14 | 0.48 |
| 1:G:196:HIS:HB3 | 7:G:2032:HOH:O | 2.12 | 0.48 |
| 1:G:377:LEU:O | 1:G:381:VAL:HG23 | 2.13 | 0.48 |
| 1:H:300:ASN:OD1 | 1:H:305:HIS:HE1 | 1.96 | 0.48 |
| 1:L:476:LEU:HD13 | 1:L:527:ALA:CB | 2.43 | 0.48 |
| 1:O:369:HIS:HD1 | 1:O:370:CYS:N | 2.12 | 0.48 |
| 1:A:117:GLY:O | 1:A:121:GLN:HG3 | 2.14 | 0.48 |
| 1:A:327:MSE:HE1 | 1:A:337:ALA:O | 2.14 | 0.48 |
| 1:B:177:MSE:O | 1:B:180:PRO:HD2 | 2.13 | 0.48 |
| 1:B:202:MSE:HE3 | 1:B:203:LEU:N | 2.28 | 0.48 |
| 1:B:295:LEU:HD11 | 1:B:302:LEU:HB2 | 1.96 | 0.48 |
| 1:B:85:LEU:HD12 | 1:B:110:ILE:HG21 | 1.96 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:476:LEU:O | 1:C:480:SER:HB2 | 2.13 | 0.48 |
| 1:C:92:ASN:ND2 | 1:C:95:LEU:H | 2.11 | 0.48 |
| 1:D:572:TRP:C | 1:D:573:PRO:O | 2.50 | 0.48 |
| 1:E:502:VAL:HG12 | 1:E:507:LEU:CD2 | 2.44 | 0.48 |
| 1:I:208:ASP:OD1 | 1:I:225:ARG:HG3 | 2.13 | 0.48 |
| 1:J:188:THR:HG21 | 1:J:195:PRO:HG3 | 1.95 | 0.48 |
| 1:K:136:THR:HG21 | 1:K:138:HIS:HB2 | 1.96 | 0.48 |
| 1:K:227:ARG:HH11 | 1:K:227:ARG:HG3 | 1.79 | 0.48 |
| 1:K:302:LEU:HB3 | 1:K:330:GLU:OE1 | 2.14 | 0.48 |
| 1:L:281:GLN:HB3 | 1:L:491:PHE:CE1 | 2.48 | 0.48 |
| 1:N:136:THR:CG2 | 1:N:137:ILE:N | 2.76 | 0.48 |
| 1:N:350:ILE:HD13 | 1:N:362:LYS:HB3 | 1.94 | 0.48 |
| 1:N:36:LYS:HE2 | 1:N:562:TYR:HB3 | 1.95 | 0.48 |
| 1:N:578:LYS:HZ1 | 1:O:222:ARG:HD3 | 1.79 | 0.48 |
| 1:B:345:ASP:CG | 1:B:354:ARG:HH22 | 2.16 | 0.48 |
| 1:D:343:MSE:HE3 | 1:D:365:PHE:CG | 2.49 | 0.48 |
| 1:E:283:THR:O | 1:E:286:VAL:HG12 | 2.13 | 0.48 |
| 1:E:396:GLY:O | 1:E:426:ALA:O | 2.32 | 0.48 |
| 1:G:59:LEU:N | 1:G:59:LEU:HD12 | 2.29 | 0.48 |
| 1:G:77:SER:O | 1:G:81:ARG:HG3 | 2.14 | 0.48 |
| 1:H:502:VAL:CG1 | 1:H:507:LEU:HD13 | 2.44 | 0.48 |
| 1:J:420:SER:HA | 2:J:1581:NAP:H1D | 1.95 | 0.48 |
| 1:J:36:LYS:HD2 | 1:J:562:TYR:CG | 2.49 | 0.48 |
| 1:K:177:MSE:HE2 | 1:K:202:MSE:HB3 | 1.95 | 0.48 |
| 1:K:250:CYS:O | 1:K:252:ILE:HD12 | 2.14 | 0.48 |
| 1:L:238:PHE:CE2 | 1:L:239:MSE:HE3 | 2.48 | 0.48 |
| 1:M:454:LEU:HD12 | 1:M:454:LEU:N | 2.29 | 0.48 |
| 1:N:61:GLN:HA | 1:N:64:GLN:HE21 | 1.79 | 0.48 |
| 1:O:30:ARG:O | 1:P:30:ARG:HD3 | 2.14 | 0.48 |
| 1:O:327:MSE:HB3 | 1:O:332:VAL:CG1 | 2.42 | 0.48 |
| 1:A:301:ARG:NH1 | 1:A:330:GLU:HG2 | 2.28 | 0.48 |
| 1:B:417:PHE:CD1 | 1:B:444:ALA:HB3 | 2.49 | 0.48 |
| 1:C:136:THR:HG22 | 1:C:137:ILE:N | 2.27 | 0.48 |
| 1:D:41:THR:HG22 | 1:D:43:GLU:N | 2.20 | 0.48 |
| 1:I:172:LEU:O | 1:I:175:TYR:HB2 | 2.13 | 0.48 |
| 1:J:202:MSE:HE2 | 1:J:204:ASP:HB2 | 1.96 | 0.48 |
| 1:K:296:ARG:HB2 | 1:K:507:LEU:HD21 | 1.96 | 0.48 |
| 1:L:104:ILE:CG1 | 1:L:108:MSE:CE | 2.91 | 0.48 |
| 1:L:88:LEU:HD13 | 1:L:96:PHE:HA | 1.96 | 0.48 |
| 1:N:314:GLU:HB2 | 2:N:1581:NAP:O1N | 2.14 | 0.48 |
| 1:N:433:LEU:CD1 | 1:N:443:PHE:HB2 | 2.44 | 0.48 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:184:LEU:O | 1:O:187:TYR:HB2 | 2.14 | 0.48 |
| 1:P:133:LEU:HB3 | 1:P:201:VAL:HG22 | 1.95 | 0.48 |
| 1:A:260:ALA:HB3 | 7:A:2018:HOH:O | 2.13 | 0.48 |
| 1:G:336:GLU:HG3 | 7:G:2038:HOH:O | 2.13 | 0.48 |
| 1:G:528:VAL:HG22 | 1:G:553:ILE:HD12 | 1.96 | 0.48 |
| 1:I:104:ILE:CD1 | 1:I:108:MSE:HE3 | 2.42 | 0.48 |
| 1:J:152:GLU:HG3 | 1:J:155:ILE:HD12 | 1.96 | 0.48 |
| 1:J:183:LYS:HE3 | 1:J:255:GLU:OE1 | 2.14 | 0.48 |
| 1:L:75:LEU:HD11 | 1:L:84:LEU:HD22 | 1.95 | 0.48 |
| 1:M:104:ILE:HG23 | 1:M:105:GLU:N | 2.29 | 0.48 |
| 1:M:320:ALA:O | 1:M:324:VAL:HG23 | 2.14 | 0.48 |
| 1:M:374:MSE:HE1 | 1:M:379:ASP:O | 2.14 | 0.48 |
| 1:M:467:ASN:HD22 | 1:M:468:SER:N | 2.11 | 0.48 |
| 1:O:160:VAL:HG21 | 1:O:238:PHE:CE2 | 2.49 | 0.48 |
| 1:O:429:THR:CB | 1:O:432:GLN:HG2 | 2.39 | 0.48 |
| 1:O:543:TYR:HA | 1:O:544:PRO:C | 2.33 | 0.48 |
| 1:P:113:THR:HG22 | 1:P:114:PRO:HA | 1.94 | 0.48 |
| 1:B:136:THR:CG2 | 1:B:137:ILE:N | 2.77 | 0.47 |
| 1:B:429:THR:HG23 | 1:B:449:PHE:CE2 | 2.49 | 0.47 |
| 1:B:108:MSE:HE1 | 1:B:516:LEU:HG | 1.96 | 0.47 |
| 1:C:86:MSE:CE | 1:C:89:GLN:NE2 | 2.77 | 0.47 |
| 1:C:129:ARG:HG3 | 1:D:91:ARG:HD3 | 1.96 | 0.47 |
| 1:E:433:LEU:HD12 | 1:E:443:PHE:HB2 | 1.95 | 0.47 |
| 1:K:172:LEU:HA | 1:K:212:LEU:HD11 | 1.96 | 0.47 |
| 1:K:36:LYS:HG3 | 1:K:562:TYR:CG | 2.49 | 0.47 |
| 1:K:429:THR:CG2 | 1:K:430:ALA:N | 2.77 | 0.47 |
| 1:L:136:THR:HG23 | 1:L:221:LEU:HD11 | 1.96 | 0.47 |
| 1:L:411:ASN:HB2 | 1:L:414:PRO:HG3 | 1.96 | 0.47 |
| 1:L:61:GLN:HA | 1:L:64:GLN:HE21 | 1.79 | 0.47 |
| 1:M:154:VAL:O | 1:M:154:VAL:HG13 | 2.14 | 0.47 |
| 1:N:172:LEU:O | 1:N:175:TYR:HB2 | 2.14 | 0.47 |
| 1:P:493:THR:O | 1:P:497:VAL:HG23 | 2.14 | 0.47 |
| 1:C:137:ILE:HB | 1:C:205:VAL:HG12 | 1.95 | 0.47 |
| 1:F:335:GLU:O | 1:F:339:LYS:HG2 | 2.15 | 0.47 |
| 1:F:36:LYS:HD2 | 1:F:562:TYR:CG | 2.49 | 0.47 |
| 1:G:243:THR:HG22 | 1:G:247:GLY:O | 2.14 | 0.47 |
| 1:G:429:THR:CG2 | 1:G:430:ALA:N | 2.76 | 0.47 |
| 1:G:296:ARG:HB2 | 1:G:507:LEU:HD21 | 1.96 | 0.47 |
| 1:G:572:TRP:C | 1:G:573:PRO:O | 2.52 | 0.47 |
| 1:H:165:ARG:HD2 | 1:H:165:ARG:C | 2.34 | 0.47 |
| 1:I:112:TYR:CG | 1:I:186:LEU:HD11 | 2.49 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:24:LYS:HZ2 | 1:L:24:LYS:HD2 | 1.78 | 0.47 |
| 1:K:529:ARG:NH1 | 1:K:529:ARG:HG2 | 2.28 | 0.47 |
| 1:K:56:PRO:HG2 | 1:L:220:GLY:HA2 | 1.96 | 0.47 |
| 1:O:108:MSE:N | 1:O:109:PRO:CD | 2.77 | 0.47 |
| 1:O:109:PRO:HA | 1:O:113:THR:O | 2.14 | 0.47 |
| 1:O:258:ALA:N | 5:O:1589:CL:CL | 2.76 | 0.47 |
| 1:P:381:VAL:HG11 | 1:P:407:MSE:HE1 | 1.95 | 0.47 |
| 1:P:428:CYS:HB2 | 1:P:432:GLN:NE2 | 2.29 | 0.47 |
| 1:P:500:GLN:HE21 | 1:P:500:GLN:N | 2.13 | 0.47 |
| 1:A:24:LYS:CD | 1:A:24:LYS:O | 2.63 | 0.47 |
| 1:B:61:GLN:HE22 | 1:B:560:THR:HG23 | 1.79 | 0.47 |
| 1:B:24:LYS:CE | 1:D:24:LYS:HD3 | 2.44 | 0.47 |
| 1:E:133:LEU:HD23 | 1:E:134:PHE:N | 2.29 | 0.47 |
| 1:F:104:ILE:CG1 | 1:F:108:MSE:HE3 | 2.44 | 0.47 |
| 1:F:375:LYS:HG2 | 7:F:2053:HOH:O | 2.15 | 0.47 |
| 1:H:78:ASP:HA | 1:H:81:ARG:HH11 | 1.79 | 0.47 |
| 1:K:64:GLN:HB3 | 1:K:95:LEU:CD2 | 2.44 | 0.47 |
| 1:O:151:PRO:HG2 | 1:O:152:GLU:OE1 | 2.15 | 0.47 |
| 1:A:229:GLN:HE21 | 1:A:229:GLN:CA | 2.26 | 0.47 |
| 1:D:429:THR:HB | 1:D:432:GLN:HG3 | 1.96 | 0.47 |
| 1:E:433:LEU:HD13 | 1:E:433:LEU:C | 2.35 | 0.47 |
| 1:F:210:GLU:OE2 | 1:F:224:LYS:HE2 | 2.14 | 0.47 |
| 1:G:401:GLN:HA | 1:G:436:TYR:CD2 | 2.50 | 0.47 |
| 1:G:492:LEU:O | 1:G:496:GLU:HG3 | 2.14 | 0.47 |
| 1:H:433:LEU:HG | 1:H:443:PHE:CD1 | 2.49 | 0.47 |
| 1:J:467:ASN:HB3 | 1:J:471:PHE:HD2 | 1.80 | 0.47 |
| 1:K:36:LYS:HE2 | 1:K:562:TYR:HB3 | 1.96 | 0.47 |
| 1:K:572:TRP:C | 1:K:573:PRO:O | 2.51 | 0.47 |
| 1:M:300:ASN:OD1 | 1:M:305:HIS:CE1 | 2.67 | 0.47 |
| 1:M:399:PHE:HB2 | 1:M:428:CYS:HB3 | 1.96 | 0.47 |
| 1:M:56:PRO:HG2 | 1:N:220:GLY:HA2 | 1.96 | 0.47 |
| 1:O:136:THR:CG2 | 1:O:137:ILE:N | 2.77 | 0.47 |
| 1:A:265:LEU:CD2 | 1:A:269:TYR:HE1 | 2.25 | 0.47 |
| 1:A:316:ALA:HB1 | 1:A:343:MSE:HE1 | 1.93 | 0.47 |
| 1:B:177:MSE:HG2 | 7:B:2012:HOH:O | 2.14 | 0.47 |
| 1:B:543:TYR:HA | 1:B:544:PRO:C | 2.35 | 0.47 |
| 1:C:324:VAL:HA | 1:C:327:MSE:HE3 | 1.95 | 0.47 |
| 1:C:356:ALA:HB2 | 1:I:230:ALA:CB | 2.45 | 0.47 |
| 1:C:402:GLN:NE2 | 1:C:402:GLN:H | 2.11 | 0.47 |
| 1:C:431:GLU:OE2 | 1:C:452:VAL:HG22 | 2.14 | 0.47 |
| 1:C:554:ARG:NH1 | 1:C:554:ARG:HG2 | 2.29 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:578:LYS:HZ3 | 1:C:578:LYS:HB3 | 1.79 | 0.47 |
| 1:E:402:GLN:CD | 1:E:402:GLN:N | 2.68 | 0.47 |
| 1:F:125:LEU:C | 1:F:125:LEU:HD13 | 2.35 | 0.47 |
| 1:F:239:MSE:CE | 1:F:239:MSE:HA | 2.40 | 0.47 |
| 1:F:72:PHE:CE1 | 1:F:81:ARG:HB3 | 2.50 | 0.47 |
| 1:H:253:GLN:HE21 | 1:H:255:GLU:HG2 | 1.80 | 0.47 |
| 1:H:321:ASN:HB2 | 7:H:2041:HOH:O | 2.14 | 0.47 |
| 1:H:376:ASN:O | 1:H:380:ILE:HG13 | 2.14 | 0.47 |
| 1:I:354:ARG:HG2 | 1:I:356:ALA:N | 2.30 | 0.47 |
| 1:I:59:LEU:HD13 | 1:I:64:GLN:HG2 | 1.96 | 0.47 |
| 1:J:140:ARG:NH2 | 1:J:230:ALA:HA | 2.30 | 0.47 |
| 1:J:41:THR:HG22 | 1:J:42:LEU:N | 2.30 | 0.47 |
| 1:K:24:LYS:HA | 1:K:28:VAL:HG23 | 1.96 | 0.47 |
| 1:L:401:GLN:HB2 | 1:L:436:TYR:CE1 | 2.50 | 0.47 |
| 1:L:59:LEU:HD13 | 1:L:64:GLN:CG | 2.44 | 0.47 |
| 1:M:36:LYS:HD2 | 1:M:562:TYR:HB3 | 1.96 | 0.47 |
| 1:M:433:LEU:HG | 1:M:443:PHE:CB | 2.38 | 0.47 |
| 1:O:359:THR:OG1 | 1:O:360:PRO:HD2 | 2.14 | 0.47 |
| 1:P:401:GLN:HG3 | 1:P:402:GLN:HE22 | 1.79 | 0.47 |
| 1:B:296:ARG:CB | 1:B:507:LEU:HD21 | 2.44 | 0.47 |
| 1:C:315:ALA:O | 1:C:319:ILE:HG13 | 2.15 | 0.47 |
| 1:C:56:PRO:HG2 | 1:D:220:GLY:HA2 | 1.96 | 0.47 |
| 1:D:309:PHE:HB2 | 1:D:343:MSE:HG2 | 1.96 | 0.47 |
| 1:E:61:GLN:O | 1:E:65:VAL:HG23 | 2.14 | 0.47 |
| 1:G:72:PHE:CE2 | 1:G:81:ARG:HD3 | 2.50 | 0.47 |
| 1:H:327:MSE:HE3 | 1:H:337:ALA:CB | 2.31 | 0.47 |
| 1:H:467:ASN:ND2 | 3:H:1582:OXL:O2 | 2.48 | 0.47 |
| 1:I:207:THR:HA | 1:I:225:ARG:HG2 | 1.96 | 0.47 |
| 1:I:469:TYR:OH | 1:I:516:LEU:HD13 | 2.14 | 0.47 |
| 1:K:401:GLN:HG3 | 1:K:436:TYR:CG | 2.50 | 0.47 |
| 1:L:146:MSE:O | 1:L:149:SER:HB3 | 2.15 | 0.47 |
| 1:M:429:THR:CG2 | 1:M:430:ALA:N | 2.77 | 0.47 |
| 1:N:59:LEU:HA | 1:P:580:LYS:H | 1.79 | 0.47 |
| 1:O:471:PHE:CG | 1:O:472:PRO:HD3 | 2.49 | 0.47 |
| 1:P:162:ASP:O | 1:P:225:ARG:NH2 | 2.30 | 0.47 |
| 1:B:420:SER:HA | 2:B:1581:NAP:H1D | 1.96 | 0.47 |
| 1:B:459:THR:HG22 | 1:B:461:TYR:CE1 | 2.49 | 0.47 |
| 1:D:41:THR:CG2 | 1:D:42:LEU:N | 2.77 | 0.47 |
| 1:D:285:SER:HB3 | 1:D:470:VAL:HG21 | 1.97 | 0.47 |
| 1:E:162:ASP:HA | 1:E:202:MSE:CE | 2.44 | 0.47 |
| 1:G:288:VAL:HG21 | 1:G:322:LEU:CD1 | 2.45 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:155:ILE:HD13 | 1:H:246:TYR:CE2 | 2.50 | 0.47 |
| 1:I:166:ILE:HG21 | 1:I:172:LEU:HD12 | 1.97 | 0.47 |
| 1:I:467:ASN:HD22 | 1:I:468:SER:N | 2.12 | 0.47 |
| 1:K:381:VAL:HG13 | 1:K:407:MSE:HE1 | 1.96 | 0.47 |
| 1:M:136:THR:CG2 | 1:M:138:HIS:N | 2.72 | 0.47 |
| 1:M:23:LYS:O | 1:M:24:LYS:HE3 | 2.15 | 0.47 |
| 1:M:578:LYS:NZ | 1:M:580:LYS:CD | 2.78 | 0.47 |
| 1:N:399:PHE:HB2 | 1:N:428:CYS:HB3 | 1.95 | 0.47 |
| 1:M:133:LEU:HD23 | 1:N:52:GLY:O | 2.14 | 0.47 |
| 1:N:86:MSE:HE1 | 1:N:89:GLN:NE2 | 2.30 | 0.47 |
| 1:A:352:LYS:HA | 1:A:352:LYS:HD3 | 1.68 | 0.47 |
| 1:C:245:ARG:HH11 | 1:C:245:ARG:HG2 | 1.80 | 0.47 |
| 1:D:404:LEU:HD22 | 1:D:433:LEU:HD23 | 1.96 | 0.47 |
| 1:F:494:THR:HG23 | 1:F:526:ILE:CG2 | 2.42 | 0.47 |
| 1:G:36:LYS:HD2 | 1:G:562:TYR:CG | 2.49 | 0.47 |
| 1:H:431:GLU:HG2 | 1:H:452:VAL:HG22 | 1.97 | 0.47 |
| 1:J:270:ARG:NH1 | 1:J:270:ARG:CG | 2.75 | 0.47 |
| 1:K:23:LYS:C | 1:K:24:LYS:HD2 | 2.35 | 0.47 |
| 1:K:385:LYS:HA | 1:K:410:PHE:HE2 | 1.79 | 0.47 |
| 1:L:158:ILE:HD12 | 1:L:242:VAL:HG11 | 1.95 | 0.47 |
| 1:L:36:LYS:NZ | 1:L:44:GLU:OE1 | 2.46 | 0.47 |
| 1:M:548:ASP:OD2 | 1:M:551:ALA:HB2 | 2.15 | 0.47 |
| 1:O:270:ARG:CG | 1:O:270:ARG:HH11 | 2.28 | 0.47 |
| 1:A:254:PHE:HE2 | 1:A:265:LEU:HD13 | 1.80 | 0.47 |
| 1:B:165:ARG:NH1 | 2:B:1581:NAP:O1N | 2.47 | 0.47 |
| 1:B:195:PRO:HD2 | 7:B:2015:HOH:O | 2.15 | 0.47 |
| 1:D:23:LYS:HB3 | 1:D:23:LYS:HE2 | 1.63 | 0.47 |
| 1:D:369:HIS:ND1 | 1:D:370:CYS:O | 2.41 | 0.47 |
| 1:D:41:THR:HG22 | 1:D:42:LEU:N | 2.28 | 0.47 |
| 1:E:164:GLU:CG | 1:E:258:ALA:HB2 | 2.44 | 0.47 |
| 1:E:61:GLN:HA | 1:E:64:GLN:HE21 | 1.79 | 0.47 |
| 1:F:90:ASP:OD1 | 1:F:131:ARG:NH1 | 2.48 | 0.47 |
| 1:J:354:ARG:NE | 1:J:358:LEU:HD21 | 2.30 | 0.47 |
| 1:J:59:LEU:O | 1:J:59:LEU:HD12 | 2.15 | 0.47 |
| 1:K:135:ILE:HD12 | 1:K:135:ILE:N | 2.30 | 0.47 |
| 1:K:239:MSE:HE1 | 1:K:252:ILE:HG12 | 1.97 | 0.47 |
| 1:L:301:ARG:HG3 | 7:L:2040:HOH:O | 2.15 | 0.47 |
| 1:O:396:GLY:O | 1:O:426:ALA:O | 2.32 | 0.47 |
| 1:B:23:LYS:HG2 | 1:B:24:LYS:N | 2.30 | 0.47 |
| 1:B:243:THR:HG21 | 1:B:273:TYR:CD2 | 2.50 | 0.47 |
| 1:B:471:PHE:CE1 | 1:B:472:PRO:HG3 | 2.50 | 0.47 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:274:CYS:SG | 1:C:478:VAL:HG11 | 2.55 | 0.47 |
| 1:C:354:ARG:HD2 | 1:C:356:ALA:N | 2.30 | 0.47 |
| 1:E:41:THR:O | 1:E:45:ARG:HG3 | 2.15 | 0.47 |
| 1:H:314:GLU:HB2 | 2:H:1581:NAP:O1N | 2.15 | 0.47 |
| 1:H:332:VAL:CG1 | 1:H:336:GLU:HB2 | 2.45 | 0.47 |
| 1:I:61:GLN:HA | 1:I:64:GLN:HE21 | 1.79 | 0.47 |
| 1:I:74:ARG:HD3 | 1:J:125:LEU:HD21 | 1.96 | 0.47 |
| 1:J:359:THR:HG22 | 1:J:362:LYS:CB | 2.44 | 0.47 |
| 1:K:420:SER:HA | 2:K:1581:NAP:H1D | 1.96 | 0.47 |
| 1:K:315:ALA:O | 1:K:319:ILE:HG13 | 2.14 | 0.47 |
| 1:K:404:LEU:HD13 | 1:K:433:LEU:HA | 1.95 | 0.47 |
| 1:K:476:LEU:HB3 | 1:K:527:ALA:HB2 | 1.96 | 0.47 |
| 1:L:209:ASN:OD1 | 1:L:211:THR:HB | 2.15 | 0.47 |
| 1:O:575:GLU:O | 1:O:578:LYS:HB3 | 2.15 | 0.47 |
| 1:P:109:PRO:HA | 1:P:113:THR:O | 2.15 | 0.47 |
| 1:A:274:CYS:SG | 1:A:478:VAL:HG11 | 2.54 | 0.47 |
| 1:A:359:THR:CG2 | 1:A:362:LYS:HG3 | 2.44 | 0.47 |
| 1:D:35:ASN:HD21 | 1:D:37:GLY:H | 1.56 | 0.47 |
| 1:E:162:ASP:HA | 1:E:202:MSE:HE1 | 1.98 | 0.47 |
| 1:I:323:ILE:O | 1:I:327:MSE:HG3 | 2.15 | 0.47 |
| 1:I:374:MSE:CE | 1:I:379:ASP:HB3 | 2.44 | 0.47 |
| 1:L:152:GLU:HG2 | 1:L:196:HIS:O | 2.15 | 0.47 |
| 1:N:88:LEU:HD13 | 1:N:96:PHE:HA | 1.96 | 0.47 |
| 1:O:145:THR:O | 1:O:148:GLN:HB2 | 2.15 | 0.47 |
| 1:O:317:LEU:HD23 | 1:O:343:MSE:HE1 | 1.96 | 0.47 |
| 1:O:33:HIS:HD2 | 1:O:93:GLU:OE2 | 1.98 | 0.47 |
| 1:A:135:ILE:HB | 1:A:203:LEU:HD23 | 1.97 | 0.46 |
| 1:C:359:THR:HG23 | 1:C:360:PRO:HD2 | 1.97 | 0.46 |
| 1:F:24:LYS:HG2 | 1:H:24:LYS:NZ | 2.29 | 0.46 |
| 1:H:374:MSE:CE | 1:H:379:ASP:HB3 | 2.44 | 0.46 |
| 1:I:77:SER:HB2 | 1:I:80:ASP:OD2 | 2.14 | 0.46 |
| 1:K:556:GLN:HE21 | 1:K:556:GLN:CA | 2.28 | 0.46 |
| 1:K:77:SER:O | 1:K:81:ARG:HG3 | 2.14 | 0.46 |
| 1:L:420:SER:HA | 2:L:1581:NAP:H1D | 1.96 | 0.46 |
| 1:L:137:ILE:HA | 1:L:234:LEU:HD22 | 1.97 | 0.46 |
| 1:L:574:GLU:OE1 | 1:L:577:MSE:HE2 | 2.15 | 0.46 |
| 1:L:60:GLY:O | 1:L:64:GLN:HG3 | 2.15 | 0.46 |
| 1:N:165:ARG:HD2 | 1:N:165:ARG:O | 2.15 | 0.46 |
| 1:P:467:ASN:HB3 | 1:P:471:PHE:HD2 | 1.80 | 0.46 |
| 1:B:113:THR:CG2 | 1:B:114:PRO:HA | 2.44 | 0.46 |
| 1:B:529:ARG:NH1 | 1:B:529:ARG:HG2 | 2.30 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:89:GLN:HG3 | 1:C:96:PHE:CD2 | 2.50 | 0.46 |
| 1:D:504:GLU:HG3 | 1:D:508:GLN:HE21 | 1.78 | 0.46 |
| 1:D:575:GLU:OE2 | 1:D:576:ALA:HB2 | 2.14 | 0.46 |
| 1:F:154:VAL:HG13 | 1:F:154:VAL:O | 2.15 | 0.46 |
| 1:F:467:ASN:ND2 | 3:F:1582:OXL:O2 | 2.48 | 0.46 |
| 1:F:78:ASP:HA | 1:F:81:ARG:HH11 | 1.81 | 0.46 |
| 1:G:202:MSE:CE | 1:G:204:ASP:HA | 2.46 | 0.46 |
| 1:G:429:THR:HG22 | 1:G:431:GLU:H | 1.79 | 0.46 |
| 1:H:433:LEU:HD13 | 1:H:433:LEU:C | 2.35 | 0.46 |
| 1:I:154:VAL:HG13 | 1:I:154:VAL:O | 2.14 | 0.46 |
| 1:N:104:ILE:HG23 | 1:N:105:GLU:N | 2.30 | 0.46 |
| 1:N:184:LEU:HD22 | 1:N:198:CYS:HB3 | 1.96 | 0.46 |
| 1:N:368:GLU:O | 1:N:368:GLU:HG3 | 2.15 | 0.46 |
| 1:P:158:ILE:HD12 | 1:P:242:VAL:HG11 | 1.97 | 0.46 |
| 1:E:288:VAL:HG12 | 1:E:292:LEU:HD13 | 1.98 | 0.46 |
| 1:E:476:LEU:O | 1:E:480:SER:HB2 | 2.15 | 0.46 |
| 1:E:543:TYR:HA | 1:E:544:PRO:C | 2.35 | 0.46 |
| 1:I:354:ARG:HG2 | 1:I:356:ALA:H | 1.79 | 0.46 |
| 1:K:359:THR:HG22 | 1:K:362:LYS:CD | 2.45 | 0.46 |
| 1:K:58:PHE:N | 1:K:58:PHE:CD1 | 2.83 | 0.46 |
| 1:L:321:ASN:HB2 | 7:L:2044:HOH:O | 2.13 | 0.46 |
| 1:N:160:VAL:HG12 | 1:N:161:THR:N | 2.30 | 0.46 |
| 1:O:328:GLN:CD | 1:O:334:LYS:HD2 | 2.35 | 0.46 |
| 1:P:162:ASP:HA | 1:P:202:MSE:CE | 2.45 | 0.46 |
| 1:B:381:VAL:CG1 | 1:B:407:MSE:HE1 | 2.46 | 0.46 |
| 1:C:161:THR:HG22 | 1:C:180:PRO:HG2 | 1.96 | 0.46 |
| 1:C:533:GLU:OE1 | 1:C:536:ARG:NH1 | 2.48 | 0.46 |
| 1:D:381:VAL:HG13 | 1:D:407:MSE:HE1 | 1.97 | 0.46 |
| 1:F:202:MSE:HE3 | 1:F:204:ASP:HA | 1.98 | 0.46 |
| 1:F:239:MSE:HE1 | 1:F:252:ILE:HD13 | 1.97 | 0.46 |
| 1:F:264:ARG:NH1 | 1:F:264:ARG:HG2 | 2.28 | 0.46 |
| 1:H:98:LYS:HD3 | 1:H:560:THR:CG2 | 2.45 | 0.46 |
| 1:I:70:LYS:HA | 1:I:70:LYS:HD3 | 1.78 | 0.46 |
| 1:L:152:GLU:HB3 | 1:L:155:ILE:HD11 | 1.98 | 0.46 |
| 1:M:86:MSE:HE1 | 1:M:89:GLN:NE2 | 2.31 | 0.46 |
| 1:O:328:GLN:HE22 | 1:O:334:LYS:HD2 | 1.77 | 0.46 |
| 1:O:350:ILE:HD11 | 1:O:362:LYS:HD2 | 1.98 | 0.46 |
| 1:O:428:CYS:HB2 | 1:O:432:GLN:HE21 | 1.80 | 0.46 |
| 1:P:433:LEU:HG | 1:P:443:PHE:CD1 | 2.50 | 0.46 |
| 1:A:202:MSE:HE2 | 1:A:204:ASP:HA | 1.97 | 0.46 |
| 1:A:89:GLN:HB2 | 1:A:96:PHE:CE1 | 2.51 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:391:GLY:HA3 | 1:B:427:GLU:HG2 | 1.97 | 0.46 |
| 1:B:192:GLY:HA3 | 1:B:557:VAL:HG13 | 1.96 | 0.46 |
| 1:F:108:MSE:HB3 | 1:F:109:PRO:HD3 | 1.97 | 0.46 |
| 1:G:44:GLU:O | 1:G:48:LEU:HB2 | 2.16 | 0.46 |
| 1:J:108:MSE:N | 1:J:109:PRO:CD | 2.79 | 0.46 |
| 1:K:179:ILE:HB | 1:K:180:PRO:HD3 | 1.96 | 0.46 |
| 1:M:24:LYS:HB2 | 1:M:24:LYS:HZ2 | 1.77 | 0.46 |
| 1:N:164:GLU:CG | 1:N:258:ALA:HB2 | 2.40 | 0.46 |
| 1:O:177:MSE:CE | 1:O:177:MSE:CA | 2.91 | 0.46 |
| 1:P:407:MSE:O | 1:P:411:ASN:HB2 | 2.15 | 0.46 |
| 1:A:188:THR:OG1 | 1:A:195:PRO:HG3 | 2.16 | 0.46 |
| 1:A:215:ASP:OD1 | 1:A:216:PRO:HD2 | 2.16 | 0.46 |
| 1:A:91:ARG:HB3 | 1:A:91:ARG:HE | 1.49 | 0.46 |
| 1:C:404:LEU:HD22 | 1:C:433:LEU:HD23 | 1.96 | 0.46 |
| 1:C:554:ARG:HH11 | 1:C:554:ARG:HG2 | 1.79 | 0.46 |
| 1:D:324:VAL:HG12 | 1:D:328:GLN:NE2 | 2.21 | 0.46 |
| 1:D:376:ASN:O | 1:D:380:ILE:HG13 | 2.15 | 0.46 |
| 1:E:340:ARG:HH11 | 1:E:340:ARG:CG | 2.29 | 0.46 |
| 1:G:123:TYR:HB3 | 1:G:175:TYR:CD2 | 2.51 | 0.46 |
| 1:G:335:GLU:OE2 | 1:G:339:LYS:NZ | 2.44 | 0.46 |
| 1:J:192:GLY:HA3 | 1:J:557:VAL:HG13 | 1.98 | 0.46 |
| 1:L:314:GLU:HB2 | 2:L:1581:NAP:O1N | 2.16 | 0.46 |
| 1:L:454:LEU:CD2 | 1:L:460:LEU:HG | 2.42 | 0.46 |
| 1:N:476:LEU:HB3 | 1:N:527:ALA:HB2 | 1.98 | 0.46 |
| 1:P:376:ASN:O | 1:P:380:ILE:HG13 | 2.15 | 0.46 |
| 1:A:172:LEU:O | 1:A:175:TYR:HB2 | 2.15 | 0.46 |
| 1:B:160:VAL:HG21 | 1:B:238:PHE:CE2 | 2.50 | 0.46 |
| 1:B:238:PHE:CE2 | 1:B:239:MSE:HE3 | 2.50 | 0.46 |
| 1:B:332:VAL:HG12 | 1:B:333:SER:N | 2.30 | 0.46 |
| 1:C:108:MSE:HB3 | 1:C:109:PRO:HD3 | 1.97 | 0.46 |
| 1:D:458:GLN:HE21 | 1:D:460:LEU:HD21 | 1.80 | 0.46 |
| 1:D:524:LEU:O | 1:D:528:VAL:HG23 | 2.16 | 0.46 |
| 1:E:90:ASP:OD1 | 1:E:131:ARG:NH1 | 2.48 | 0.46 |
| 1:E:202:MSE:HE3 | 1:E:203:LEU:C | 2.35 | 0.46 |
| 1:K:543:TYR:HA | 1:K:544:PRO:C | 2.35 | 0.46 |
| 1:L:131:ARG:O | 1:L:177:MSE:HE3 | 2.16 | 0.46 |
| 1:L:323:ILE:HG22 | 1:L:327:MSE:HE2 | 1.98 | 0.46 |
| 1:M:270:ARG:HG2 | 1:M:270:ARG:HH11 | 1.80 | 0.46 |
| 1:N:177:MSE:O | 1:N:180:PRO:HD2 | 2.16 | 0.46 |
| 1:O:239:MSE:HE1 | 1:O:252:ILE:HG21 | 1.97 | 0.46 |
| 1:P:155:ILE:HB | 1:P:246:TYR:CE2 | 2.51 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:385:LYS:HA | 1:P:410:PHE:CE2 | 2.51 | 0.46 |
| 1:P:407:MSE:HG2 | 1:P:416:ILE:HD11 | 1.97 | 0.46 |
| 1:A:175:TYR:CE2 | 1:A:218:TYR:HA | 2.51 | 0.46 |
| 1:B:578:LYS:O | 1:B:578:LYS:HD2 | 2.15 | 0.46 |
| 1:C:284:ALA:HA | 1:C:319:ILE:HG12 | 1.97 | 0.46 |
| 1:D:416:ILE:CG1 | 1:D:433:LEU:HD21 | 2.39 | 0.46 |
| 1:E:342:TRP:CD2 | 1:E:367:HIS:HD2 | 2.34 | 0.46 |
| 1:K:378:GLU:OE2 | 1:K:382:LYS:NZ | 2.46 | 0.46 |
| 1:K:410:PHE:CD1 | 1:K:410:PHE:N | 2.84 | 0.46 |
| 1:M:516:LEU:HA | 1:M:516:LEU:HD12 | 1.75 | 0.46 |
| 1:M:92:ASN:ND2 | 1:M:92:ASN:C | 2.58 | 0.46 |
| 1:N:69:LEU:HD22 | 1:N:106:ARG:HH12 | 1.79 | 0.46 |
| 1:O:92:ASN:ND2 | 1:O:92:ASN:C | 2.69 | 0.46 |
| 1:A:332:VAL:CG1 | 1:A:333:SER:N | 2.79 | 0.46 |
| 1:A:404:LEU:HD22 | 1:A:433:LEU:HD23 | 1.98 | 0.46 |
| 1:B:35:ASN:ND2 | 1:B:37:GLY:H | 2.14 | 0.46 |
| 1:C:141:GLY:N | 1:C:237:GLU:OE1 | 2.39 | 0.46 |
| 1:C:580:LYS:HG3 | 1:C:580:LYS:O | 2.15 | 0.46 |
| 1:E:283:THR:CG2 | 1:E:284:ALA:N | 2.79 | 0.46 |
| 1:G:254:PHE:HE2 | 1:G:265:LEU:HD13 | 1.81 | 0.46 |
| 1:J:41:THR:CG2 | 7:J:2006:HOH:O | 2.64 | 0.46 |
| 1:K:184:LEU:HD12 | 1:K:200:PRO:HB3 | 1.97 | 0.46 |
| 1:K:164:GLU:CG | 1:K:258:ALA:HB2 | 2.38 | 0.46 |
| 1:P:327:MSE:O | 1:P:332:VAL:HG12 | 2.16 | 0.46 |
| 1:P:502:VAL:CG1 | 1:P:507:LEU:HD13 | 2.46 | 0.46 |
| 1:A:476:LEU:HB3 | 1:A:527:ALA:HB2 | 1.97 | 0.46 |
| 1:A:64:GLN:O | 1:A:68:ILE:HG12 | 2.15 | 0.46 |
| 1:B:120:CYS:O | 1:B:175:TYR:HB3 | 2.16 | 0.46 |
| 1:B:222:ARG:HH11 | 1:B:222:ARG:HG3 | 1.80 | 0.46 |
| 1:B:59:LEU:N | 1:B:59:LEU:HD12 | 2.30 | 0.46 |
| 1:D:159:VAL:HG23 | 1:D:184:LEU:HD21 | 1.98 | 0.46 |
| 1:F:103:ASP:HB3 | 1:F:107:PHE:CE1 | 2.50 | 0.46 |
| 1:G:177:MSE:O | 1:G:180:PRO:HD2 | 2.16 | 0.46 |
| 1:G:61:GLN:HA | 1:G:64:GLN:HE21 | 1.80 | 0.46 |
| 1:H:351:VAL:HG12 | 1:H:369:HIS:HB3 | 1.97 | 0.46 |
| 1:J:137:ILE:HA | 1:J:234:LEU:HD22 | 1.97 | 0.46 |
| 1:J:47:GLN:NE2 | 1:J:566:VAL:HG13 | 2.31 | 0.46 |
| 1:K:288:VAL:HG21 | 1:K:322:LEU:HB3 | 1.98 | 0.46 |
| 1:K:407:MSE:HG2 | 1:K:416:ILE:HD11 | 1.98 | 0.46 |
| 1:K:454:LEU:CD1 | 1:K:454:LEU:N | 2.79 | 0.46 |
| 1:K:516:LEU:O | 1:K:519:ILE:HG22 | 2.16 | 0.46 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:414:PRO:HD2 | 1:L:441:GLY:HA2 | 1.98 | 0.46 |
| 1:I:222:ARG:HD2 | 1:L:580:LYS:CE | 2.45 | 0.46 |
| 1:M:578:LYS:HZ1 | 1:M:580:LYS:CD | 2.26 | 0.46 |
| 1:P:524:LEU:O | 1:P:528:VAL:HG23 | 2.15 | 0.46 |
| 1:P:543:TYR:HA | 1:P:544:PRO:C | 2.36 | 0.46 |
| 1:B:415:ILE:CG1 | 1:B:442:ILE:HD12 | 2.46 | 0.45 |
| 1:C:132:GLY:HA2 | 1:C:200:PRO:HG2 | 1.98 | 0.45 |
| 1:C:165:ARG:HD2 | 1:C:165:ARG:O | 2.15 | 0.45 |
| 1:C:38:MSE:SE | 1:C:55:PRO:HG2 | 2.66 | 0.45 |
| 1:E:184:LEU:HD22 | 1:E:198:CYS:HB3 | 1.98 | 0.45 |
| 1:F:184:LEU:HD12 | 1:F:200:PRO:HB3 | 1.97 | 0.45 |
| 1:F:291:LEU:HD21 | 1:F:388:VAL:HG11 | 1.98 | 0.45 |
| 1:G:133:LEU:HB2 | 1:G:199:LEU:HD11 | 1.98 | 0.45 |
| 1:G:257:PHE:O | 1:G:314:GLU:OE2 | 2.35 | 0.45 |
| 1:G:36:LYS:HD3 | 1:G:562:TYR:HB3 | 1.98 | 0.45 |
| 1:G:502:VAL:HG12 | 1:G:507:LEU:HD13 | 1.98 | 0.45 |
| 1:H:145:THR:HA | 1:H:148:GLN:NE2 | 2.30 | 0.45 |
| 1:H:386:PRO:CG | 1:H:407:MSE:HE1 | 2.33 | 0.45 |
| 1:I:108:MSE:N | 1:I:109:PRO:CD | 2.79 | 0.45 |
| 1:I:117:GLY:O | 1:I:121:GLN:HG3 | 2.16 | 0.45 |
| 1:I:369:HIS:ND1 | 1:I:370:CYS:N | 2.63 | 0.45 |
| 1:K:470:VAL:HG13 | 1:K:494:THR:HG21 | 1.97 | 0.45 |
| 1:K:38:MSE:SE | 1:K:57:CYS:SG | 3.24 | 0.45 |
| 1:L:296:ARG:O | 1:L:299:LYS:HE3 | 2.15 | 0.45 |
| 1:O:381:VAL:HG13 | 1:O:407:MSE:CE | 2.41 | 0.45 |
| 1:O:74:ARG:HD3 | 1:P:125:LEU:HD21 | 1.98 | 0.45 |
| 1:P:572:TRP:C | 1:P:573:PRO:O | 2.54 | 0.45 |
| 1:P:580:LYS:HB3 | 1:P:580:LYS:HE2 | 1.58 | 0.45 |
| 1:A:229:GLN:HA | 1:A:229:GLN:HE21 | 1.81 | 0.45 |
| 1:A:322:LEU:HD23 | 1:A:322:LEU:HA | 1.75 | 0.45 |
| 1:A:91:ARG:HB2 | 1:B:129:ARG:HH12 | 1.81 | 0.45 |
| 1:C:41:THR:CG2 | 1:C:43:GLU:H | 2.30 | 0.45 |
| 1:E:309:PHE:HB2 | 1:E:343:MSE:HG2 | 1.98 | 0.45 |
| 1:H:35:ASN:ND2 | 1:H:37:GLY:H | 2.14 | 0.45 |
| 1:I:322:LEU:HD23 | 1:I:322:LEU:HA | 1.76 | 0.45 |
| 7:J:2027:HOH:O | 1:K:580:LYS:HD2 | 2.15 | 0.45 |
| 1:N:202:MSE:HE1 | 1:N:204:ASP:HA | 1.99 | 0.45 |
| 1:A:156:LYS:HD3 | 1:A:479:ILE:HG23 | 1.98 | 0.45 |
| 1:A:214:LYS:HD3 | 7:A:2015:HOH:O | 2.15 | 0.45 |
| 1:A:33:HIS:HD2 | 1:A:93:GLU:OE2 | 1.97 | 0.45 |
| 1:C:23:LYS:O | 1:C:24:LYS:HG3 | 2.16 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:433:LEU:O | 1:C:437:THR:HG23 | 2.17 | 0.45 |
| 1:G:152:GLU:OE2 | 1:G:154:VAL:HG13 | 2.17 | 0.45 |
| 1:H:108:MSE:N | 1:H:109:PRO:CD | 2.78 | 0.45 |
| 1:I:163:GLY:HA2 | 1:I:166:ILE:HD11 | 1.97 | 0.45 |
| 1:K:64:GLN:HB3 | 1:K:95:LEU:HD21 | 1.97 | 0.45 |
| 1:L:117:GLY:O | 1:L:121:GLN:HG3 | 2.15 | 0.45 |
| 1:L:354:ARG:NE | 1:L:358:LEU:HD21 | 2.32 | 0.45 |
| 1:L:578:LYS:HB3 | 1:L:578:LYS:HE2 | 1.82 | 0.45 |
| 1:M:324:VAL:HA | 1:M:327:MSE:HE3 | 1.97 | 0.45 |
| 1:P:389:LEU:HD22 | 1:P:399:PHE:CZ | 2.51 | 0.45 |
| 1:A:194:LYS:HA | 1:A:195:PRO:HD3 | 1.87 | 0.45 |
| 1:D:184:LEU:O | 1:D:187:TYR:HB2 | 2.17 | 0.45 |
| 1:D:543:TYR:HA | 1:D:544:PRO:C | 2.36 | 0.45 |
| 1:F:36:LYS:CD | 1:F:562:TYR:HB3 | 2.47 | 0.45 |
| 1:K:376:ASN:O | 1:K:380:ILE:HG13 | 2.16 | 0.45 |
| 1:M:427:GLU:O | 1:M:428:CYS:HB3 | 2.17 | 0.45 |
| 1:M:543:TYR:HA | 1:M:544:PRO:C | 2.36 | 0.45 |
| 1:N:253:GLN:NE2 | 1:N:255:GLU:OE1 | 2.47 | 0.45 |
| 1:A:316:ALA:HB1 | 1:A:343:MSE:HE2 | 1.96 | 0.45 |
| 1:A:466:ASN:HA | 2:A:1581:NAP:N7N | 2.20 | 0.45 |
| 1:C:174:CYS:SG | 1:C:219:ILE:CD1 | 3.04 | 0.45 |
| 1:C:204:ASP:HA | 7:C:2026:HOH:O | 2.16 | 0.45 |
| 1:C:42:LEU:O | 1:C:46:GLN:HG3 | 2.16 | 0.45 |
| 1:H:543:TYR:HA | 1:H:544:PRO:C | 2.37 | 0.45 |
| 1:I:136:THR:CG2 | 1:I:221:LEU:HD11 | 2.47 | 0.45 |
| 1:L:120:CYS:O | 1:L:175:TYR:HB3 | 2.16 | 0.45 |
| 1:M:136:THR:OG1 | 1:M:221:LEU:HD11 | 2.17 | 0.45 |
| 1:M:161:THR:HA | 1:M:257:PHE:CE1 | 2.52 | 0.45 |
| 1:M:36:LYS:HE2 | 1:M:40:PHE:CD2 | 2.52 | 0.45 |
| 1:M:378:GLU:OE1 | 1:M:382:LYS:HE2 | 2.15 | 0.45 |
| 1:M:88:LEU:CD1 | 1:M:96:PHE:HA | 2.46 | 0.45 |
| 1:N:44:GLU:O | 1:N:48:LEU:HB2 | 2.15 | 0.45 |
| 1:N:572:TRP:C | 1:N:573:PRO:O | 2.54 | 0.45 |
| 1:A:429:THR:HG22 | 1:A:430:ALA:H | 1.82 | 0.45 |
| 1:A:401:GLN:HG2 | 1:A:436:TYR:CZ | 2.51 | 0.45 |
| 1:A:82:TYR:CE2 | 1:A:86:MSE:HG3 | 2.51 | 0.45 |
| 1:B:535:TYR:HE2 | 1:B:549:LEU:HD21 | 1.81 | 0.45 |
| 1:D:328:GLN:HA | 1:D:332:VAL:O | 2.17 | 0.45 |
| 1:D:435:LYS:HE3 | 1:D:436:TYR:CE1 | 2.52 | 0.45 |
| 1:F:350:ILE:HG22 | 1:F:350:ILE:O | 2.17 | 0.45 |
| 1:G:136:THR:HG23 | 1:G:221:LEU:HD11 | 1.99 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:64:GLN:NE2 | 1:G:562:TYR:OH | 2.50 | 0.45 |
| 1:G:77:SER:HB2 | 1:G:80:ASP:OD2 | 2.17 | 0.45 |
| 1:K:467:ASN:N | 2:K:1581:NAP:H72N | 2.15 | 0.45 |
| 1:L:300:ASN:OD1 | 1:L:305:HIS:HE1 | 1.99 | 0.45 |
| 1:O:340:ARG:HG2 | 1:O:340:ARG:NH1 | 2.32 | 0.45 |
| 1:P:162:ASP:HA | 1:P:202:MSE:HE1 | 1.98 | 0.45 |
| 1:P:276:PHE:HB2 | 1:P:281:GLN:OE1 | 2.17 | 0.45 |
| 1:P:98:LYS:HD3 | 1:P:560:THR:CG2 | 2.47 | 0.45 |
| 1:A:469:TYR:OH | 1:A:516:LEU:HD12 | 2.17 | 0.45 |
| 1:C:494:THR:CG2 | 1:C:526:ILE:HD12 | 2.25 | 0.45 |
| 1:C:32:PRO:HD2 | 1:D:30:ARG:NH2 | 2.32 | 0.45 |
| 1:D:429:THR:H | 1:D:432:GLN:NE2 | 2.15 | 0.45 |
| 1:D:90:ASP:OD2 | 1:D:131:ARG:NH1 | 2.50 | 0.45 |
| 1:E:260:ALA:O | 1:E:264:ARG:HG2 | 2.16 | 0.45 |
| 1:H:412:LYS:O | 1:H:413:ARG:HD2 | 2.17 | 0.45 |
| 1:J:402:GLN:HG3 | 7:J:2041:HOH:O | 2.17 | 0.45 |
| 1:K:245:ARG:HG2 | 1:K:245:ARG:NH1 | 2.32 | 0.45 |
| 1:K:359:THR:HG22 | 1:K:362:LYS:CG | 2.47 | 0.45 |
| 1:L:243:THR:HG21 | 1:L:273:TYR:HD2 | 1.81 | 0.45 |
| 1:L:454:LEU:HD22 | 1:L:454:LEU:H | 1.81 | 0.45 |
| 1:N:309:PHE:HB2 | 1:N:343:MSE:HG2 | 1.98 | 0.45 |
| 1:O:120:CYS:O | 1:O:175:TYR:HB3 | 2.16 | 0.45 |
| 1:O:571:THR:HG23 | 1:O:572:TRP:N | 2.32 | 0.45 |
| 1:P:222:ARG:HH11 | 1:P:222:ARG:HG3 | 1.82 | 0.45 |
| 1:A:456:SER:HB3 | 7:A:2023:HOH:O | 2.16 | 0.45 |
| 1:A:470:VAL:HG13 | 1:A:494:THR:HG21 | 1.99 | 0.45 |
| 1:C:252:ILE:HD12 | 1:C:252:ILE:N | 2.32 | 0.45 |
| 1:C:312:ALA:CB | 1:C:362:LYS:HE2 | 2.47 | 0.45 |
| 1:E:112:TYR:CG | 1:E:186:LEU:HD11 | 2.52 | 0.45 |
| 1:F:33:HIS:HD2 | 1:F:93:GLU:OE2 | 2.00 | 0.45 |
| 1:H:427:GLU:CD | 1:H:427:GLU:H | 2.19 | 0.45 |
| 1:I:399:PHE:HB2 | 1:I:428:CYS:HB3 | 1.98 | 0.45 |
| 1:J:429:THR:HG22 | 1:J:431:GLU:N | 2.30 | 0.45 |
| 1:J:61:GLN:HE21 | 1:J:98:LYS:HE2 | 1.82 | 0.45 |
| 1:L:68:ILE:HD13 | 7:L:2009:HOH:O | 2.17 | 0.45 |
| 1:N:138:HIS:NE2 | 1:N:223:HIS:CE1 | 2.83 | 0.45 |
| 1:N:350:ILE:HG23 | 1:N:358:LEU:CD1 | 2.47 | 0.45 |
| 1:N:493:THR:HG23 | 1:N:529:ARG:NH1 | 2.32 | 0.45 |
| 1:P:454:LEU:HD21 | 1:P:460:LEU:CD1 | 2.44 | 0.45 |
| 1:A:136:THR:CG2 | 1:A:137:ILE:N | 2.80 | 0.45 |
| 1:H:483:LEU:HD12 | 1:H:539:THR:HB | 1.99 | 0.45 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:61:GLN:O | 1:H:65:VAL:HG23 | 2.17 | 0.45 |
| 1:I:359:THR:HG22 | 1:I:362:LYS:HG3 | 1.98 | 0.45 |
| 1:I:376:ASN:O | 1:I:380:ILE:HG13 | 2.16 | 0.45 |
| 1:K:314:GLU:HB2 | 2:K:1581:NAP:O1N | 2.17 | 0.45 |
| 1:K:288:VAL:HG12 | 1:K:292:LEU:HD22 | 1.98 | 0.45 |
| 1:L:442:ILE:HG22 | 1:L:512:LEU:HD11 | 1.99 | 0.45 |
| 1:O:189:ALA:O | 1:O:520:GLN:NE2 | 2.41 | 0.45 |
| 1:O:357:SER:C | 1:O:358:LEU:HD12 | 2.35 | 0.45 |
| 1:P:132:GLY:HA2 | 1:P:200:PRO:HG2 | 1.98 | 0.45 |
| 1:A:270:ARG:HH11 | 1:A:270:ARG:HG2 | 1.81 | 0.45 |
| 1:C:556:GLN:CA | 1:C:556:GLN:HE21 | 2.29 | 0.45 |
| 1:D:160:VAL:HG11 | 1:D:238:PHE:CZ | 2.51 | 0.45 |
| 1:E:343:MSE:HE3 | 1:E:365:PHE:CG | 2.51 | 0.45 |
| 1:G:454:LEU:HB3 | 1:G:455:PRO:HD2 | 1.99 | 0.45 |
| 1:G:528:VAL:CG1 | 1:G:532:LYS:HE2 | 2.47 | 0.45 |
| 1:H:284:ALA:O | 1:H:288:VAL:HG23 | 2.17 | 0.45 |
| 1:H:359:THR:HG23 | 1:H:361:GLU:N | 2.31 | 0.45 |
| 1:J:319:ILE:O | 1:J:323:ILE:HG13 | 2.17 | 0.45 |
| 1:L:183:LYS:NZ | 1:L:467:ASN:ND2 | 2.65 | 0.45 |
| 1:L:137:ILE:HB | 1:L:205:VAL:HG12 | 1.98 | 0.45 |
| 1:L:285:SER:HB3 | 1:L:470:VAL:HG21 | 1.98 | 0.45 |
| 1:M:529:ARG:NH1 | 1:M:529:ARG:HG2 | 2.32 | 0.45 |
| 1:M:578:LYS:NZ | 1:M:580:LYS:CA | 2.79 | 0.45 |
| 1:N:108:MSE:N | 1:N:109:PRO:CD | 2.80 | 0.45 |
| 1:D:529:ARG:HA | 1:D:529:ARG:HD2 | 1.81 | 0.44 |
| 1:E:305:HIS:O | 1:E:340:ARG:NH1 | 2.50 | 0.44 |
| 1:E:420:SER:HA | 2:E:1581:NAP:H1D | 1.99 | 0.44 |
| 1:G:335:GLU:HG3 | 1:G:336:GLU:N | 2.33 | 0.44 |
| 1:H:327:MSE:HE1 | 1:H:337:ALA:O | 2.17 | 0.44 |
| 1:H:324:VAL:HG12 | 1:H:328:GLN:HE21 | 1.81 | 0.44 |
| 1:I:533:GLU:HG3 | 1:I:537:ASN:HD21 | 1.80 | 0.44 |
| 1:K:209:ASN:OD1 | 1:K:211:THR:HB | 2.17 | 0.44 |
| 1:K:220:GLY:HA2 | 1:L:56:PRO:HG2 | 1.98 | 0.44 |
| 1:M:162:ASP:O | 1:M:225:ARG:NH2 | 2.39 | 0.44 |
| 1:M:132:GLY:HA2 | 1:M:200:PRO:HG2 | 1.98 | 0.44 |
| 1:M:368:GLU:HG3 | 7:M:2044:HOH:O | 2.17 | 0.44 |
| 1:N:494:THR:HG23 | 1:N:526:ILE:HD13 | 1.98 | 0.44 |
| 1:O:146:MSE:HE3 | 1:P:51:HIS:NE2 | 2.31 | 0.44 |
| 1:P:61:GLN:HE21 | 1:P:98:LYS:HE3 | 1.82 | 0.44 |
| 1:B:276:PHE:HB2 | 1:B:281:GLN:OE1 | 2.16 | 0.44 |
| 1:B:332:VAL:HG13 | 1:B:336:GLU:HB3 | 1.98 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:322:LEU:HD21 | 1:C:492:LEU:HB2 | 2.00 | 0.44 |
| 1:A:42:LEU:CD2 | 1:C:577:MSE:HE3 | 2.36 | 0.44 |
| 1:G:303:SER:O | 1:G:340:ARG:CZ | 2.66 | 0.44 |
| 1:J:476:LEU:HD23 | 1:J:476:LEU:O | 2.18 | 0.44 |
| 1:K:24:LYS:N | 1:K:24:LYS:HD2 | 2.32 | 0.44 |
| 1:K:331:GLY:HA3 | 1:O:300:ASN:HA | 1.98 | 0.44 |
| 1:O:572:TRP:C | 1:O:573:PRO:O | 2.55 | 0.44 |
| 1:P:33:HIS:HD2 | 1:P:93:GLU:OE2 | 2.00 | 0.44 |
| 1:P:429:THR:CG2 | 1:P:430:ALA:N | 2.80 | 0.44 |
| 1:A:261:ASN:OD1 | 1:A:264:ARG:NH1 | 2.49 | 0.44 |
| 1:A:378:GLU:HA | 1:A:403:ILE:HD13 | 1.99 | 0.44 |
| 1:B:162:ASP:C | 1:B:202:MSE:HE1 | 2.37 | 0.44 |
| 1:B:92:ASN:ND2 | 1:B:92:ASN:C | 2.70 | 0.44 |
| 1:C:133:LEU:HB2 | 1:C:199:LEU:HD11 | 1.98 | 0.44 |
| 1:G:33:HIS:HD2 | 1:G:93:GLU:OE2 | 2.00 | 0.44 |
| 1:J:401:GLN:O | 1:J:405:GLN:HB2 | 2.18 | 0.44 |
| 1:K:154:VAL:C | 1:K:155:ILE:HD12 | 2.37 | 0.44 |
| 1:M:95:LEU:O | 1:M:99:VAL:HG23 | 2.17 | 0.44 |
| 1:O:327:MSE:HE1 | 1:O:341:ILE:CD1 | 2.47 | 0.44 |
| 1:O:94:LYS:HD3 | 1:O:558:TYR:OH | 2.18 | 0.44 |
| 1:B:332:VAL:CG1 | 1:B:333:SER:N | 2.80 | 0.44 |
| 1:B:389:LEU:CD1 | 1:B:407:MSE:HE3 | 2.44 | 0.44 |
| 1:C:261:ASN:O | 1:C:265:LEU:HG | 2.18 | 0.44 |
| 1:C:192:GLY:HA3 | 1:C:557:VAL:HG13 | 2.00 | 0.44 |
| 1:D:284:ALA:HA | 1:D:319:ILE:HG12 | 2.00 | 0.44 |
| 1:D:401:GLN:HG3 | 1:D:436:TYR:CD1 | 2.53 | 0.44 |
| 1:D:61:GLN:HE22 | 1:D:560:THR:HG23 | 1.83 | 0.44 |
| 1:F:227:ARG:HD3 | 7:F:2045:HOH:O | 2.16 | 0.44 |
| 1:F:92:ASN:C | 1:F:92:ASN:ND2 | 2.68 | 0.44 |
| 1:H:104:ILE:HG23 | 1:H:105:GLU:N | 2.31 | 0.44 |
| 1:L:466:ASN:HA | 2:L:1581:NAP:N7N | 2.24 | 0.44 |
| 1:M:222:ARG:HH11 | 1:M:222:ARG:HG3 | 1.83 | 0.44 |
| 1:M:30:ARG:O | 1:N:30:ARG:HD3 | 2.16 | 0.44 |
| 1:N:470:VAL:O | 1:N:474:VAL:HG23 | 2.17 | 0.44 |
| 1:O:110:ILE:O | 1:O:115:THR:HB | 2.18 | 0.44 |
| 1:P:35:ASN:ND2 | 1:P:37:GLY:H | 2.14 | 0.44 |
| 1:P:429:THR:HG23 | 7:P:2064:HOH:O | 2.17 | 0.44 |
| 1:A:284:ALA:O | 1:A:288:VAL:HG23 | 2.17 | 0.44 |
| 1:A:57:CYS:HB3 | 1:B:219:ILE:O | 2.18 | 0.44 |
| 1:B:100:LEU:HD21 | 1:B:111:VAL:HG21 | 1.99 | 0.44 |
| 1:C:154:VAL:HG13 | 1:C:154:VAL:O | 2.17 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:283:THR:HG23 | 1:E:284:ALA:N | 2.33 | 0.44 |
| 1:F:23:LYS:C | 1:F:24:LYS:HD2 | 2.38 | 0.44 |
| 1:K:188:THR:OG1 | 1:K:195:PRO:HG3 | 2.17 | 0.44 |
| 1:K:300:ASN:HD22 | 1:K:304:ASP:HB2 | 1.82 | 0.44 |
| 1:K:284:ALA:HA | 1:K:319:ILE:HG12 | 1.98 | 0.44 |
| 1:K:284:ALA:HB1 | 1:K:322:LEU:HB2 | 1.99 | 0.44 |
| 1:K:429:THR:HG23 | 1:K:449:PHE:CD2 | 2.52 | 0.44 |
| 1:L:35:ASN:HD21 | 1:L:37:GLY:H | 1.60 | 0.44 |
| 1:N:415:ILE:HG12 | 1:N:442:ILE:HD12 | 1.99 | 0.44 |
| 1:O:429:THR:H | 1:O:432:GLN:HG3 | 1.83 | 0.44 |
| 1:O:285:SER:HB3 | 1:O:470:VAL:HG21 | 1.99 | 0.44 |
| 1:P:227:ARG:HG3 | 1:P:227:ARG:NH1 | 2.31 | 0.44 |
| 1:P:340:ARG:NH1 | 1:P:340:ARG:HG2 | 2.32 | 0.44 |
| 1:A:358:LEU:CD2 | 1:A:363:GLU:HG3 | 2.39 | 0.44 |
| 1:B:301:ARG:HH11 | 1:B:301:ARG:CB | 2.26 | 0.44 |
| 1:B:572:TRP:C | 1:B:573:PRO:O | 2.54 | 0.44 |
| 1:C:172:LEU:O | 1:C:175:TYR:HB2 | 2.17 | 0.44 |
| 1:C:556:GLN:CA | 1:C:556:GLN:NE2 | 2.80 | 0.44 |
| 1:C:92:ASN:C | 1:C:92:ASN:ND2 | 2.71 | 0.44 |
| 1:E:184:LEU:O | 1:E:187:TYR:HB2 | 2.18 | 0.44 |
| 1:F:324:VAL:O | 1:F:328:GLN:HG3 | 2.18 | 0.44 |
| 1:G:467:ASN:HB3 | 1:G:471:PHE:HD2 | 1.83 | 0.44 |
| 1:H:359:THR:CG2 | 1:H:361:GLU:HB2 | 2.48 | 0.44 |
| 1:I:165:ARG:NH2 | 1:I:279:ASP:OD1 | 2.48 | 0.44 |
| 1:J:33:HIS:HD2 | 1:J:93:GLU:OE1 | 1.98 | 0.44 |
| 1:L:41:THR:CG2 | 1:L:42:LEU:N | 2.81 | 0.44 |
| 1:L:61:GLN:HG3 | 1:L:562:TYR:CE1 | 2.52 | 0.44 |
| 1:N:401:GLN:HG2 | 1:N:436:TYR:CZ | 2.53 | 0.44 |
| 1:O:158:ILE:HG12 | 1:O:199:LEU:HB3 | 1.99 | 0.44 |
| 1:O:41:THR:HG21 | 7:O:2006:HOH:O | 2.18 | 0.44 |
| 1:O:471:PHE:CD1 | 1:O:472:PRO:HD3 | 2.52 | 0.44 |
| 1:P:136:THR:CG2 | 1:P:137:ILE:N | 2.80 | 0.44 |
| 1:A:151:PRO:HG2 | 1:A:152:GLU:OE1 | 2.17 | 0.44 |
| 1:A:172:LEU:HA | 1:A:212:LEU:HD11 | 2.00 | 0.44 |
| 1:B:188:THR:HG21 | 1:B:195:PRO:HG3 | 2.00 | 0.44 |
| 1:B:433:LEU:C | 1:B:433:LEU:HD13 | 2.37 | 0.44 |
| 1:C:507:LEU:HD12 | 1:C:507:LEU:HA | 1.79 | 0.44 |
| 1:C:533:GLU:HG3 | 1:C:537:ASN:HD21 | 1.83 | 0.44 |
| 1:E:133:LEU:HB3 | 1:E:201:VAL:HG22 | 1.98 | 0.44 |
| 1:E:476:LEU:HB3 | 1:E:527:ALA:HB2 | 1.98 | 0.44 |
| 1:F:429:THR:HG23 | 1:F:449:PHE:CE2 | 2.53 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:399:PHE:CD1 | 1:G:399:PHE:N | 2.86 | 0.44 |
| 1:G:61:GLN:NE2 | 1:G:98:LYS:HD3 | 2.33 | 0.44 |
| 1:I:110:ILE:O | 1:I:115:THR:HB | 2.18 | 0.44 |
| 1:I:401:GLN:HG3 | 1:I:402:GLN:NE2 | 2.33 | 0.44 |
| 1:K:159:VAL:HG23 | 1:K:184:LEU:HD21 | 2.00 | 0.44 |
| 1:L:266:LEU:O | 1:L:270:ARG:HB2 | 2.18 | 0.44 |
| 1:M:578:LYS:HZ1 | 1:M:580:LYS:CB | 2.22 | 0.44 |
| 1:O:284:ALA:HA | 1:O:319:ILE:HG12 | 2.00 | 0.44 |
| 1:B:165:ARG:O | 1:B:256:ASP:HB3 | 2.17 | 0.44 |
| 1:C:177:MSE:HG2 | 1:C:202:MSE:CG | 2.47 | 0.44 |
| 1:C:351:VAL:O | 1:C:354:ARG:HB2 | 2.18 | 0.44 |
| 1:D:152:GLU:OE1 | 1:D:196:HIS:NE2 | 2.51 | 0.44 |
| 1:F:227:ARG:CG | 1:F:227:ARG:NH1 | 2.79 | 0.44 |
| 1:H:123:TYR:HB3 | 1:H:175:TYR:CD2 | 2.52 | 0.44 |
| 1:I:401:GLN:HB2 | 1:I:436:TYR:CD1 | 2.53 | 0.44 |
| 1:I:578:LYS:HE3 | 1:I:580:LYS:HB2 | 2.00 | 0.44 |
| 1:J:381:VAL:HG13 | 1:J:407:MSE:HE1 | 2.00 | 0.44 |
| 1:K:137:ILE:HD13 | 1:K:226:ILE:HB | 2.00 | 0.44 |
| 1:K:66:TYR:C | 1:K:66:TYR:CD1 | 2.91 | 0.44 |
| 1:L:172:LEU:O | 1:L:175:TYR:HB2 | 2.18 | 0.44 |
| 1:L:399:PHE:HB2 | 1:L:428:CYS:HB3 | 2.00 | 0.44 |
| 1:L:401:GLN:HB2 | 1:L:436:TYR:CG | 2.53 | 0.44 |
| 1:N:50:ILE:HA | 1:N:53:LEU:HD12 | 1.99 | 0.44 |
| 1:O:160:VAL:HG12 | 1:O:161:THR:N | 2.32 | 0.44 |
| 1:O:36:LYS:HD2 | 1:O:562:TYR:CG | 2.53 | 0.44 |
| 1:P:264:ARG:HG3 | 1:P:265:LEU:N | 2.31 | 0.44 |
| 1:P:274:CYS:SG | 1:P:478:VAL:HG11 | 2.58 | 0.44 |
| 1:P:516:LEU:O | 1:P:519:ILE:HG22 | 2.18 | 0.44 |
| 1:A:342:TRP:CE2 | 1:A:384:ILE:HD12 | 2.53 | 0.44 |
| 1:A:570:TYR:CE2 | 1:D:142:HIS:CG | 3.06 | 0.44 |
| 1:B:324:VAL:HG12 | 1:B:328:GLN:HE21 | 1.83 | 0.44 |
| 1:D:120:CYS:O | 1:D:175:TYR:HB3 | 2.18 | 0.44 |
| 1:E:315:ALA:O | 1:E:319:ILE:HG13 | 2.17 | 0.44 |
| 1:E:433:LEU:CD1 | 1:E:443:PHE:HB2 | 2.47 | 0.44 |
| 1:E:77:SER:HB3 | 1:E:80:ASP:OD2 | 2.18 | 0.44 |
| 1:F:327:MSE:HE1 | 1:F:337:ALA:O | 2.17 | 0.44 |
| 1:G:251:LEU:HD23 | 1:G:274:CYS:SG | 2.58 | 0.44 |
| 1:G:315:ALA:O | 1:G:319:ILE:HG13 | 2.18 | 0.44 |
| 1:G:327:MSE:HE2 | 1:G:337:ALA:HA | 2.00 | 0.44 |
| 1:G:493:THR:HG23 | 1:G:529:ARG:NH1 | 2.33 | 0.44 |
| 1:G:572:TRP:O | 1:G:577:MSE:HE2 | 2.18 | 0.44 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:296:ARG:O | 1:H:299:LYS:NZ | 2.51 | 0.44 |
| 1:H:394:ALA:HA | 1:H:420:SER:HB3 | 1.99 | 0.44 |
| 1:F:46:GLN:OE1 | 1:H:569:SER:HA | 2.18 | 0.44 |
| 1:I:162:ASP:C | 1:I:162:ASP:OD1 | 2.57 | 0.44 |
| 1:J:184:LEU:O | 1:J:187:TYR:HB2 | 2.17 | 0.44 |
| 1:J:312:ALA:HB3 | 1:J:362:LYS:HE2 | 1.98 | 0.44 |
| 1:L:138:HIS:NE2 | 1:L:223:HIS:HE1 | 2.16 | 0.44 |
| 1:M:145:THR:O | 1:M:148:GLN:HB2 | 2.17 | 0.44 |
| 1:N:471:PHE:CG | 1:N:472:PRO:HD3 | 2.52 | 0.44 |
| 1:O:154:VAL:HG22 | 1:O:154:VAL:O | 2.18 | 0.44 |
| 1:O:41:THR:CG2 | 1:O:42:LEU:N | 2.80 | 0.44 |
| 1:P:433:LEU:C | 1:P:433:LEU:HD13 | 2.38 | 0.44 |
| 1:B:123:TYR:HB3 | 1:B:175:TYR:CD2 | 2.53 | 0.43 |
| 1:D:152:GLU:HB3 | 1:D:155:ILE:HD11 | 2.00 | 0.43 |
| 1:B:24:LYS:CD | 1:D:24:LYS:NZ | 2.81 | 0.43 |
| 1:F:100:LEU:HD23 | 1:F:107:PHE:HB3 | 1.99 | 0.43 |
| 1:F:108:MSE:HE2 | 1:F:190:CYS:SG | 2.58 | 0.43 |
| 1:F:354:ARG:HG2 | 1:F:356:ALA:H | 1.81 | 0.43 |
| 1:F:350:ILE:CD1 | 1:F:362:LYS:HD3 | 2.43 | 0.43 |
| 1:G:471:PHE:CG | 1:G:472:PRO:HD3 | 2.53 | 0.43 |
| 1:I:334:LYS:O | 1:I:338:ILE:HG13 | 2.18 | 0.43 |
| 1:I:416:ILE:CG1 | 1:I:433:LEU:HD21 | 2.46 | 0.43 |
| 1:K:74:ARG:HD3 | 1:L:125:LEU:HD11 | 2.00 | 0.43 |
| 1:L:108:MSE:N | 1:L:109:PRO:CD | 2.81 | 0.43 |
| 1:L:42:LEU:O | 1:L:46:GLN:HG3 | 2.17 | 0.43 |
| 1:M:164:GLU:HG2 | 1:M:258:ALA:HB2 | 1.99 | 0.43 |
| 1:M:478:VAL:HG13 | 1:M:483:LEU:HB3 | 2.00 | 0.43 |
| 1:M:33:HIS:HD2 | 1:M:93:GLU:OE2 | 2.00 | 0.43 |
| 1:N:270:ARG:NH1 | 1:N:270:ARG:HG2 | 2.30 | 0.43 |
| 1:A:165:ARG:O | 1:A:256:ASP:HB3 | 2.18 | 0.43 |
| 1:B:165:ARG:O | 1:B:165:ARG:NE | 2.49 | 0.43 |
| 1:C:174:CYS:HB2 | 1:C:220:GLY:HA3 | 1.99 | 0.43 |
| 1:E:132:GLY:CA | 1:E:200:PRO:HG2 | 2.47 | 0.43 |
| 1:E:412:LYS:O | 1:E:413:ARG:HD2 | 2.18 | 0.43 |
| 1:F:284:ALA:HA | 1:F:319:ILE:HG12 | 2.00 | 0.43 |
| 1:F:554:ARG:HG2 | 1:F:554:ARG:NH1 | 2.32 | 0.43 |
| 1:G:136:THR:CG2 | 1:G:137:ILE:N | 2.81 | 0.43 |
| 1:H:157:ALA:HB2 | 1:H:479:ILE:HD11 | 1.99 | 0.43 |
| 1:H:160:VAL:HG21 | 1:H:238:PHE:CE2 | 2.52 | 0.43 |
| 1:H:268:LYS:HG2 | 1:H:269:TYR:CE2 | 2.52 | 0.43 |
| 1:J:314:GLU:HB2 | 2:J:1581:NAP:O1N | 2.18 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:516:LEU:H | 1:J:516:LEU:HD22 | 1.82 | 0.43 |
| 1:K:359:THR:HG22 | 1:K:362:LYS:HG3 | 2.00 | 0.43 |
| 1:J:24:LYS:CD | 1:L:24:LYS:HD2 | 2.48 | 0.43 |
| 1:N:85:LEU:HD12 | 1:N:110:ILE:CG2 | 2.48 | 0.43 |
| 1:N:389:LEU:HD22 | 1:N:399:PHE:CZ | 2.52 | 0.43 |
| 1:N:557:VAL:HG12 | 1:N:558:TYR:N | 2.33 | 0.43 |
| 1:P:530:ILE:HG12 | 7:P:2072:HOH:O | 2.19 | 0.43 |
| 1:B:171:ASP:OD2 | 1:B:225:ARG:HD2 | 2.19 | 0.43 |
| 1:B:166:ILE:HG21 | 1:B:172:LEU:HD12 | 2.01 | 0.43 |
| 1:B:41:THR:CG2 | 1:B:42:LEU:N | 2.81 | 0.43 |
| 1:C:404:LEU:HD13 | 1:C:433:LEU:HA | 2.00 | 0.43 |
| 1:C:413:ARG:HD2 | 7:C:2047:HOH:O | 2.18 | 0.43 |
| 1:D:359:THR:HG23 | 1:D:360:PRO:CD | 2.44 | 0.43 |
| 1:H:156:LYS:HD2 | 1:H:197:GLN:OE1 | 2.19 | 0.43 |
| 1:H:266:LEU:O | 1:H:270:ARG:HB2 | 2.18 | 0.43 |
| 1:H:98:LYS:HD3 | 1:H:560:THR:HG21 | 2.00 | 0.43 |
| 1:I:374:MSE:HE1 | 1:I:379:ASP:HB3 | 1.99 | 0.43 |
| 1:I:41:THR:CG2 | 1:I:42:LEU:N | 2.81 | 0.43 |
| 1:K:172:LEU:O | 1:K:175:TYR:HB2 | 2.18 | 0.43 |
| 1:K:196:HIS:HB2 | 7:K:2017:HOH:O | 2.18 | 0.43 |
| 1:K:322:LEU:HD21 | 1:K:492:LEU:HB2 | 2.00 | 0.43 |
| 1:L:529:ARG:HH11 | 1:L:529:ARG:HG3 | 1.82 | 0.43 |
| 1:O:165:ARG:C | 1:O:165:ARG:HD2 | 2.39 | 0.43 |
| 1:O:327:MSE:HE1 | 1:O:341:ILE:HD11 | 2.00 | 0.43 |
| 1:P:82:TYR:CE2 | 1:P:86:MSE:HG3 | 2.53 | 0.43 |
| 1:A:229:GLN:NE2 | 1:A:229:GLN:CA | 2.81 | 0.43 |
| 1:B:23:LYS:HG2 | 1:B:24:LYS:H | 1.82 | 0.43 |
| 1:B:303:SER:HB2 | 1:B:332:VAL:HG21 | 1.98 | 0.43 |
| 1:B:428:CYS:CB | 1:B:432:GLN:HE21 | 2.31 | 0.43 |
| 1:D:573:PRO:O | 1:D:577:MSE:HE2 | 2.19 | 0.43 |
| 1:F:428:CYS:HA | 1:F:432:GLN:HE22 | 1.84 | 0.43 |
| 1:G:334:LYS:O | 1:G:338:ILE:HG13 | 2.18 | 0.43 |
| 1:G:375:LYS:HB2 | 1:G:375:LYS:HE3 | 1.89 | 0.43 |
| 1:H:322:LEU:HD23 | 1:H:322:LEU:HA | 1.88 | 0.43 |
| 1:J:374:MSE:CE | 1:J:379:ASP:HB3 | 2.49 | 0.43 |
| 1:J:507:LEU:HD13 | 1:J:511:ARG:O | 2.18 | 0.43 |
| 1:K:245:ARG:NH1 | 7:K:2015:HOH:O | 2.50 | 0.43 |
| 1:L:483:LEU:CD1 | 1:L:539:THR:HB | 2.44 | 0.43 |
| 1:N:245:ARG:HG2 | 1:N:246:TYR:CD2 | 2.52 | 0.43 |
| 1:O:104:ILE:CG1 | 1:O:108:MSE:CE | 2.92 | 0.43 |
| 1:P:38:MSE:HE3 | 5:P:1589:CL:CL | 2.55 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:104:ILE:HD11 | 1:A:108:MSE:CE | 2.48 | 0.43 |
| 1:A:406:ASP:HB3 | 1:A:410:PHE:CZ | 2.54 | 0.43 |
| 1:A:429:THR:CG2 | 1:A:430:ALA:H | 2.30 | 0.43 |
| 1:A:401:GLN:HG2 | 1:A:436:TYR:CD1 | 2.53 | 0.43 |
| 1:A:91:ARG:HB2 | 1:B:129:ARG:NH1 | 2.34 | 0.43 |
| 1:B:429:THR:H | 1:B:432:GLN:HE21 | 1.66 | 0.43 |
| 1:B:98:LYS:HD3 | 1:B:560:THR:HG23 | 1.99 | 0.43 |
| 1:C:166:ILE:HG23 | 1:C:179:ILE:HG13 | 2.00 | 0.43 |
| 1:C:471:PHE:CG | 1:C:472:PRO:HD3 | 2.54 | 0.43 |
| 1:C:63:ALA:O | 1:C:66:TYR:HB3 | 2.18 | 0.43 |
| 1:D:155:ILE:HD13 | 1:D:246:TYR:CZ | 2.53 | 0.43 |
| 1:D:98:LYS:HD3 | 1:D:560:THR:HG23 | 1.99 | 0.43 |
| 1:E:215:ASP:O | 1:E:222:ARG:NH2 | 2.49 | 0.43 |
| 1:E:529:ARG:HG2 | 1:E:529:ARG:HH11 | 1.82 | 0.43 |
| 1:F:136:THR:HB | 1:F:139:ASP:OD2 | 2.18 | 0.43 |
| 1:F:177:MSE:HE2 | 1:F:180:PRO:HD2 | 2.01 | 0.43 |
| 1:F:188:THR:OG1 | 1:F:195:PRO:HG3 | 2.17 | 0.43 |
| 1:H:194:LYS:HD2 | 1:H:197:GLN:HE22 | 1.83 | 0.43 |
| 1:K:387:THR:HG22 | 1:K:411:ASN:OD1 | 2.18 | 0.43 |
| 1:L:165:ARG:NH2 | 2:L:1581:NAP:O1N | 2.50 | 0.43 |
| 1:L:374:MSE:HE1 | 1:L:379:ASP:C | 2.39 | 0.43 |
| 1:O:515:PRO:HG2 | 5:O:1588:CL:CL | 2.56 | 0.43 |
| 1:O:494:THR:HG23 | 1:O:526:ILE:HD13 | 2.00 | 0.43 |
| 1:O:78:ASP:HA | 1:O:81:ARG:NH1 | 2.34 | 0.43 |
| 1:P:177:MSE:HE2 | 1:P:202:MSE:HB3 | 2.00 | 0.43 |
| 1:P:388:VAL:HG22 | 1:P:415:ILE:HB | 2.00 | 0.43 |
| 1:B:136:THR:CG2 | 1:B:221:LEU:HD11 | 2.45 | 0.43 |
| 1:B:352:LYS:CE | 1:B:353:GLY:N | 2.80 | 0.43 |
| 1:C:117:GLY:O | 1:C:121:GLN:HG3 | 2.18 | 0.43 |
| 1:C:174:CYS:HB3 | 1:C:219:ILE:HD12 | 2.00 | 0.43 |
| 1:E:137:ILE:HA | 1:E:234:LEU:CD2 | 2.47 | 0.43 |
| 1:E:445:SER:HG | 1:E:449:PHE:HD1 | 1.61 | 0.43 |
| 1:F:420:SER:HA | 2:F:1581:NAP:H1D | 2.01 | 0.43 |
| 1:G:26:TYR:HE1 | 1:G:30:ARG:NH1 | 2.17 | 0.43 |
| 1:H:309:PHE:HB2 | 1:H:343:MSE:HG2 | 2.01 | 0.43 |
| 1:H:442:ILE:HG22 | 1:H:512:LEU:HD11 | 2.01 | 0.43 |
| 1:K:104:ILE:O | 1:K:108:MSE:HB2 | 2.18 | 0.43 |
| 1:K:120:CYS:O | 1:K:175:TYR:HB3 | 2.19 | 0.43 |
| 1:N:117:GLY:O | 1:N:121:GLN:HG3 | 2.18 | 0.43 |
| 1:N:322:LEU:HD23 | 1:N:322:LEU:HA | 1.83 | 0.43 |
| 1:N:578:LYS:HE3 | 1:N:580:LYS:HB2 | 2.01 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:86:MSE:CE | 1:N:89:GLN:NE2 | 2.81 | 0.43 |
| 1:O:137:ILE:HA | 1:O:234:LEU:HD22 | 1.99 | 0.43 |
| 1:O:71:ASN:OD1 | 1:P:125:LEU:HD23 | 2.19 | 0.43 |
| 1:A:394:ALA:HB2 | 2:A:1581:NAP:O3D | 2.18 | 0.43 |
| 1:A:132:GLY:CA | 1:A:200:PRO:HG2 | 2.48 | 0.43 |
| 1:B:467:ASN:O | 1:B:470:VAL:N | 2.41 | 0.43 |
| 1:C:174:CYS:SG | 1:C:219:ILE:HD12 | 2.58 | 0.43 |
| 1:D:135:ILE:HB | 1:D:203:LEU:HD23 | 1.99 | 0.43 |
| 1:D:86:MSE:HE1 | 1:D:89:GLN:NE2 | 2.34 | 0.43 |
| 1:H:229:GLN:HG3 | 1:H:233:ASP:OD2 | 2.18 | 0.43 |
| 1:I:245:ARG:HH11 | 1:I:245:ARG:CG | 2.31 | 0.43 |
| 1:J:512:LEU:HA | 1:J:512:LEU:HD23 | 1.86 | 0.43 |
| 1:J:570:TYR:OH | 1:K:139:ASP:HB3 | 2.19 | 0.43 |
| 1:K:165:ARG:C | 1:K:165:ARG:HD2 | 2.39 | 0.43 |
| 1:N:392:VAL:HG23 | 1:N:392:VAL:O | 2.18 | 0.43 |
| 1:N:536:ARG:CG | 1:N:536:ARG:HH11 | 2.32 | 0.43 |
| 1:P:100:LEU:HD21 | 1:P:111:VAL:HG21 | 2.01 | 0.43 |
| 1:P:340:ARG:HG2 | 1:P:340:ARG:HH11 | 1.83 | 0.43 |
| 1:P:516:LEU:HD12 | 1:P:516:LEU:HA | 1.81 | 0.43 |
| 1:B:36:LYS:H | 1:B:40:PHE:HE1 | 1.65 | 0.43 |
| 1:B:413:ARG:NH1 | 1:B:413:ARG:HG3 | 2.34 | 0.43 |
| 1:B:77:SER:O | 1:B:81:ARG:HG3 | 2.18 | 0.43 |
| 1:C:285:SER:HB3 | 1:C:470:VAL:HG21 | 2.00 | 0.43 |
| 1:D:376:ASN:HB3 | 1:D:379:ASP:OD2 | 2.18 | 0.43 |
| 1:D:516:LEU:O | 1:D:519:ILE:HG22 | 2.19 | 0.43 |
| 1:E:274:CYS:SG | 1:E:478:VAL:HG11 | 2.59 | 0.43 |
| 1:E:374:MSE:CE | 1:E:379:ASP:HB3 | 2.48 | 0.43 |
| 1:E:56:PRO:HG2 | 1:F:220:GLY:HA2 | 2.01 | 0.43 |
| 1:F:286:VAL:HG22 | 1:F:513:TYR:CE2 | 2.54 | 0.43 |
| 1:F:521:GLN:HE22 | 1:F:554:ARG:HH22 | 1.66 | 0.43 |
| 1:G:56:PRO:HG2 | 1:H:220:GLY:HA2 | 2.01 | 0.43 |
| 1:J:165:ARG:C | 1:J:165:ARG:HD2 | 2.39 | 0.43 |
| 1:J:164:GLU:OE2 | 1:J:227:ARG:NH2 | 2.52 | 0.43 |
| 1:K:79:LEU:HD13 | 1:K:118:LEU:CD1 | 2.48 | 0.43 |
| 1:K:352:LYS:HD3 | 1:K:368:GLU:HG2 | 2.00 | 0.43 |
| 1:K:534:ALA:HA | 1:K:539:THR:OG1 | 2.19 | 0.43 |
| 1:N:210:GLU:HA | 1:N:213:LEU:HD12 | 1.99 | 0.43 |
| 1:N:215:ASP:HA | 1:N:216:PRO:HD2 | 1.92 | 0.43 |
| 1:O:172:LEU:O | 1:O:175:TYR:HB2 | 2.18 | 0.43 |
| 1:O:218:TYR:HB3 | 1:O:222:ARG:HH12 | 1.83 | 0.43 |
| 1:O:58:PHE:CD1 | 1:O:58:PHE:N | 2.86 | 0.43 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:148:GLN:HA | 1:C:245:ARG:HH21 | 1.84 | 0.43 |
| 1:D:243:THR:HG21 | 1:D:273:TYR:CD2 | 2.54 | 0.43 |
| 1:E:284:ALA:HA | 1:E:319:ILE:HG12 | 2.01 | 0.43 |
| 1:F:545:GLN:HA | 1:F:546:PRO:HD3 | 1.87 | 0.43 |
| 1:G:105:GLU:HG2 | 1:G:516:LEU:HD23 | 2.01 | 0.43 |
| 1:G:164:GLU:HB2 | 1:G:225:ARG:NH2 | 2.34 | 0.43 |
| 1:G:448:PRO:HD3 | 1:G:464:GLN:NE2 | 2.33 | 0.43 |
| 1:H:61:GLN:HG3 | 1:H:562:TYR:CE1 | 2.54 | 0.43 |
| 1:L:207:THR:O | 1:L:224:LYS:HA | 2.19 | 0.43 |
| 1:M:417:PHE:CD1 | 1:M:444:ALA:HB3 | 2.54 | 0.43 |
| 1:N:160:VAL:HG21 | 1:N:238:PHE:HE2 | 1.84 | 0.43 |
| 1:O:385:LYS:HE3 | 1:O:410:PHE:CD1 | 2.53 | 0.43 |
| 1:O:305:HIS:CD2 | 1:O:387:THR:OG1 | 2.72 | 0.43 |
| 1:B:245:ARG:HG2 | 1:B:246:TYR:CE2 | 2.54 | 0.43 |
| 1:B:78:ASP:HA | 1:B:81:ARG:HH11 | 1.84 | 0.43 |
| 1:D:239:MSE:HE1 | 1:D:252:ILE:HG21 | 2.01 | 0.43 |
| 1:E:284:ALA:O | 1:E:288:VAL:HG23 | 2.18 | 0.43 |
| 1:E:466:ASN:HA | 2:E:1581:NAP:H72N | 1.83 | 0.43 |
| 1:H:167:LEU:HB3 | 1:H:168:GLY:H | 1.67 | 0.43 |
| 1:J:92:ASN:ND2 | 1:J:92:ASN:C | 2.72 | 0.43 |
| 1:O:174:CYS:SG | 1:O:219:ILE:HD12 | 2.59 | 0.43 |
| 1:O:59:LEU:HB2 | 1:O:63:ALA:HB3 | 2.01 | 0.43 |
| 1:A:404:LEU:HD22 | 1:A:433:LEU:CD2 | 2.49 | 0.42 |
| 1:A:492:LEU:O | 1:A:496:GLU:HG3 | 2.19 | 0.42 |
| 1:A:516:LEU:O | 1:A:519:ILE:HG22 | 2.19 | 0.42 |
| 1:B:39:ALA:CB | 1:B:562:TYR:CE1 | 3.02 | 0.42 |
| 1:C:177:MSE:O | 1:C:180:PRO:HD2 | 2.19 | 0.42 |
| 1:C:261:ASN:HA | 1:C:264:ARG:NH1 | 2.34 | 0.42 |
| 1:C:497:VAL:CG1 | 1:C:526:ILE:HD13 | 2.48 | 0.42 |
| 1:D:140:ARG:NH1 | 1:D:230:ALA:HA | 2.34 | 0.42 |
| 1:D:359:THR:CG2 | 1:D:360:PRO:HD2 | 2.47 | 0.42 |
| 1:D:47:GLN:HE22 | 1:D:566:VAL:CG1 | 2.32 | 0.42 |
| 1:E:166:ILE:HG23 | 1:E:179:ILE:HG13 | 2.01 | 0.42 |
| 1:E:136:THR:CG2 | 1:E:221:LEU:HD11 | 2.49 | 0.42 |
| 1:E:471:PHE:N | 1:E:472:PRO:CD | 2.82 | 0.42 |
| 1:F:100:LEU:HD23 | 1:F:107:PHE:CB | 2.49 | 0.42 |
| 1:F:164:GLU:HG2 | 1:F:258:ALA:HB2 | 2.01 | 0.42 |
| 1:G:376:ASN:OD1 | 1:G:378:GLU:N | 2.52 | 0.42 |
| 1:J:402:GLN:CD | 1:J:402:GLN:N | 2.72 | 0.42 |
| 1:L:467:ASN:ND2 | 3:L:1582:OXL:O2 | 2.51 | 0.42 |
| 1:L:500:GLN:HE21 | 1:L:500:GLN:CA | 2.31 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:M:467:ASN:H | 2:M:1581:NAP:H72N | 1.67 | 0.42 |
| 1:M:471:PHE:CG | 1:M:472:PRO:HD3 | 2.54 | 0.42 |
| 1:N:152:GLU:CD | 1:N:196:HIS:NE2 | 2.73 | 0.42 |
| 1:O:210:GLU:HG2 | 7:O:2040:HOH:O | 2.18 | 0.42 |
| 1:O:354:ARG:HG3 | 1:O:373:GLU:OE2 | 2.19 | 0.42 |
| 1:P:202:MSE:HE2 | 1:P:203:LEU:C | 2.40 | 0.42 |
| 1:P:467:ASN:ND2 | 3:P:1582:OXL:O2 | 2.52 | 0.42 |
| 1:P:554:ARG:HG2 | 1:P:554:ARG:HH11 | 1.84 | 0.42 |
| 1:P:59:LEU:HB2 | 1:P:63:ALA:HB3 | 2.01 | 0.42 |
| 1:A:136:THR:HG23 | 1:A:137:ILE:N | 2.34 | 0.42 |
| 1:A:315:ALA:O | 1:A:319:ILE:HG13 | 2.20 | 0.42 |
| 1:A:408:ALA:HB1 | 1:A:440:ARG:HH22 | 1.84 | 0.42 |
| 1:A:388:VAL:HG22 | 1:A:415:ILE:HB | 2.00 | 0.42 |
| 1:B:431:GLU:OE1 | 1:B:452:VAL:HG13 | 2.19 | 0.42 |
| 1:C:61:GLN:HA | 1:C:64:GLN:HE21 | 1.84 | 0.42 |
| 1:E:323:ILE:HG22 | 1:E:327:MSE:HE2 | 2.01 | 0.42 |
| 1:E:546:PRO:HB2 | 1:E:549:LEU:HD23 | 2.01 | 0.42 |
| 1:F:113:THR:CG2 | 1:F:114:PRO:HA | 2.49 | 0.42 |
| 1:F:153:SER:HA | 1:F:245:ARG:HH12 | 1.84 | 0.42 |
| 1:F:132:GLY:CA | 1:F:200:PRO:HG2 | 2.49 | 0.42 |
| 1:F:442:ILE:HG21 | 1:F:512:LEU:HD21 | 2.00 | 0.42 |
| 1:H:162:ASP:O | 1:H:225:ARG:NH2 | 2.52 | 0.42 |
| 1:H:359:THR:HG22 | 1:H:362:LYS:N | 2.15 | 0.42 |
| 1:J:303:SER:O | 1:J:340:ARG:CZ | 2.67 | 0.42 |
| 1:J:359:THR:HG22 | 1:J:362:LYS:HG3 | 2.00 | 0.42 |
| 1:J:78:ASP:HA | 1:J:81:ARG:HH11 | 1.83 | 0.42 |
| 1:M:319:ILE:O | 1:M:323:ILE:HG13 | 2.19 | 0.42 |
| 1:A:283:THR:O | 1:A:286:VAL:HG12 | 2.19 | 0.42 |
| 1:A:474:VAL:O | 1:A:478:VAL:HG23 | 2.19 | 0.42 |
| 1:B:359:THR:HG23 | 1:B:362:LYS:HD2 | 2.01 | 0.42 |
| 1:B:533:GLU:HG3 | 1:B:537:ASN:ND2 | 2.34 | 0.42 |
| 1:B:61:GLN:HE21 | 1:B:98:LYS:NZ | 2.17 | 0.42 |
| 1:C:401:GLN:HG3 | 1:C:436:TYR:CD1 | 2.55 | 0.42 |
| 1:L:300:ASN:OD1 | 1:L:305:HIS:CE1 | 2.73 | 0.42 |
| 1:N:514:PRO:HA | 1:N:515:PRO:HD3 | 1.96 | 0.42 |
| 1:N:578:LYS:NZ | 1:O:222:ARG:HD3 | 2.35 | 0.42 |
| 1:P:165:ARG:O | 1:P:165:ARG:HD2 | 2.20 | 0.42 |
| 1:P:202:MSE:HE2 | 1:P:204:ASP:HA | 2.01 | 0.42 |
| 1:A:368:GLU:O | 1:A:369:HIS:HB2 | 2.19 | 0.42 |
| 1:A:394:ALA:HA | 1:A:420:SER:HB3 | 2.00 | 0.42 |
| 1:C:433:LEU:HD13 | 1:C:433:LEU:C | 2.40 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:396:GLY:O | 1:D:426:ALA:O | 2.37 | 0.42 |
| 1:D:505:GLU:O | 1:D:509:GLU:HG3 | 2.19 | 0.42 |
| 1:C:129:ARG:CG | 1:D:91:ARG:HD3 | 2.49 | 0.42 |
| 1:E:162:ASP:CA | 1:E:202:MSE:HE1 | 2.49 | 0.42 |
| 1:G:553:ILE:O | 1:G:557:VAL:HG23 | 2.18 | 0.42 |
| 1:H:580:LYS:O | 1:H:580:LYS:HD3 | 2.19 | 0.42 |
| 1:I:389:LEU:CD1 | 1:I:407:MSE:HE3 | 2.48 | 0.42 |
| 1:J:381:VAL:CG1 | 1:J:407:MSE:HE1 | 2.49 | 0.42 |
| 1:J:157:ALA:HB2 | 1:J:479:ILE:HD11 | 2.00 | 0.42 |
| 1:J:575:GLU:CD | 1:J:575:GLU:H | 2.21 | 0.42 |
| 1:J:59:LEU:HD13 | 1:J:64:GLN:CG | 2.48 | 0.42 |
| 1:K:166:ILE:HD12 | 1:K:179:ILE:HG13 | 2.00 | 0.42 |
| 1:K:325:MSE:HE2 | 1:K:492:LEU:HD22 | 2.01 | 0.42 |
| 1:K:375:LYS:HB2 | 1:K:375:LYS:HE3 | 1.62 | 0.42 |
| 1:L:356:ALA:O | 1:L:358:LEU:HD23 | 2.19 | 0.42 |
| 1:L:378:GLU:CA | 1:L:403:ILE:HD11 | 2.48 | 0.42 |
| 1:L:548:ASP:C | 1:L:548:ASP:OD2 | 2.56 | 0.42 |
| 1:M:194:LYS:HA | 1:M:195:PRO:HD3 | 1.91 | 0.42 |
| 1:M:374:MSE:CE | 1:M:379:ASP:HB3 | 2.48 | 0.42 |
| 1:N:551:ALA:O | 1:N:554:ARG:HG2 | 2.19 | 0.42 |
| 1:A:279:ASP:O | 1:A:283:THR:CG2 | 2.66 | 0.42 |
| 1:C:358:LEU:HD12 | 1:C:358:LEU:HA | 1.90 | 0.42 |
| 1:C:359:THR:HG23 | 1:C:361:GLU:OE1 | 2.20 | 0.42 |
| 1:D:300:ASN:OD1 | 1:D:305:HIS:HE1 | 2.03 | 0.42 |
| 1:F:356:ALA:HB2 | 7:F:2051:HOH:O | 2.18 | 0.42 |
| 1:F:36:LYS:HD2 | 1:F:562:TYR:HB3 | 2.02 | 0.42 |
| 1:G:91:ARG:HD3 | 1:H:129:ARG:CG | 2.49 | 0.42 |
| 1:H:342:TRP:CD2 | 1:H:367:HIS:HD2 | 2.38 | 0.42 |
| 1:J:47:GLN:HE22 | 1:J:566:VAL:HG13 | 1.84 | 0.42 |
| 1:K:416:ILE:HG13 | 1:K:433:LEU:CD2 | 2.38 | 0.42 |
| 1:L:354:ARG:HE | 1:L:358:LEU:HD21 | 1.85 | 0.42 |
| 1:N:243:THR:HG21 | 1:N:273:TYR:CD2 | 2.53 | 0.42 |
| 1:O:24:LYS:HE3 | 1:O:47:GLN:O | 2.20 | 0.42 |
| 1:A:154:VAL:O | 1:A:154:VAL:HG13 | 2.20 | 0.42 |
| 1:B:138:HIS:NE2 | 1:B:223:HIS:HE1 | 2.17 | 0.42 |
| 1:D:288:VAL:O | 1:D:292:LEU:HD13 | 2.19 | 0.42 |
| 1:D:401:GLN:O | 1:D:405:GLN:HG3 | 2.19 | 0.42 |
| 1:D:467:ASN:HD21 | 3:D:1582:OXL:C2 | 2.32 | 0.42 |
| 1:D:270:ARG:NH2 | 1:D:488:ASP:OD1 | 2.53 | 0.42 |
| 1:E:263:PHE:CZ | 1:E:314:GLU:HA | 2.55 | 0.42 |
| 1:F:354:ARG:NH2 | 1:F:358:LEU:HD12 | 2.34 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:204:ASP:OD1 | 1:F:56:PRO:HG3 | 2.20 | 0.42 |
| 1:G:229:GLN:HA | 1:G:229:GLN:NE2 | 2.35 | 0.42 |
| 1:I:578:LYS:HZ3 | 1:L:222:ARG:HD3 | 1.85 | 0.42 |
| 1:M:222:ARG:HH12 | 1:P:580:LYS:HD2 | 1.85 | 0.42 |
| 1:M:248:MSE:HG3 | 1:P:544:PRO:CD | 2.50 | 0.42 |
| 1:M:24:LYS:HD3 | 1:M:48:LEU:HD23 | 2.02 | 0.42 |
| 1:N:474:VAL:O | 1:N:478:VAL:HG23 | 2.18 | 0.42 |
| 1:O:194:LYS:HA | 1:O:195:PRO:HD3 | 1.84 | 0.42 |
| 1:P:296:ARG:HB2 | 1:P:507:LEU:HD21 | 2.02 | 0.42 |
| 1:B:104:ILE:CG1 | 1:B:108:MSE:CE | 2.96 | 0.42 |
| 1:B:323:ILE:O | 1:B:327:MSE:HG3 | 2.20 | 0.42 |
| 1:E:224:LYS:CE | 7:E:2029:HOH:O | 2.68 | 0.42 |
| 1:F:569:SER:HA | 1:H:46:GLN:OE1 | 2.20 | 0.42 |
| 1:H:184:LEU:HD12 | 1:H:200:PRO:HB3 | 2.01 | 0.42 |
| 1:I:146:MSE:HE2 | 1:J:52:GLY:HA3 | 2.02 | 0.42 |
| 1:K:354:ARG:HG2 | 1:K:356:ALA:H | 1.84 | 0.42 |
| 1:L:493:THR:O | 1:L:497:VAL:HG23 | 2.20 | 0.42 |
| 1:M:104:ILE:CG2 | 1:M:105:GLU:N | 2.82 | 0.42 |
| 1:M:548:ASP:OD2 | 1:M:551:ALA:CB | 2.68 | 0.42 |
| 1:N:137:ILE:HB | 1:N:205:VAL:HG12 | 2.01 | 0.42 |
| 1:O:160:VAL:HG21 | 1:O:238:PHE:CZ | 2.55 | 0.42 |
| 1:B:158:ILE:HG22 | 1:B:160:VAL:HG23 | 2.01 | 0.42 |
| 1:C:270:ARG:NH1 | 1:C:270:ARG:CG | 2.82 | 0.42 |
| 1:C:467:ASN:O | 1:C:470:VAL:N | 2.40 | 0.42 |
| 1:D:502:VAL:HG22 | 1:D:514:PRO:HD3 | 2.02 | 0.42 |
| 1:E:322:LEU:HD23 | 1:E:322:LEU:HA | 1.78 | 0.42 |
| 1:E:374:MSE:HE1 | 1:E:379:ASP:CB | 2.49 | 0.42 |
| 1:F:548:ASP:OD2 | 1:F:551:ALA:HB2 | 2.19 | 0.42 |
| 1:F:61:GLN:NE2 | 1:F:98:LYS:HG2 | 2.34 | 0.42 |
| 1:H:148:GLN:HA | 1:H:245:ARG:NH2 | 2.35 | 0.42 |
| 1:H:145:THR:O | 1:H:148:GLN:HB2 | 2.20 | 0.42 |
| 1:H:166:ILE:HD12 | 1:H:179:ILE:HG13 | 2.01 | 0.42 |
| 1:K:352:LYS:HG3 | 1:K:366:ALA:O | 2.20 | 0.42 |
| 1:K:378:GLU:OE1 | 1:K:402:GLN:HB2 | 2.20 | 0.42 |
| 1:K:454:LEU:HD12 | 1:K:454:LEU:N | 2.35 | 0.42 |
| 1:L:301:ARG:NH2 | 7:L:2039:HOH:O | 2.53 | 0.42 |
| 1:L:399:PHE:CD2 | 1:L:427:GLU:HB3 | 2.54 | 0.42 |
| 1:N:460:LEU:HA | 1:N:509:GLU:O | 2.20 | 0.42 |
| 1:O:166:ILE:HD12 | 1:O:179:ILE:CG1 | 2.50 | 0.42 |
| 1:P:160:VAL:CG1 | 1:P:161:THR:N | 2.83 | 0.42 |
| 1:A:433:LEU:CD1 | 1:A:443:PHE:HB2 | 2.49 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:91:ARG:NH1 | 1:B:128:ARG:HA | 2.34 | 0.42 |
| 1:B:31:ASP:HA | 1:B:32:PRO:HD2 | 1.90 | 0.42 |
| 1:B:401:GLN:O | 1:B:405:GLN:HB2 | 2.20 | 0.42 |
| 1:B:429:THR:CG2 | 1:B:430:ALA:N | 2.83 | 0.42 |
| 1:C:259:ASN:HB3 | 7:C:2034:HOH:O | 2.19 | 0.42 |
| 1:C:349:LEU:HB2 | 1:C:380:ILE:CD1 | 2.50 | 0.42 |
| 1:C:389:LEU:HG | 1:C:407:MSE:HE3 | 2.01 | 0.42 |
| 1:C:431:GLU:OE2 | 1:C:452:VAL:HG13 | 2.19 | 0.42 |
| 1:D:150:TRP:HA | 1:D:151:PRO:HD2 | 1.84 | 0.42 |
| 1:D:270:ARG:HH12 | 1:D:487:GLY:HA2 | 1.84 | 0.42 |
| 1:E:177:MSE:HE2 | 1:E:202:MSE:CB | 2.50 | 0.42 |
| 1:E:395:ILE:O | 1:E:396:GLY:C | 2.58 | 0.42 |
| 1:E:467:ASN:ND2 | 3:E:1582:OXL:O2 | 2.53 | 0.42 |
| 1:G:104:ILE:O | 1:G:108:MSE:HB2 | 2.19 | 0.42 |
| 1:H:386:PRO:HG2 | 1:H:407:MSE:CE | 2.34 | 0.42 |
| 1:K:207:THR:HA | 1:K:225:ARG:HG2 | 2.02 | 0.42 |
| 1:M:248:MSE:HG3 | 1:P:544:PRO:HD2 | 2.01 | 0.42 |
| 1:M:502:VAL:HG12 | 1:M:507:LEU:HD13 | 2.00 | 0.42 |
| 1:O:238:PHE:O | 1:O:242:VAL:HG23 | 2.20 | 0.42 |
| 1:O:36:LYS:HD2 | 1:O:562:TYR:HB3 | 2.01 | 0.42 |
| 1:P:222:ARG:NH1 | 1:P:222:ARG:HG3 | 2.34 | 0.42 |
| 1:A:160:VAL:HG13 | 1:A:201:VAL:HB | 2.02 | 0.42 |
| 1:C:345:ASP:OD1 | 1:C:354:ARG:NH2 | 2.52 | 0.42 |
| 1:C:359:THR:CG2 | 1:C:361:GLU:H | 2.33 | 0.42 |
| 1:D:554:ARG:NH1 | 1:D:554:ARG:HG2 | 2.34 | 0.42 |
| 1:E:297:ILE:CG1 | 1:E:507:LEU:HD12 | 2.49 | 0.42 |
| 1:G:155:ILE:HD13 | 1:G:246:TYR:CZ | 2.55 | 0.42 |
| 1:G:160:VAL:HG11 | 1:G:238:PHE:CZ | 2.55 | 0.42 |
| 1:G:378:GLU:O | 1:G:382:LYS:HG3 | 2.20 | 0.42 |
| 1:H:154:VAL:O | 1:H:154:VAL:CG1 | 2.66 | 0.42 |
| 1:H:72:PHE:CZ | 1:H:81:ARG:HD3 | 2.55 | 0.42 |
| 1:I:328:GLN:HA | 1:I:332:VAL:O | 2.19 | 0.42 |
| 1:K:389:LEU:HD13 | 1:K:399:PHE:CZ | 2.54 | 0.42 |
| 1:L:133:LEU:HA | 1:L:133:LEU:HD23 | 1.88 | 0.42 |
| 1:L:23:LYS:HD2 | 1:L:27:GLU:HG2 | 2.00 | 0.42 |
| 1:L:315:ALA:O | 1:L:319:ILE:HG13 | 2.19 | 0.42 |
| 1:L:394:ALA:HA | 1:L:420:SER:HB3 | 2.02 | 0.42 |
| 1:M:435:LYS:HE3 | 1:M:436:TYR:CZ | 2.55 | 0.42 |
| 1:M:512:LEU:HD23 | 1:M:512:LEU:HA | 1.89 | 0.42 |
| 1:M:51:HIS:CD2 | 1:N:146:MSE:HE3 | 2.54 | 0.42 |
| 1:N:59:LEU:HD12 | 1:N:59:LEU:O | 2.19 | 0.42 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:96:PHE:CZ | 1:N:100:LEU:HD11 | 2.54 | 0.42 |
| 1:O:428:CYS:CB | 1:O:432:GLN:HE21 | 2.33 | 0.42 |
| 1:P:108:MSE:N | 1:P:109:PRO:CD | 2.83 | 0.42 |
| 1:B:250:CYS:O | 1:B:252:ILE:HD12 | 2.20 | 0.41 |
| 1:C:261:ASN:OD1 | 1:C:264:ARG:NH1 | 2.50 | 0.41 |
| 1:C:317:LEU:HD23 | 1:C:343:MSE:HE1 | 2.01 | 0.41 |
| 1:D:442:ILE:CG2 | 1:D:512:LEU:HD21 | 2.50 | 0.41 |
| 1:E:571:THR:OG1 | 1:E:577:MSE:SE | 2.88 | 0.41 |
| 1:F:113:THR:HG23 | 1:F:114:PRO:HA | 2.01 | 0.41 |
| 1:F:418:ALA:O | 1:F:445:SER:HA | 2.20 | 0.41 |
| 1:F:514:PRO:HA | 1:F:515:PRO:HD3 | 1.97 | 0.41 |
| 1:I:309:PHE:HE1 | 1:I:341:ILE:HG23 | 1.84 | 0.41 |
| 1:J:401:GLN:HG2 | 1:J:436:TYR:CE2 | 2.54 | 0.41 |
| 1:K:108:MSE:HB3 | 1:K:109:PRO:HD3 | 2.02 | 0.41 |
| 1:K:395:ILE:O | 1:K:396:GLY:C | 2.58 | 0.41 |
| 1:L:564:CYS:SG | 1:L:566:VAL:HB | 2.60 | 0.41 |
| 1:N:225:ARG:HB2 | 1:N:227:ARG:NH1 | 2.35 | 0.41 |
| 1:O:23:LYS:HG3 | 1:O:24:LYS:N | 2.34 | 0.41 |
| 1:P:429:THR:CG2 | 1:P:431:GLU:H | 2.26 | 0.41 |
| 1:C:497:VAL:HG11 | 1:C:526:ILE:HD13 | 2.02 | 0.41 |
| 1:D:162:ASP:O | 1:D:225:ARG:NH2 | 2.43 | 0.41 |
| 1:D:343:MSE:HB2 | 1:D:350:ILE:HD12 | 2.03 | 0.41 |
| 1:E:136:THR:CG2 | 1:E:137:ILE:N | 2.83 | 0.41 |
| 1:E:74:ARG:HD3 | 1:F:125:LEU:HD11 | 2.02 | 0.41 |
| 1:H:342:TRP:CZ3 | 1:H:367:HIS:HB2 | 2.55 | 0.41 |
| 1:I:264:ARG:NH1 | 1:I:264:ARG:HB3 | 2.35 | 0.41 |
| 1:J:215:ASP:HB3 | 1:J:218:TYR:HB2 | 2.01 | 0.41 |
| 1:J:158:ILE:HD12 | 1:J:242:VAL:HG11 | 2.02 | 0.41 |
| 1:L:104:ILE:HG23 | 1:L:105:GLU:N | 2.35 | 0.41 |
| 1:L:165:ARG:HD2 | 1:L:165:ARG:C | 2.40 | 0.41 |
| 1:L:322:LEU:HD23 | 1:L:322:LEU:HA | 1.92 | 0.41 |
| 1:M:108:MSE:N | 1:M:109:PRO:CD | 2.83 | 0.41 |
| 1:M:314:GLU:HB2 | 2:M:1581:NAP:O1N | 2.19 | 0.41 |
| 1:N:202:MSE:HE2 | 1:N:204:ASP:HB2 | 2.02 | 0.41 |
| 1:O:504:GLU:HG3 | 1:O:508:GLN:NE2 | 2.35 | 0.41 |
| 1:P:92:ASN:ND2 | 1:P:95:LEU:H | 2.17 | 0.41 |
| 1:A:276:PHE:HB2 | 1:A:281:GLN:OE1 | 2.20 | 0.41 |
| 1:B:172:LEU:O | 1:B:175:TYR:HB2 | 2.19 | 0.41 |
| 1:B:215:ASP:OD1 | 1:B:216:PRO:HD2 | 2.20 | 0.41 |
| 1:C:118:LEU:HD11 | 5:C:1588:CL:CL | 2.57 | 0.41 |
| 1:D:136:THR:HG22 | 1:D:139:ASP:OD1 | 2.20 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:152:GLU:OE2 | 1:E:196:HIS:CE1 | 2.73 | 0.41 |
| 1:E:160:VAL:HG11 | 1:E:238:PHE:CZ | 2.55 | 0.41 |
| 1:E:327:MSE:HE1 | 1:E:337:ALA:O | 2.20 | 0.41 |
| 1:E:401:GLN:HG3 | 7:E:2038:HOH:O | 2.20 | 0.41 |
| 1:F:209:ASN:OD1 | 1:F:211:THR:HB | 2.20 | 0.41 |
| 1:G:165:ARG:O | 1:G:256:ASP:HB3 | 2.21 | 0.41 |
| 1:H:274:CYS:SG | 1:H:478:VAL:HG11 | 2.61 | 0.41 |
| 1:H:526:ILE:O | 1:H:530:ILE:HG13 | 2.20 | 0.41 |
| 1:I:471:PHE:CG | 1:I:472:PRO:HD3 | 2.56 | 0.41 |
| 1:I:297:ILE:CD1 | 1:I:507:LEU:HD12 | 2.49 | 0.41 |
| 1:J:243:THR:HG21 | 1:J:273:TYR:CD2 | 2.54 | 0.41 |
| 1:L:297:ILE:HD11 | 1:L:507:LEU:HG | 2.01 | 0.41 |
| 1:L:65:VAL:O | 1:L:69:LEU:HG | 2.21 | 0.41 |
| 1:M:574:GLU:HA | 1:M:577:MSE:HE2 | 2.01 | 0.41 |
| 1:N:33:HIS:HD2 | 1:N:93:GLU:OE2 | 2.02 | 0.41 |
| 1:O:476:LEU:HB3 | 1:O:527:ALA:HB2 | 2.01 | 0.41 |
| 1:P:141:GLY:H | 1:P:237:GLU:CD | 2.23 | 0.41 |
| 1:B:322:LEU:HA | 1:B:322:LEU:HD23 | 1.86 | 0.41 |
| 1:C:458:GLN:HB3 | 1:C:458:GLN:HE21 | 1.66 | 0.41 |
| 1:C:72:PHE:CE1 | 1:C:81:ARG:HB3 | 2.55 | 0.41 |
| 1:D:92:ASN:ND2 | 1:D:92:ASN:C | 2.64 | 0.41 |
| 1:E:386:PRO:HG2 | 1:E:407:MSE:CE | 2.28 | 0.41 |
| 1:F:150:TRP:HA | 1:F:151:PRO:HD2 | 1.84 | 0.41 |
| 1:F:195:PRO:HD2 | 1:F:558:TYR:CE1 | 2.55 | 0.41 |
| 1:F:68:ILE:HG13 | 1:F:95:LEU:HD11 | 2.01 | 0.41 |
| 1:G:239:MSE:HE1 | 1:G:252:ILE:HG21 | 2.02 | 0.41 |
| 1:G:239:MSE:O | 1:G:243:THR:OG1 | 2.39 | 0.41 |
| 1:G:242:VAL:HG13 | 1:G:246:TYR:CD1 | 2.53 | 0.41 |
| 1:G:429:THR:HG23 | 1:G:449:PHE:CD2 | 2.55 | 0.41 |
| 1:H:194:LYS:HA | 1:H:195:PRO:HD3 | 1.82 | 0.41 |
| 1:H:402:GLN:HG3 | 7:H:2045:HOH:O | 2.19 | 0.41 |
| 1:I:554:ARG:HG2 | 1:I:554:ARG:NH1 | 2.34 | 0.41 |
| 1:J:429:THR:CG2 | 1:J:430:ALA:N | 2.83 | 0.41 |
| 1:J:471:PHE:CG | 1:J:472:PRO:HD3 | 2.55 | 0.41 |
| 1:K:254:PHE:CE2 | 1:K:265:LEU:HD13 | 2.56 | 0.41 |
| 1:L:252:ILE:N | 1:L:252:ILE:HD12 | 2.36 | 0.41 |
| 1:L:380:ILE:O | 1:L:384:ILE:HG12 | 2.20 | 0.41 |
| 1:L:572:TRP:O | 1:L:573:PRO:C | 2.58 | 0.41 |
| 1:M:141:GLY:H | 1:M:237:GLU:CD | 2.22 | 0.41 |
| 1:P:323:ILE:HG22 | 1:P:327:MSE:HE2 | 2.02 | 0.41 |
| 1:A:100:LEU:HD21 | 1:A:111:VAL:HG21 | 2.01 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:150:TRP:CD1 | 1:A:155:ILE:HD11 | 2.55 | 0.41 |
| 1:A:207:THR:HA | 1:A:225:ARG:NH1 | 2.34 | 0.41 |
| 1:A:36:LYS:HE2 | 1:A:562:TYR:HB3 | 2.02 | 0.41 |
| 1:B:207:THR:HA | 1:B:225:ARG:HG2 | 2.02 | 0.41 |
| 1:B:307:VAL:HG22 | 1:B:388:VAL:HB | 2.02 | 0.41 |
| 1:C:500:GLN:HB3 | 7:C:2063:HOH:O | 2.19 | 0.41 |
| 1:D:433:LEU:CD1 | 1:D:443:PHE:HB2 | 2.51 | 0.41 |
| 1:D:547:GLU:OE2 | 1:D:547:GLU:N | 2.50 | 0.41 |
| 1:F:194:LYS:HA | 1:F:195:PRO:HD3 | 1.95 | 0.41 |
| 1:F:158:ILE:HG12 | 1:F:199:LEU:HB3 | 2.01 | 0.41 |
| 1:F:401:GLN:CG | 1:F:436:TYR:CZ | 3.01 | 0.41 |
| 1:F:467:ASN:HB3 | 1:F:471:PHE:HD2 | 1.84 | 0.41 |
| 1:K:274:CYS:SG | 1:K:478:VAL:HG11 | 2.60 | 0.41 |
| 1:K:61:GLN:HA | 1:K:64:GLN:HE21 | 1.85 | 0.41 |
| 1:M:90:ASP:OD1 | 1:M:131:ARG:NH1 | 2.53 | 0.41 |
| 1:N:141:GLY:H | 1:N:237:GLU:CD | 2.21 | 0.41 |
| 1:N:466:ASN:OD1 | 1:N:467:ASN:N | 2.53 | 0.41 |
| 1:N:59:LEU:HD11 | 1:N:64:GLN:HG3 | 2.03 | 0.41 |
| 1:O:105:GLU:HB2 | 7:O:2024:HOH:O | 2.19 | 0.41 |
| 1:P:184:LEU:HD22 | 1:P:198:CYS:HB3 | 2.01 | 0.41 |
| 1:P:292:LEU:HA | 1:P:292:LEU:HD12 | 1.94 | 0.41 |
| 1:P:61:GLN:HE22 | 1:P:98:LYS:HE3 | 1.84 | 0.41 |
| 1:A:243:THR:HG21 | 1:A:273:TYR:CD2 | 2.55 | 0.41 |
| 1:B:212:LEU:HD13 | 1:B:218:TYR:CE1 | 2.55 | 0.41 |
| 1:B:85:LEU:HD12 | 1:B:110:ILE:CG2 | 2.51 | 0.41 |
| 1:G:50:ILE:HA | 1:G:53:LEU:HD12 | 2.02 | 0.41 |
| 1:H:177:MSE:O | 1:H:180:PRO:HD2 | 2.21 | 0.41 |
| 1:K:79:LEU:HD13 | 1:K:118:LEU:HD12 | 2.03 | 0.41 |
| 1:K:498:ILE:CD1 | 1:K:526:ILE:HD11 | 2.48 | 0.41 |
| 1:M:144:ALA:HB2 | 7:M:2022:HOH:O | 2.20 | 0.41 |
| 1:N:420:SER:HA | 2:N:1581:NAP:H1D | 2.02 | 0.41 |
| 1:O:350:ILE:CD1 | 1:O:362:LYS:HD2 | 2.50 | 0.41 |
| 1:P:202:MSE:HE3 | 1:P:203:LEU:C | 2.41 | 0.41 |
| 1:P:350:ILE:HD11 | 1:P:362:LYS:HD3 | 2.01 | 0.41 |
| 1:D:174:CYS:HA | 1:D:202:MSE:HE3 | 2.02 | 0.41 |
| 1:D:416:ILE:HG13 | 1:D:433:LEU:CD2 | 2.41 | 0.41 |
| 1:F:393:ALA:HB3 | 7:F:2057:HOH:O | 2.20 | 0.41 |
| 1:G:239:MSE:CE | 1:G:254:PHE:CZ | 3.02 | 0.41 |
| 1:G:395:ILE:O | 1:G:396:GLY:C | 2.59 | 0.41 |
| 1:G:389:LEU:HD22 | 1:G:399:PHE:CZ | 2.56 | 0.41 |
| 1:H:77:SER:O | 1:H:81:ARG:HG3 | 2.21 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:284:ALA:HB1 | 1:L:322:LEU:HB2 | 2.02 | 0.41 |
| 1:L:429:THR:CG2 | 1:L:430:ALA:N | 2.84 | 0.41 |
| 1:M:86:MSE:CE | 1:M:89:GLN:NE2 | 2.84 | 0.41 |
| 1:N:140:ARG:HG2 | 1:N:234:LEU:HD13 | 2.03 | 0.41 |
| 1:N:265:LEU:HA | 1:N:265:LEU:HD23 | 1.84 | 0.41 |
| 1:N:502:VAL:CG1 | 1:N:507:LEU:HD13 | 2.50 | 0.41 |
| 1:O:460:LEU:HA | 1:O:509:GLU:O | 2.20 | 0.41 |
| 1:P:332:VAL:CG2 | 1:P:336:GLU:HB3 | 2.51 | 0.41 |
| 1:P:44:GLU:O | 1:P:48:LEU:HB2 | 2.20 | 0.41 |
| 1:B:350:ILE:HG12 | 1:B:354:ARG:NH2 | 2.35 | 0.41 |
| 1:C:120:CYS:O | 1:C:175:TYR:HB3 | 2.21 | 0.41 |
| 1:C:194:LYS:HA | 1:C:195:PRO:HD3 | 1.87 | 0.41 |
| 1:C:26:TYR:H | 1:C:26:TYR:HD2 | 1.69 | 0.41 |
| 1:B:24:LYS:HZ3 | 1:D:24:LYS:HD3 | 1.86 | 0.41 |
| 1:E:232:ASP:OD1 | 1:E:264:ARG:NH2 | 2.54 | 0.41 |
| 1:E:394:ALA:HA | 1:E:420:SER:HB3 | 2.03 | 0.41 |
| 1:G:30:ARG:HD3 | 1:H:30:ARG:O | 2.20 | 0.41 |
| 1:G:285:SER:HB3 | 1:G:470:VAL:HG21 | 2.03 | 0.41 |
| 1:I:121:GLN:NE2 | 1:I:169:LEU:HD13 | 2.36 | 0.41 |
| 1:I:266:LEU:O | 1:I:270:ARG:HB2 | 2.21 | 0.41 |
| 1:I:58:PHE:CD1 | 1:I:58:PHE:N | 2.89 | 0.41 |
| 1:J:328:GLN:HA | 1:J:332:VAL:O | 2.21 | 0.41 |
| 1:J:404:LEU:HD13 | 1:J:433:LEU:HA | 2.02 | 0.41 |
| 1:K:381:VAL:HG21 | 1:K:403:ILE:HD12 | 2.03 | 0.41 |
| 1:L:395:ILE:O | 1:L:396:GLY:C | 2.59 | 0.41 |
| 1:N:140:ARG:HB3 | 1:N:140:ARG:CZ | 2.50 | 0.41 |
| 1:O:151:PRO:HB3 | 1:P:26:TYR:CE2 | 2.55 | 0.41 |
| 1:O:245:ARG:CG | 1:O:245:ARG:HH11 | 2.34 | 0.41 |
| 1:A:150:TRP:CE2 | 1:A:199:LEU:HD13 | 2.56 | 0.41 |
| 1:B:266:LEU:O | 1:B:270:ARG:HB2 | 2.21 | 0.41 |
| 1:B:399:PHE:CG | 1:B:427:GLU:HB3 | 2.56 | 0.41 |
| 1:C:350:ILE:HG23 | 1:C:358:LEU:HD11 | 2.01 | 0.41 |
| 1:D:194:LYS:HA | 1:D:195:PRO:HD3 | 1.89 | 0.41 |
| 1:D:23:LYS:CG | 1:D:24:LYS:N | 2.73 | 0.41 |
| 1:C:127:PHE:CE2 | 1:D:38:MSE:HE2 | 2.56 | 0.41 |
| 1:E:172:LEU:O | 1:E:175:TYR:HB2 | 2.21 | 0.41 |
| 1:E:394:ALA:HB2 | 2:E:1581:NAP:O3D | 2.21 | 0.41 |
| 1:E:471:PHE:CG | 1:E:472:PRO:HD3 | 2.55 | 0.41 |
| 1:F:177:MSE:CE | 1:F:180:PRO:HG2 | 2.51 | 0.41 |
| 1:F:192:GLY:CA | 1:F:557:VAL:HG13 | 2.50 | 0.41 |
| 1:G:183:LYS:HZ2 | 1:G:467:ASN:HD22 | 1.68 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:143:ILE:HG13 | 1:J:237:GLU:OE2 | 2.21 | 0.41 |
| 1:K:343:MSE:HE3 | 1:K:350:ILE:HD12 | 2.02 | 0.41 |
| 1:L:109:PRO:HA | 1:L:113:THR:O | 2.21 | 0.41 |
| 1:M:177:MSE:C | 1:M:180:PRO:HD2 | 2.40 | 0.41 |
| 1:M:270:ARG:NH2 | 1:M:488:ASP:OD1 | 2.54 | 0.41 |
| 1:O:136:THR:HG22 | 1:O:137:ILE:N | 2.35 | 0.41 |
| 1:O:467:ASN:H | 2:O:1581:NAP:H72N | 1.69 | 0.41 |
| 1:O:64:GLN:NE2 | 1:O:562:TYR:OH | 2.51 | 0.41 |
| 1:O:78:ASP:HA | 1:O:81:ARG:HH11 | 1.86 | 0.41 |
| 1:P:473:GLY:N | 5:P:1590:CL:CL | 2.84 | 0.41 |
| 1:P:207:THR:HA | 1:P:225:ARG:HG2 | 2.03 | 0.41 |
| 1:P:143:ILE:CD1 | 1:P:237:GLU:HG2 | 2.40 | 0.41 |
| 1:A:51:HIS:NE2 | 1:B:139:ASP:OD2 | 2.44 | 0.41 |
| 1:D:154:VAL:C | 1:D:155:ILE:HD12 | 2.41 | 0.41 |
| 1:D:471:PHE:N | 1:D:472:PRO:CD | 2.84 | 0.41 |
| 1:D:72:PHE:CE1 | 1:D:81:ARG:HB3 | 2.56 | 0.41 |
| 1:E:110:ILE:O | 1:E:115:THR:HB | 2.20 | 0.41 |
| 1:E:207:THR:HA | 1:E:225:ARG:HG2 | 2.03 | 0.41 |
| 1:E:52:GLY:O | 1:F:133:LEU:HD23 | 2.21 | 0.41 |
| 1:F:190:CYS:HB3 | 1:F:519:ILE:HG12 | 2.02 | 0.41 |
| 1:F:59:LEU:HB2 | 1:F:63:ALA:HB3 | 2.02 | 0.41 |
| 1:H:466:ASN:HA | 2:H:1581:NAP:N7N | 2.33 | 0.41 |
| 1:H:89:GLN:HG3 | 1:H:96:PHE:CD2 | 2.55 | 0.41 |
| 1:J:359:THR:HG23 | 1:J:362:LYS:N | 2.22 | 0.41 |
| 1:J:41:THR:CG2 | 1:J:42:LEU:N | 2.83 | 0.41 |
| 1:K:136:THR:CG2 | 1:K:138:HIS:HB2 | 2.51 | 0.41 |
| 1:K:156:LYS:NZ | 1:K:197:GLN:NE2 | 2.69 | 0.41 |
| 1:K:243:THR:HG21 | 1:K:273:TYR:CD2 | 2.56 | 0.41 |
| 1:K:29:LEU:HA | 1:K:35:ASN:ND2 | 2.36 | 0.41 |
| 1:N:123:TYR:HB3 | 1:N:175:TYR:CD2 | 2.56 | 0.41 |
| 1:N:184:LEU:O | 1:N:187:TYR:HB2 | 2.21 | 0.41 |
| 1:O:155:ILE:N | 1:O:155:ILE:HD12 | 2.35 | 0.41 |
| 1:O:270:ARG:CG | 1:O:270:ARG:NH1 | 2.84 | 0.41 |
| 1:O:359:THR:HG22 | 1:O:362:LYS:CE | 2.47 | 0.41 |
| 1:P:162:ASP:CA | 1:P:202:MSE:HE1 | 2.50 | 0.41 |
| 1:P:342:TRP:CD2 | 1:P:367:HIS:HD2 | 2.39 | 0.41 |
| 1:P:471:PHE:N | 1:P:472:PRO:CD | 2.84 | 0.41 |
| 1:P:504:GLU:CG | 1:P:508:GLN:HE22 | 2.15 | 0.41 |
| 1:A:59:LEU:HD13 | 1:A:64:GLN:CG | 2.52 | 0.41 |
| 1:B:104:ILE:CG2 | 1:B:105:GLU:N | 2.83 | 0.41 |
| 1:B:125:LEU:HD13 | 1:B:125:LEU:C | 2.41 | 0.41 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:154:VAL:C | 1:B:155:ILE:HD12 | 2.41 | 0.41 |
| 1:B:303:SER:CB | 1:B:332:VAL:HG21 | 2.51 | 0.41 |
| 1:E:194:LYS:HA | 1:E:195:PRO:HD3 | 1.89 | 0.41 |
| 1:E:443:PHE:CG | 1:E:444:ALA:N | 2.89 | 0.41 |
| 1:F:109:PRO:HA | 1:F:113:THR:O | 2.20 | 0.41 |
| 1:F:23:LYS:N | 1:F:24:LYS:NZ | 2.64 | 0.41 |
| 1:G:119:ALA:O | 1:G:123:TYR:N | 2.54 | 0.41 |
| 1:G:352:LYS:HZ1 | 1:G:366:ALA:HB3 | 1.86 | 0.41 |
| 1:J:164:GLU:CG | 1:J:258:ALA:HB2 | 2.48 | 0.41 |
| 1:J:315:ALA:O | 1:J:319:ILE:HG13 | 2.20 | 0.41 |
| 1:K:343:MSE:O | 1:K:349:LEU:HD12 | 2.20 | 0.41 |
| 1:K:421:ASN:HB3 | 1:K:422:PRO:HA | 2.03 | 0.41 |
| 1:L:100:LEU:HD21 | 1:L:111:VAL:HG21 | 2.03 | 0.41 |
| 1:L:407:MSE:HG2 | 1:L:416:ILE:HD11 | 2.01 | 0.41 |
| 1:M:384:ILE:O | 1:M:385:LYS:C | 2.60 | 0.41 |
| 1:N:202:MSE:HE3 | 1:N:204:ASP:N | 2.36 | 0.41 |
| 1:N:471:PHE:CD1 | 1:N:472:PRO:HD3 | 2.56 | 0.41 |
| 1:N:551:ALA:HA | 1:N:554:ARG:HD2 | 2.03 | 0.41 |
| 1:N:59:LEU:CD1 | 1:N:64:GLN:HG3 | 2.50 | 0.41 |
| 1:P:160:VAL:HG21 | 1:P:238:PHE:CZ | 2.56 | 0.41 |
| 1:P:374:MSE:HE1 | 1:P:379:ASP:C | 2.41 | 0.41 |
| 1:A:113:THR:CG2 | 1:A:114:PRO:HA | 2.51 | 0.40 |
| 1:A:414:PRO:HG2 | 1:A:441:GLY:HA2 | 2.02 | 0.40 |
| 1:A:92:ASN:ND2 | 1:A:95:LEU:H | 2.19 | 0.40 |
| 1:C:467:ASN:ND2 | 3:C:1582:OXL:C2 | 2.84 | 0.40 |
| 1:C:399:PHE:HB2 | 1:C:428:CYS:HB3 | 2.03 | 0.40 |
| 1:C:484:LYS:HB3 | 1:C:485:HIS:CD2 | 2.56 | 0.40 |
| 1:D:61:GLN:NE2 | 1:D:560:THR:HG23 | 2.35 | 0.40 |
| 1:E:165:ARG:C | 1:E:165:ARG:HD2 | 2.41 | 0.40 |
| 1:F:429:THR:N | 1:F:432:GLN:NE2 | 2.51 | 0.40 |
| 1:G:502:VAL:CG1 | 1:G:507:LEU:HD13 | 2.51 | 0.40 |
| 1:G:59:LEU:HB2 | 1:G:63:ALA:HB3 | 2.03 | 0.40 |
| 1:H:268:LYS:HG2 | 1:H:269:TYR:CD2 | 2.57 | 0.40 |
| 1:H:168:GLY:O | 1:H:425:LYS:HE3 | 2.21 | 0.40 |
| 1:I:120:CYS:O | 1:I:175:TYR:HB3 | 2.22 | 0.40 |
| 1:J:145:THR:O | 1:J:148:GLN:HB2 | 2.20 | 0.40 |
| 1:J:177:MSE:CE | 1:J:202:MSE:HB2 | 2.50 | 0.40 |
| 1:J:429:THR:HB | 1:J:432:GLN:CG | 2.39 | 0.40 |
| 1:J:516:LEU:N | 1:J:516:LEU:HD22 | 2.36 | 0.40 |
| 1:K:354:ARG:HB3 | 1:K:358:LEU:HD11 | 2.02 | 0.40 |
| 1:K:365:PHE:CD1 | 1:K:365:PHE:N | 2.88 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:M:94:LYS:HB2 | 1:M:562:TYR:CE2 | 2.56 | 0.40 |
| 1:N:431:GLU:OE2 | 1:N:452:VAL:HG22 | 2.21 | 0.40 |
| 1:O:332:VAL:HG22 | 1:O:333:SER:N | 2.36 | 0.40 |
| 1:O:416:ILE:HG13 | 1:O:433:LEU:CD2 | 2.48 | 0.40 |
| 1:P:133:LEU:HD22 | 1:P:135:ILE:CG1 | 2.46 | 0.40 |
| 1:A:235:LEU:HA | 1:A:235:LEU:HD13 | 1.85 | 0.40 |
| 1:A:231:TYR:O | 1:A:235:LEU:HD23 | 2.21 | 0.40 |
| 1:A:245:ARG:HG2 | 1:A:246:TYR:CE2 | 2.56 | 0.40 |
| 1:A:417:PHE:CE1 | 1:A:444:ALA:HB3 | 2.57 | 0.40 |
| 1:C:186:LEU:HD22 | 1:C:190:CYS:SG | 2.62 | 0.40 |
| 1:C:152:GLU:OE1 | 1:C:196:HIS:CE1 | 2.75 | 0.40 |
| 1:D:212:LEU:HD13 | 1:D:218:TYR:CE1 | 2.56 | 0.40 |
| 1:E:202:MSE:CE | 1:E:203:LEU:O | 2.70 | 0.40 |
| 1:E:84:LEU:HD23 | 1:E:84:LEU:C | 2.41 | 0.40 |
| 1:F:59:LEU:HD13 | 1:F:64:GLN:CG | 2.51 | 0.40 |
| 1:F:66:TYR:O | 1:F:70:LYS:HG2 | 2.21 | 0.40 |
| 1:G:494:THR:HG23 | 1:G:526:ILE:HG23 | 2.03 | 0.40 |
| 1:G:36:LYS:CD | 1:G:562:TYR:HB3 | 2.51 | 0.40 |
| 1:H:136:THR:HG22 | 1:H:137:ILE:N | 2.36 | 0.40 |
| 1:I:223:HIS:C | 1:I:223:HIS:CD2 | 2.94 | 0.40 |
| 1:I:352:LYS:HD3 | 1:I:352:LYS:HA | 1.84 | 0.40 |
| 1:J:502:VAL:CG1 | 1:J:507:LEU:HD22 | 2.46 | 0.40 |
| 1:J:88:LEU:O | 1:J:88:LEU:HD23 | 2.20 | 0.40 |
| 1:K:270:ARG:NH2 | 1:K:488:ASP:OD1 | 2.53 | 0.40 |
| 1:L:108:MSE:HB3 | 1:L:109:PRO:HD3 | 2.03 | 0.40 |
| 1:L:471:PHE:CG | 1:L:472:PRO:HD3 | 2.56 | 0.40 |
| 1:M:109:PRO:HA | 1:M:113:THR:O | 2.22 | 0.40 |
| 1:N:413:ARG:HD3 | 7:N:2047:HOH:O | 2.20 | 0.40 |
| 1:P:131:ARG:HH11 | 1:P:131:ARG:HB2 | 1.84 | 0.40 |
| 1:P:135:ILE:HD13 | 1:P:143:ILE:HG23 | 2.03 | 0.40 |
| 1:P:26:TYR:N | 1:P:26:TYR:CD2 | 2.89 | 0.40 |
| 1:P:350:ILE:HG23 | 1:P:358:LEU:HD11 | 2.02 | 0.40 |
| 1:A:142:HIS:O | 1:A:146:MSE:HG3 | 2.21 | 0.40 |
| 1:B:128:ARG:HH11 | 1:B:128:ARG:HG2 | 1.86 | 0.40 |
| 1:B:88:LEU:HD13 | 1:B:96:PHE:HA | 2.02 | 0.40 |
| 1:C:110:ILE:O | 1:C:115:THR:HB | 2.22 | 0.40 |
| 1:D:276:PHE:C | 1:D:276:PHE:CD1 | 2.94 | 0.40 |
| 1:E:157:ALA:HB2 | 1:E:479:ILE:HD11 | 2.04 | 0.40 |
| 1:F:215:ASP:HA | 1:F:216:PRO:HD2 | 1.96 | 0.40 |
| 1:F:383:ASP:C | 1:F:383:ASP:OD1 | 2.59 | 0.40 |
| 1:G:466:ASN:HA | 2:G:1581:NAP:H72N | 1.87 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:503:SER:O | 1:G:506:ASN:HB2 | 2.20 | 0.40 |
| 1:H:167:LEU:CD1 | 1:H:179:ILE:HD11 | 2.51 | 0.40 |
| 1:H:38:MSE:HB2 | 1:H:59:LEU:HD11 | 2.02 | 0.40 |
| 1:J:493:THR:HG23 | 1:J:529:ARG:NH1 | 2.36 | 0.40 |
| 1:J:575:GLU:OE2 | 1:J:575:GLU:N | 2.37 | 0.40 |
| 1:K:270:ARG:HH12 | 1:K:487:GLY:HA2 | 1.85 | 0.40 |
| 1:L:281:GLN:HB3 | 1:L:491:PHE:CD1 | 2.56 | 0.40 |
| 1:M:401:GLN:HG3 | 1:M:436:TYR:CD1 | 2.56 | 0.40 |
| 1:M:59:LEU:HD13 | 1:M:64:GLN:CG | 2.50 | 0.40 |
| 1:N:112:TYR:CG | 1:N:186:LEU:HD11 | 2.56 | 0.40 |
| 1:N:235:LEU:HA | 1:N:235:LEU:HD13 | 1.90 | 0.40 |
| 1:N:416:ILE:HG21 | 1:N:433:LEU:HD23 | 2.03 | 0.40 |
| 1:N:433:LEU:HD13 | 1:N:433:LEU:C | 2.41 | 0.40 |
| 1:N:470:VAL:HG13 | 1:N:494:THR:HG21 | 2.03 | 0.40 |
| 1:N:69:LEU:HD22 | 1:N:106:ARG:NH1 | 2.36 | 0.40 |
| 1:O:354:ARG:HE | 1:O:358:LEU:CD1 | 2.32 | 0.40 |
| 1:O:359:THR:HG22 | 1:O:362:LYS:HG3 | 2.03 | 0.40 |
| 1:O:413:ARG:HA | 1:O:414:PRO:HD2 | 1.96 | 0.40 |
| 1:P:154:VAL:O | 1:P:154:VAL:CG1 | 2.66 | 0.40 |
| 1:P:199:LEU:HG | 1:P:201:VAL:HG23 | 2.03 | 0.40 |
| 1:P:404:LEU:HD22 | 1:P:433:LEU:HD23 | 2.03 | 0.40 |
| 1:A:433:LEU:HD12 | 1:A:434:TYR:CE2 | 2.57 | 0.40 |
| 1:B:202:MSE:HE2 | 1:B:204:ASP:HA | 2.04 | 0.40 |
| 1:D:467:ASN:O | 1:D:470:VAL:N | 2.40 | 0.40 |
| 1:D:564:CYS:SG | 1:D:566:VAL:HG23 | 2.62 | 0.40 |
| 1:E:226:ILE:HA | 1:E:226:ILE:HD13 | 1.96 | 0.40 |
| 1:F:177:MSE:CE | 1:F:177:MSE:CA | 2.96 | 0.40 |
| 1:G:399:PHE:HB2 | 1:G:428:CYS:HB3 | 2.02 | 0.40 |
| 1:G:412:LYS:HB3 | 7:G:2042:HOH:O | 2.22 | 0.40 |
| 1:H:259:ASN:HB3 | 7:H:2035:HOH:O | 2.22 | 0.40 |
| 1:H:417:PHE:CD1 | 1:H:444:ALA:HB3 | 2.56 | 0.40 |
| 1:H:44:GLU:O | 1:H:48:LEU:HB2 | 2.22 | 0.40 |
| 1:H:507:LEU:HD12 | 1:H:511:ARG:O | 2.21 | 0.40 |
| 1:I:215:ASP:HA | 1:I:216:PRO:HD2 | 1.94 | 0.40 |
| 1:I:242:VAL:HG13 | 1:I:246:TYR:HD1 | 1.87 | 0.40 |
| 1:I:536:ARG:HD3 | 7:I:2069:HOH:O | 2.21 | 0.40 |
| 1:K:209:ASN:HB3 | 1:K:212:LEU:HD12 | 2.04 | 0.40 |
| 1:K:36:LYS:O | 1:K:39:ALA:HB3 | 2.22 | 0.40 |
| 1:L:132:GLY:HA3 | 1:L:177:MSE:HE3 | 2.02 | 0.40 |
| 1:L:158:ILE:HG22 | 1:L:160:VAL:HG23 | 2.04 | 0.40 |
| 1:L:194:LYS:HA | 1:L:195:PRO:HD3 | 1.84 | 0.40 |

Continued on next page...

Continued from previous page...

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:136:THR:CG2 | 1:M:138:HIS:HB2 | 2.51 | 0.40 |
| 1:M:261:ASN:OD1 | 1:M:264:ARG:NH2 | 2.54 | 0.40 |
| 1:N:72:PHE:CZ | 1:N:81:ARG:HD3 | 2.56 | 0.40 |
| 1:O:429:THR:HG22 | 1:O:430:ALA:H | 1.86 | 0.40 |
| 1:P:165:ARG:HD2 | 1:P:165:ARG:C | 2.41 | 0.40 |
| 1:A:303:SER:HB3 | 1:A:332:VAL:HG21 | 2.03 | 0.40 |
| 1:C:26:TYR:N | 1:C:26:TYR:CD2 | 2.90 | 0.40 |
| 1:C:412:LYS:O | 1:C:440:ARG:NH1 | 2.48 | 0.40 |
| 1:C:505:GLU:HG3 | 7:C:2064:HOH:O | 2.20 | 0.40 |
| 1:C:533:GLU:CD | 1:C:536:ARG:HH11 | 2.25 | 0.40 |
| 1:D:166:ILE:HD12 | 1:D:179:ILE:CG1 | 2.51 | 0.40 |
| 1:F:395:ILE:O | 1:F:396:GLY:C | 2.60 | 0.40 |
| 1:G:174:CYS:HB2 | 1:G:220:GLY:HA3 | 2.04 | 0.40 |
| 1:G:388:VAL:HG22 | 1:G:415:ILE:HD12 | 2.03 | 0.40 |
| 1:G:514:PRO:HA | 1:G:515:PRO:HD3 | 1.93 | 0.40 |
| 1:I:108:MSE:CE | 1:I:190:CYS:SG | 3.08 | 0.40 |
| 1:J:432:GLN:H | 1:J:432:GLN:HG2 | 1.69 | 0.40 |
| 1:J:531:ALA:HB1 | 1:J:549:LEU:HD22 | 2.04 | 0.40 |
| 1:J:572:TRP:C | 1:J:573:PRO:O | 2.58 | 0.40 |
| 1:K:92:ASN:ND2 | 1:K:92:ASN:C | 2.75 | 0.40 |
| 1:L:312:ALA:HA | 1:L:316:ALA:HB3 | 2.03 | 0.40 |
| 1:L:157:ALA:HB2 | 1:L:479:ILE:HD11 | 2.04 | 0.40 |
| 1:N:194:LYS:HA | 1:N:195:PRO:HD3 | 1.93 | 0.40 |
| 1:N:184:LEU:HD12 | 1:N:200:PRO:HB3 | 2.04 | 0.40 |
| 1:N:395:ILE:O | 1:N:396:GLY:C | 2.60 | 0.40 |
| 1:O:316:ALA:HB1 | 1:O:343:MSE:HE2 | 2.02 | 0.40 |
| 1:O:98:LYS:HD3 | 1:O:560:THR:HG21 | 2.04 | 0.40 |
| 1:P:162:ASP:C | 1:P:162:ASP:OD1 | 2.60 | 0.40 |
| 1:P:243:THR:HG21 | 1:P:273:TYR:HD2 | 1.86 | 0.40 |
| 1:P:48:LEU:O | 1:P:49:ASN:HB2 | 2.21 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 553/555 (100%) | 524 (95%) | 23 (4%) | 6 (1%) | 17 | 29 |
| 1 | B | 553/555 (100%) | 530 (96%) | 21 (4%) | 2 (0%) | 38 | 59 |
| 1 | C | 553/555 (100%) | 530 (96%) | 21 (4%) | 2 (0%) | 38 | 59 |
| 1 | D | 553/555 (100%) | 530 (96%) | 21 (4%) | 2 (0%) | 38 | 59 |
| 1 | E | 553/555 (100%) | 530 (96%) | 22 (4%) | 1 (0%) | 51 | 73 |
| 1 | F | 553/555 (100%) | 529 (96%) | 22 (4%) | 2 (0%) | 38 | 59 |
| 1 | G | 553/555 (100%) | 531 (96%) | 19 (3%) | 3 (0%) | 32 | 53 |
| 1 | H | 553/555 (100%) | 534 (97%) | 16 (3%) | 3 (0%) | 32 | 53 |
| 1 | I | 553/555 (100%) | 535 (97%) | 17 (3%) | 1 (0%) | 51 | 73 |
| 1 | J | 553/555 (100%) | 531 (96%) | 19 (3%) | 3 (0%) | 32 | 53 |
| 1 | K | 553/555 (100%) | 524 (95%) | 27 (5%) | 2 (0%) | 38 | 59 |
| 1 | L | 553/555 (100%) | 534 (97%) | 14 (2%) | 5 (1%) | 20 | 36 |
| 1 | M | 553/555 (100%) | 528 (96%) | 23 (4%) | 2 (0%) | 38 | 59 |
| 1 | N | 553/555 (100%) | 528 (96%) | 21 (4%) | 4 (1%) | 25 | 43 |
| 1 | O | 553/555 (100%) | 531 (96%) | 18 (3%) | 4 (1%) | 25 | 43 |
| 1 | P | 553/555 (100%) | 532 (96%) | 18 (3%) | 3 (0%) | 32 | 53 |
| All | All | 8848/8880 (100%) | 8481 (96%) | 322 (4%) | 45 (0%) | 32 | 53 |

All (45) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 396 | GLY |
| 1 | A | 573 | PRO |
| 1 | B | 396 | GLY |
| 1 | C | 396 | GLY |
| 1 | D | 396 | GLY |
| 1 | D | 573 | PRO |
| 1 | E | 396 | GLY |
| 1 | F | 573 | PRO |
| 1 | G | 396 | GLY |
| 1 | G | 573 | PRO |
| 1 | H | 396 | GLY |
| 1 | I | 396 | GLY |
| 1 | J | 396 | GLY |
| 1 | J | 573 | PRO |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 396 | GLY |
| 1 | L | 396 | GLY |
| 1 | M | 396 | GLY |
| 1 | N | 352 | LYS |
| 1 | N | 396 | GLY |
| 1 | N | 573 | PRO |
| 1 | O | 396 | GLY |
| 1 | P | 396 | GLY |
| 1 | P | 573 | PRO |
| 1 | B | 468 | SER |
| 1 | C | 468 | SER |
| 1 | F | 396 | GLY |
| 1 | H | 468 | SER |
| 1 | P | 468 | SER |
| 1 | A | 259 | ASN |
| 1 | A | 468 | SER |
| 1 | L | 259 | ASN |
| 1 | O | 573 | PRO |
| 1 | L | 468 | SER |
| 1 | A | 25 | GLY |
| 1 | G | 392 | VAL |
| 1 | J | 392 | VAL |
| 1 | L | 392 | VAL |
| 1 | O | 392 | VAL |
| 1 | H | 392 | VAL |
| 1 | K | 392 | VAL |
| 1 | N | 392 | VAL |
| 1 | A | 392 | VAL |
| 1 | L | 56 | PRO |
| 1 | M | 56 | PRO |
| 1 | O | 56 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|----------|-------------|----|
| 1 | A | 467/453 (103%) | 438 (94%) | 29 (6%) | 21 | 39 |
| 1 | B | 467/453 (103%) | 438 (94%) | 29 (6%) | 21 | 39 |
| 1 | C | 467/453 (103%) | 437 (94%) | 30 (6%) | 20 | 38 |
| 1 | D | 467/453 (103%) | 439 (94%) | 28 (6%) | 22 | 41 |
| 1 | E | 467/453 (103%) | 431 (92%) | 36 (8%) | 15 | 28 |
| 1 | F | 467/453 (103%) | 434 (93%) | 33 (7%) | 17 | 32 |
| 1 | G | 467/453 (103%) | 441 (94%) | 26 (6%) | 25 | 45 |
| 1 | H | 467/453 (103%) | 437 (94%) | 30 (6%) | 20 | 38 |
| 1 | I | 467/453 (103%) | 439 (94%) | 28 (6%) | 22 | 41 |
| 1 | J | 467/453 (103%) | 437 (94%) | 30 (6%) | 20 | 38 |
| 1 | K | 467/453 (103%) | 443 (95%) | 24 (5%) | 28 | 50 |
| 1 | L | 467/453 (103%) | 437 (94%) | 30 (6%) | 20 | 38 |
| 1 | M | 467/453 (103%) | 432 (92%) | 35 (8%) | 16 | 29 |
| 1 | N | 467/453 (103%) | 443 (95%) | 24 (5%) | 28 | 50 |
| 1 | O | 467/453 (103%) | 437 (94%) | 30 (6%) | 20 | 38 |
| 1 | P | 467/453 (103%) | 430 (92%) | 37 (8%) | 14 | 27 |
| All | All | 7472/7248 (103%) | 6993 (94%) | 479 (6%) | 20 | 38 |

All (479) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 24 | LYS |
| 1 | A | 57 | CYS |
| 1 | A | 59 | LEU |
| 1 | A | 77 | SER |
| 1 | A | 88 | LEU |
| 1 | A | 92 | ASN |
| 1 | A | 114 | PRO |
| 1 | A | 118 | LEU |
| 1 | A | 125 | LEU |
| 1 | A | 136 | THR |
| 1 | A | 160 | VAL |
| 1 | A | 187 | TYR |
| 1 | A | 196 | HIS |
| 1 | A | 251 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 322 | LEU |
| 1 | A | 347 | LYS |
| 1 | A | 359 | THR |
| 1 | A | 389 | LEU |
| 1 | A | 402 | GLN |
| 1 | A | 410 | PHE |
| 1 | A | 458 | GLN |
| 1 | A | 459 | THR |
| 1 | A | 476 | LEU |
| 1 | A | 500 | GLN |
| 1 | A | 507 | LEU |
| 1 | A | 533 | GLU |
| 1 | A | 556 | GLN |
| 1 | A | 573 | PRO |
| 1 | A | 575 | GLU |
| 1 | B | 27 | GLU |
| 1 | B | 43 | GLU |
| 1 | B | 57 | CYS |
| 1 | B | 59 | LEU |
| 1 | B | 73 | GLU |
| 1 | B | 88 | LEU |
| 1 | B | 92 | ASN |
| 1 | B | 100 | LEU |
| 1 | B | 105 | GLU |
| 1 | B | 113 | THR |
| 1 | B | 125 | LEU |
| 1 | B | 133 | LEU |
| 1 | B | 165 | ARG |
| 1 | B | 187 | TYR |
| 1 | B | 239 | MSE |
| 1 | B | 251 | LEU |
| 1 | B | 292 | LEU |
| 1 | B | 301 | ARG |
| 1 | B | 310 | GLN |
| 1 | B | 322 | LEU |
| 1 | B | 352 | LYS |
| 1 | B | 389 | LEU |
| 1 | B | 401 | GLN |
| 1 | B | 405 | GLN |
| 1 | B | 458 | GLN |
| 1 | B | 476 | LEU |
| 1 | B | 556 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 560 | THR |
| 1 | B | 569 | SER |
| 1 | C | 41 | THR |
| 1 | C | 59 | LEU |
| 1 | C | 88 | LEU |
| 1 | C | 92 | ASN |
| 1 | C | 98 | LYS |
| 1 | C | 118 | LEU |
| 1 | C | 155 | ILE |
| 1 | C | 177 | MSE |
| 1 | C | 196 | HIS |
| 1 | C | 202 | MSE |
| 1 | C | 292 | LEU |
| 1 | C | 322 | LEU |
| 1 | C | 329 | LYS |
| 1 | C | 359 | THR |
| 1 | C | 364 | HIS |
| 1 | C | 378 | GLU |
| 1 | C | 389 | LEU |
| 1 | C | 410 | PHE |
| 1 | C | 438 | GLU |
| 1 | C | 476 | LEU |
| 1 | C | 500 | GLN |
| 1 | C | 507 | LEU |
| 1 | C | 516 | LEU |
| 1 | C | 521 | GLN |
| 1 | C | 556 | GLN |
| 1 | C | 560 | THR |
| 1 | C | 573 | PRO |
| 1 | C | 574 | GLU |
| 1 | C | 575 | GLU |
| 1 | C | 580 | LYS |
| 1 | D | 30 | ARG |
| 1 | D | 59 | LEU |
| 1 | D | 87 | SER |
| 1 | D | 88 | LEU |
| 1 | D | 92 | ASN |
| 1 | D | 133 | LEU |
| 1 | D | 136 | THR |
| 1 | D | 139 | ASP |
| 1 | D | 140 | ARG |
| 1 | D | 196 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 240 | GLU |
| 1 | D | 251 | LEU |
| 1 | D | 259 | ASN |
| 1 | D | 322 | LEU |
| 1 | D | 364 | HIS |
| 1 | D | 378 | GLU |
| 1 | D | 389 | LEU |
| 1 | D | 410 | PHE |
| 1 | D | 454 | LEU |
| 1 | D | 476 | LEU |
| 1 | D | 500 | GLN |
| 1 | D | 516 | LEU |
| 1 | D | 521 | GLN |
| 1 | D | 533 | GLU |
| 1 | D | 547 | GLU |
| 1 | D | 556 | GLN |
| 1 | D | 560 | THR |
| 1 | D | 575 | GLU |
| 1 | E | 24 | LYS |
| 1 | E | 27 | GLU |
| 1 | E | 43 | GLU |
| 1 | E | 48 | LEU |
| 1 | E | 57 | CYS |
| 1 | E | 59 | LEU |
| 1 | E | 88 | LEU |
| 1 | E | 92 | ASN |
| 1 | E | 100 | LEU |
| 1 | E | 118 | LEU |
| 1 | E | 125 | LEU |
| 1 | E | 131 | ARG |
| 1 | E | 133 | LEU |
| 1 | E | 187 | TYR |
| 1 | E | 196 | HIS |
| 1 | E | 240 | GLU |
| 1 | E | 245 | ARG |
| 1 | E | 251 | LEU |
| 1 | E | 310 | GLN |
| 1 | E | 322 | LEU |
| 1 | E | 333 | SER |
| 1 | E | 340 | ARG |
| 1 | E | 360 | PRO |
| 1 | E | 364 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 368 | GLU |
| 1 | E | 389 | LEU |
| 1 | E | 410 | PHE |
| 1 | E | 435 | LYS |
| 1 | E | 476 | LEU |
| 1 | E | 489 | ASP |
| 1 | E | 492 | LEU |
| 1 | E | 500 | GLN |
| 1 | E | 516 | LEU |
| 1 | E | 560 | THR |
| 1 | E | 573 | PRO |
| 1 | E | 575 | GLU |
| 1 | F | 24 | LYS |
| 1 | F | 30 | ARG |
| 1 | F | 57 | CYS |
| 1 | F | 59 | LEU |
| 1 | F | 88 | LEU |
| 1 | F | 92 | ASN |
| 1 | F | 129 | ARG |
| 1 | F | 133 | LEU |
| 1 | F | 140 | ARG |
| 1 | F | 152 | GLU |
| 1 | F | 177 | MSE |
| 1 | F | 196 | HIS |
| 1 | F | 227 | ARG |
| 1 | F | 244 | SER |
| 1 | F | 251 | LEU |
| 1 | F | 259 | ASN |
| 1 | F | 264 | ARG |
| 1 | F | 292 | LEU |
| 1 | F | 299 | LYS |
| 1 | F | 310 | GLN |
| 1 | F | 322 | LEU |
| 1 | F | 335 | GLU |
| 1 | F | 379 | ASP |
| 1 | F | 389 | LEU |
| 1 | F | 458 | GLN |
| 1 | F | 476 | LEU |
| 1 | F | 516 | LEU |
| 1 | F | 521 | GLN |
| 1 | F | 533 | GLU |
| 1 | F | 556 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 560 | THR |
| 1 | F | 573 | PRO |
| 1 | F | 575 | GLU |
| 1 | G | 48 | LEU |
| 1 | G | 57 | CYS |
| 1 | G | 59 | LEU |
| 1 | G | 88 | LEU |
| 1 | G | 92 | ASN |
| 1 | G | 114 | PRO |
| 1 | G | 125 | LEU |
| 1 | G | 133 | LEU |
| 1 | G | 160 | VAL |
| 1 | G | 196 | HIS |
| 1 | G | 227 | ARG |
| 1 | G | 243 | THR |
| 1 | G | 292 | LEU |
| 1 | G | 322 | LEU |
| 1 | G | 335 | GLU |
| 1 | G | 352 | LYS |
| 1 | G | 363 | GLU |
| 1 | G | 389 | LEU |
| 1 | G | 410 | PHE |
| 1 | G | 412 | LYS |
| 1 | G | 476 | LEU |
| 1 | G | 500 | GLN |
| 1 | G | 507 | LEU |
| 1 | G | 556 | GLN |
| 1 | G | 575 | GLU |
| 1 | G | 580 | LYS |
| 1 | H | 27 | GLU |
| 1 | H | 47 | GLN |
| 1 | H | 48 | LEU |
| 1 | H | 57 | CYS |
| 1 | H | 59 | LEU |
| 1 | H | 62 | ASP |
| 1 | H | 88 | LEU |
| 1 | H | 92 | ASN |
| 1 | H | 111 | VAL |
| 1 | H | 133 | LEU |
| 1 | H | 140 | ARG |
| 1 | H | 165 | ARG |
| 1 | H | 196 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 223 | HIS |
| 1 | H | 251 | LEU |
| 1 | H | 322 | LEU |
| 1 | H | 358 | LEU |
| 1 | H | 359 | THR |
| 1 | H | 389 | LEU |
| 1 | H | 476 | LEU |
| 1 | H | 500 | GLN |
| 1 | H | 505 | GLU |
| 1 | H | 507 | LEU |
| 1 | H | 516 | LEU |
| 1 | H | 539 | THR |
| 1 | H | 547 | GLU |
| 1 | H | 556 | GLN |
| 1 | H | 560 | THR |
| 1 | H | 575 | GLU |
| 1 | H | 578 | LYS |
| 1 | I | 48 | LEU |
| 1 | I | 49 | ASN |
| 1 | I | 59 | LEU |
| 1 | I | 61 | GLN |
| 1 | I | 73 | GLU |
| 1 | I | 88 | LEU |
| 1 | I | 92 | ASN |
| 1 | I | 131 | ARG |
| 1 | I | 133 | LEU |
| 1 | I | 165 | ARG |
| 1 | I | 187 | TYR |
| 1 | I | 223 | HIS |
| 1 | I | 285 | SER |
| 1 | I | 322 | LEU |
| 1 | I | 335 | GLU |
| 1 | I | 340 | ARG |
| 1 | I | 360 | PRO |
| 1 | I | 389 | LEU |
| 1 | I | 410 | PHE |
| 1 | I | 454 | LEU |
| 1 | I | 467 | ASN |
| 1 | I | 476 | LEU |
| 1 | I | 516 | LEU |
| 1 | I | 556 | GLN |
| 1 | I | 560 | THR |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 569 | SER |
| 1 | I | 575 | GLU |
| 1 | I | 578 | LYS |
| 1 | J | 27 | GLU |
| 1 | J | 59 | LEU |
| 1 | J | 67 | SER |
| 1 | J | 88 | LEU |
| 1 | J | 92 | ASN |
| 1 | J | 116 | VAL |
| 1 | J | 133 | LEU |
| 1 | J | 136 | THR |
| 1 | J | 140 | ARG |
| 1 | J | 165 | ARG |
| 1 | J | 187 | TYR |
| 1 | J | 202 | MSE |
| 1 | J | 251 | LEU |
| 1 | J | 292 | LEU |
| 1 | J | 322 | LEU |
| 1 | J | 363 | GLU |
| 1 | J | 389 | LEU |
| 1 | J | 405 | GLN |
| 1 | J | 476 | LEU |
| 1 | J | 489 | ASP |
| 1 | J | 500 | GLN |
| 1 | J | 504 | GLU |
| 1 | J | 505 | GLU |
| 1 | J | 507 | LEU |
| 1 | J | 521 | GLN |
| 1 | J | 533 | GLU |
| 1 | J | 538 | ASN |
| 1 | J | 556 | GLN |
| 1 | J | 560 | THR |
| 1 | J | 573 | PRO |
| 1 | K | 27 | GLU |
| 1 | K | 49 | ASN |
| 1 | K | 59 | LEU |
| 1 | K | 62 | ASP |
| 1 | K | 88 | LEU |
| 1 | K | 92 | ASN |
| 1 | K | 136 | THR |
| 1 | K | 139 | ASP |
| 1 | K | 165 | ARG |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 251 | LEU |
| 1 | K | 292 | LEU |
| 1 | K | 310 | GLN |
| 1 | K | 322 | LEU |
| 1 | K | 364 | HIS |
| 1 | K | 389 | LEU |
| 1 | K | 410 | PHE |
| 1 | K | 456 | SER |
| 1 | K | 476 | LEU |
| 1 | K | 489 | ASP |
| 1 | K | 533 | GLU |
| 1 | K | 556 | GLN |
| 1 | K | 560 | THR |
| 1 | K | 569 | SER |
| 1 | K | 578 | LYS |
| 1 | L | 48 | LEU |
| 1 | L | 57 | CYS |
| 1 | L | 59 | LEU |
| 1 | L | 88 | LEU |
| 1 | L | 92 | ASN |
| 1 | L | 152 | GLU |
| 1 | L | 177 | MSE |
| 1 | L | 187 | TYR |
| 1 | L | 196 | HIS |
| 1 | L | 224 | LYS |
| 1 | L | 239 | MSE |
| 1 | L | 245 | ARG |
| 1 | L | 251 | LEU |
| 1 | L | 261 | ASN |
| 1 | L | 310 | GLN |
| 1 | L | 321 | ASN |
| 1 | L | 322 | LEU |
| 1 | L | 352 | LYS |
| 1 | L | 364 | HIS |
| 1 | L | 389 | LEU |
| 1 | L | 456 | SER |
| 1 | L | 476 | LEU |
| 1 | L | 500 | GLN |
| 1 | L | 507 | LEU |
| 1 | L | 539 | THR |
| 1 | L | 547 | GLU |
| 1 | L | 556 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 557 | VAL |
| 1 | L | 575 | GLU |
| 1 | L | 580 | LYS |
| 1 | M | 24 | LYS |
| 1 | M | 27 | GLU |
| 1 | M | 57 | CYS |
| 1 | M | 59 | LEU |
| 1 | M | 88 | LEU |
| 1 | M | 92 | ASN |
| 1 | M | 105 | GLU |
| 1 | M | 125 | LEU |
| 1 | M | 133 | LEU |
| 1 | M | 136 | THR |
| 1 | M | 165 | ARG |
| 1 | M | 196 | HIS |
| 1 | M | 251 | LEU |
| 1 | M | 292 | LEU |
| 1 | M | 310 | GLN |
| 1 | M | 322 | LEU |
| 1 | M | 332 | VAL |
| 1 | M | 336 | GLU |
| 1 | M | 352 | LYS |
| 1 | M | 358 | LEU |
| 1 | M | 360 | PRO |
| 1 | M | 364 | HIS |
| 1 | M | 389 | LEU |
| 1 | M | 433 | LEU |
| 1 | M | 450 | ASP |
| 1 | M | 467 | ASN |
| 1 | M | 476 | LEU |
| 1 | M | 505 | GLU |
| 1 | M | 507 | LEU |
| 1 | M | 538 | ASN |
| 1 | M | 556 | GLN |
| 1 | M | 560 | THR |
| 1 | M | 571 | THR |
| 1 | M | 575 | GLU |
| 1 | M | 578 | LYS |
| 1 | N | 24 | LYS |
| 1 | N | 77 | SER |
| 1 | N | 88 | LEU |
| 1 | N | 92 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 105 | GLU |
| 1 | N | 125 | LEU |
| 1 | N | 133 | LEU |
| 1 | N | 139 | ASP |
| 1 | N | 152 | GLU |
| 1 | N | 187 | TYR |
| 1 | N | 196 | HIS |
| 1 | N | 310 | GLN |
| 1 | N | 321 | ASN |
| 1 | N | 322 | LEU |
| 1 | N | 389 | LEU |
| 1 | N | 410 | PHE |
| 1 | N | 456 | SER |
| 1 | N | 476 | LEU |
| 1 | N | 489 | ASP |
| 1 | N | 507 | LEU |
| 1 | N | 556 | GLN |
| 1 | N | 560 | THR |
| 1 | N | 573 | PRO |
| 1 | N | 578 | LYS |
| 1 | O | 57 | CYS |
| 1 | O | 59 | LEU |
| 1 | O | 88 | LEU |
| 1 | O | 92 | ASN |
| 1 | O | 133 | LEU |
| 1 | O | 165 | ARG |
| 1 | O | 177 | MSE |
| 1 | O | 187 | TYR |
| 1 | O | 196 | HIS |
| 1 | O | 232 | ASP |
| 1 | O | 245 | ARG |
| 1 | O | 251 | LEU |
| 1 | O | 302 | LEU |
| 1 | O | 303 | SER |
| 1 | O | 322 | LEU |
| 1 | O | 335 | GLU |
| 1 | O | 389 | LEU |
| 1 | O | 410 | PHE |
| 1 | O | 467 | ASN |
| 1 | O | 476 | LEU |
| 1 | O | 489 | ASP |
| 1 | O | 507 | LEU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 516 | LEU |
| 1 | O | 521 | GLN |
| 1 | O | 533 | GLU |
| 1 | O | 547 | GLU |
| 1 | O | 556 | GLN |
| 1 | O | 560 | THR |
| 1 | O | 571 | THR |
| 1 | O | 575 | GLU |
| 1 | P | 48 | LEU |
| 1 | P | 57 | CYS |
| 1 | P | 58 | PHE |
| 1 | P | 59 | LEU |
| 1 | P | 62 | ASP |
| 1 | P | 73 | GLU |
| 1 | P | 88 | LEU |
| 1 | P | 92 | ASN |
| 1 | P | 113 | THR |
| 1 | P | 118 | LEU |
| 1 | P | 131 | ARG |
| 1 | P | 140 | ARG |
| 1 | P | 152 | GLU |
| 1 | P | 153 | SER |
| 1 | P | 155 | ILE |
| 1 | P | 183 | LYS |
| 1 | P | 196 | HIS |
| 1 | P | 251 | LEU |
| 1 | P | 264 | ARG |
| 1 | P | 292 | LEU |
| 1 | P | 310 | GLN |
| 1 | P | 322 | LEU |
| 1 | P | 385 | LYS |
| 1 | P | 389 | LEU |
| 1 | P | 410 | PHE |
| 1 | P | 438 | GLU |
| 1 | P | 454 | LEU |
| 1 | P | 476 | LEU |
| 1 | P | 500 | GLN |
| 1 | P | 507 | LEU |
| 1 | P | 508 | GLN |
| 1 | P | 516 | LEU |
| 1 | P | 521 | GLN |
| 1 | P | 533 | GLU |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 556 | GLN |
| 1 | P | 560 | THR |
| 1 | P | 573 | PRO |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (286) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 33 | HIS |
| 1 | A | 35 | ASN |
| 1 | A | 61 | GLN |
| 1 | A | 64 | GLN |
| 1 | A | 89 | GLN |
| 1 | A | 92 | ASN |
| 1 | A | 122 | HIS |
| 1 | A | 223 | HIS |
| 1 | A | 229 | GLN |
| 1 | A | 305 | HIS |
| 1 | A | 310 | GLN |
| 1 | A | 328 | GLN |
| 1 | A | 432 | GLN |
| 1 | A | 508 | GLN |
| 1 | A | 545 | GLN |
| 1 | A | 556 | GLN |
| 1 | B | 33 | HIS |
| 1 | B | 35 | ASN |
| 1 | B | 61 | GLN |
| 1 | B | 64 | GLN |
| 1 | B | 89 | GLN |
| 1 | B | 92 | ASN |
| 1 | B | 223 | HIS |
| 1 | B | 305 | HIS |
| 1 | B | 328 | GLN |
| 1 | B | 364 | HIS |
| 1 | B | 401 | GLN |
| 1 | B | 402 | GLN |
| 1 | B | 432 | GLN |
| 1 | B | 458 | GLN |
| 1 | B | 508 | GLN |
| 1 | B | 521 | GLN |
| 1 | B | 537 | ASN |
| 1 | B | 545 | GLN |
| 1 | B | 556 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 35 | ASN |
| 1 | C | 46 | GLN |
| 1 | C | 61 | GLN |
| 1 | C | 64 | GLN |
| 1 | C | 89 | GLN |
| 1 | C | 92 | ASN |
| 1 | C | 197 | GLN |
| 1 | C | 223 | HIS |
| 1 | C | 229 | GLN |
| 1 | C | 305 | HIS |
| 1 | C | 328 | GLN |
| 1 | C | 401 | GLN |
| 1 | C | 402 | GLN |
| 1 | C | 458 | GLN |
| 1 | C | 508 | GLN |
| 1 | C | 537 | ASN |
| 1 | C | 545 | GLN |
| 1 | C | 556 | GLN |
| 1 | D | 33 | HIS |
| 1 | D | 35 | ASN |
| 1 | D | 61 | GLN |
| 1 | D | 64 | GLN |
| 1 | D | 89 | GLN |
| 1 | D | 92 | ASN |
| 1 | D | 196 | HIS |
| 1 | D | 229 | GLN |
| 1 | D | 259 | ASN |
| 1 | D | 305 | HIS |
| 1 | D | 328 | GLN |
| 1 | D | 401 | GLN |
| 1 | D | 432 | GLN |
| 1 | D | 458 | GLN |
| 1 | D | 467 | ASN |
| 1 | D | 508 | GLN |
| 1 | D | 521 | GLN |
| 1 | D | 545 | GLN |
| 1 | D | 556 | GLN |
| 1 | D | 563 | ASN |
| 1 | E | 35 | ASN |
| 1 | E | 46 | GLN |
| 1 | E | 49 | ASN |
| 1 | E | 61 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 64 | GLN |
| 1 | E | 92 | ASN |
| 1 | E | 122 | HIS |
| 1 | E | 223 | HIS |
| 1 | E | 305 | HIS |
| 1 | E | 328 | GLN |
| 1 | E | 500 | GLN |
| 1 | E | 538 | ASN |
| 1 | E | 545 | GLN |
| 1 | F | 33 | HIS |
| 1 | F | 35 | ASN |
| 1 | F | 61 | GLN |
| 1 | F | 64 | GLN |
| 1 | F | 89 | GLN |
| 1 | F | 92 | ASN |
| 1 | F | 197 | GLN |
| 1 | F | 223 | HIS |
| 1 | F | 259 | ASN |
| 1 | F | 267 | HIS |
| 1 | F | 305 | HIS |
| 1 | F | 328 | GLN |
| 1 | F | 432 | GLN |
| 1 | F | 458 | GLN |
| 1 | F | 467 | ASN |
| 1 | F | 521 | GLN |
| 1 | F | 545 | GLN |
| 1 | F | 556 | GLN |
| 1 | G | 33 | HIS |
| 1 | G | 35 | ASN |
| 1 | G | 51 | HIS |
| 1 | G | 61 | GLN |
| 1 | G | 64 | GLN |
| 1 | G | 89 | GLN |
| 1 | G | 92 | ASN |
| 1 | G | 122 | HIS |
| 1 | G | 148 | GLN |
| 1 | G | 223 | HIS |
| 1 | G | 229 | GLN |
| 1 | G | 305 | HIS |
| 1 | G | 328 | GLN |
| 1 | G | 401 | GLN |
| 1 | G | 432 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 467 | ASN |
| 1 | G | 521 | GLN |
| 1 | G | 545 | GLN |
| 1 | G | 556 | GLN |
| 1 | H | 33 | HIS |
| 1 | H | 35 | ASN |
| 1 | H | 49 | ASN |
| 1 | H | 61 | GLN |
| 1 | H | 64 | GLN |
| 1 | H | 89 | GLN |
| 1 | H | 92 | ASN |
| 1 | H | 148 | GLN |
| 1 | H | 223 | HIS |
| 1 | H | 229 | GLN |
| 1 | H | 271 | ASN |
| 1 | H | 305 | HIS |
| 1 | H | 321 | ASN |
| 1 | H | 328 | GLN |
| 1 | H | 367 | HIS |
| 1 | H | 376 | ASN |
| 1 | H | 401 | GLN |
| 1 | H | 405 | GLN |
| 1 | H | 432 | GLN |
| 1 | H | 508 | GLN |
| 1 | H | 521 | GLN |
| 1 | H | 537 | ASN |
| 1 | H | 545 | GLN |
| 1 | H | 556 | GLN |
| 1 | I | 33 | HIS |
| 1 | I | 35 | ASN |
| 1 | I | 61 | GLN |
| 1 | I | 64 | GLN |
| 1 | I | 89 | GLN |
| 1 | I | 92 | ASN |
| 1 | I | 121 | GLN |
| 1 | I | 122 | HIS |
| 1 | I | 229 | GLN |
| 1 | I | 305 | HIS |
| 1 | I | 328 | GLN |
| 1 | I | 405 | GLN |
| 1 | I | 458 | GLN |
| 1 | I | 467 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 537 | ASN |
| 1 | I | 545 | GLN |
| 1 | I | 556 | GLN |
| 1 | J | 33 | HIS |
| 1 | J | 35 | ASN |
| 1 | J | 49 | ASN |
| 1 | J | 61 | GLN |
| 1 | J | 64 | GLN |
| 1 | J | 89 | GLN |
| 1 | J | 92 | ASN |
| 1 | J | 122 | HIS |
| 1 | J | 223 | HIS |
| 1 | J | 259 | ASN |
| 1 | J | 305 | HIS |
| 1 | J | 328 | GLN |
| 1 | J | 364 | HIS |
| 1 | J | 432 | GLN |
| 1 | J | 467 | ASN |
| 1 | J | 545 | GLN |
| 1 | J | 556 | GLN |
| 1 | J | 563 | ASN |
| 1 | K | 33 | HIS |
| 1 | K | 35 | ASN |
| 1 | K | 46 | GLN |
| 1 | K | 61 | GLN |
| 1 | K | 64 | GLN |
| 1 | K | 89 | GLN |
| 1 | K | 92 | ASN |
| 1 | K | 148 | GLN |
| 1 | K | 197 | GLN |
| 1 | K | 259 | ASN |
| 1 | K | 305 | HIS |
| 1 | K | 310 | GLN |
| 1 | K | 401 | GLN |
| 1 | K | 402 | GLN |
| 1 | K | 432 | GLN |
| 1 | K | 467 | ASN |
| 1 | K | 508 | GLN |
| 1 | K | 545 | GLN |
| 1 | K | 556 | GLN |
| 1 | L | 35 | ASN |
| 1 | L | 49 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 51 | HIS |
| 1 | L | 61 | GLN |
| 1 | L | 64 | GLN |
| 1 | L | 89 | GLN |
| 1 | L | 92 | ASN |
| 1 | L | 148 | GLN |
| 1 | L | 223 | HIS |
| 1 | L | 261 | ASN |
| 1 | L | 305 | HIS |
| 1 | L | 310 | GLN |
| 1 | L | 321 | ASN |
| 1 | L | 328 | GLN |
| 1 | L | 432 | GLN |
| 1 | L | 467 | ASN |
| 1 | L | 500 | GLN |
| 1 | L | 537 | ASN |
| 1 | L | 556 | GLN |
| 1 | M | 33 | HIS |
| 1 | M | 35 | ASN |
| 1 | M | 51 | HIS |
| 1 | M | 61 | GLN |
| 1 | M | 64 | GLN |
| 1 | M | 89 | GLN |
| 1 | M | 92 | ASN |
| 1 | M | 223 | HIS |
| 1 | M | 305 | HIS |
| 1 | M | 401 | GLN |
| 1 | M | 405 | GLN |
| 1 | M | 432 | GLN |
| 1 | M | 467 | ASN |
| 1 | M | 508 | GLN |
| 1 | M | 545 | GLN |
| 1 | M | 556 | GLN |
| 1 | N | 33 | HIS |
| 1 | N | 35 | ASN |
| 1 | N | 61 | GLN |
| 1 | N | 64 | GLN |
| 1 | N | 89 | GLN |
| 1 | N | 92 | ASN |
| 1 | N | 223 | HIS |
| 1 | N | 259 | ASN |
| 1 | N | 305 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 328 | GLN |
| 1 | N | 458 | GLN |
| 1 | N | 464 | GLN |
| 1 | N | 467 | ASN |
| 1 | N | 508 | GLN |
| 1 | N | 545 | GLN |
| 1 | N | 556 | GLN |
| 1 | O | 33 | HIS |
| 1 | O | 35 | ASN |
| 1 | O | 61 | GLN |
| 1 | O | 64 | GLN |
| 1 | O | 89 | GLN |
| 1 | O | 92 | ASN |
| 1 | O | 223 | HIS |
| 1 | O | 267 | HIS |
| 1 | O | 305 | HIS |
| 1 | O | 328 | GLN |
| 1 | O | 401 | GLN |
| 1 | O | 402 | GLN |
| 1 | O | 405 | GLN |
| 1 | O | 432 | GLN |
| 1 | O | 467 | ASN |
| 1 | O | 508 | GLN |
| 1 | O | 537 | ASN |
| 1 | O | 545 | GLN |
| 1 | O | 556 | GLN |
| 1 | P | 33 | HIS |
| 1 | P | 35 | ASN |
| 1 | P | 61 | GLN |
| 1 | P | 64 | GLN |
| 1 | P | 89 | GLN |
| 1 | P | 92 | ASN |
| 1 | P | 223 | HIS |
| 1 | P | 229 | GLN |
| 1 | P | 305 | HIS |
| 1 | P | 402 | GLN |
| 1 | P | 432 | GLN |
| 1 | P | 500 | GLN |
| 1 | P | 508 | GLN |
| 1 | P | 545 | GLN |
| 1 | P | 556 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 117 ligands modelled in this entry, 85 are monoatomic - leaving 32 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 | $\# Z > 2$ |
| 2 | NAP | A | 1581 | - | 44,52,52 | 1.70 | 10 (22%) | 51,80,80 | 1.76 | 3 (5%) |
| 3 | OXL | A | 1583 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | B | 1581 | - | 44,52,52 | 1.56 | 10 (22%) | 51,80,80 | 1.73 | 4 (7%) |
| 3 | OXL | B | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | C | 1581 | - | 44,52,52 | 1.65 | 7 (15%) | 51,80,80 | 1.76 | 4 (7%) |
| 3 | OXL | C | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | D | 1581 | - | 44,52,52 | 1.60 | 9 (20%) | 51,80,80 | 1.84 | 4 (7%) |
| 3 | OXL | D | 1582 | 4,6 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | E | 1581 | - | 44,52,52 | 1.67 | 9 (20%) | 51,80,80 | 1.77 | 4 (7%) |
| 3 | OXL | E | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | F | 1581 | - | 44,52,52 | 1.60 | 8 (18%) | 51,80,80 | 1.78 | 5 (9%) |
| 3 | OXL | F | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | G | 1581 | - | 44,52,52 | 1.58 | 6 (13%) | 51,80,80 | 1.79 | 4 (7%) |
| 3 | OXL | G | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | H | 1581 | - | 44,52,52 | 1.62 | 9 (20%) | 51,80,80 | 1.78 | 5 (9%) |
| 3 | OXL | H | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | NAP | I | 1581 | - | 44,52,52 | 1.71 | 11 (25%) | 51,80,80 | 1.79 | 4 (7%) |
| 3 | OXL | I | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | J | 1581 | - | 44,52,52 | 1.62 | 8 (18%) | 51,80,80 | 1.85 | 4 (7%) |
| 3 | OXL | J | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | K | 1581 | - | 44,52,52 | 1.68 | 8 (18%) | 51,80,80 | 1.81 | 5 (9%) |
| 3 | OXL | K | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | L | 1581 | - | 44,52,52 | 1.77 | 11 (25%) | 51,80,80 | 1.78 | 3 (5%) |
| 3 | OXL | L | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | M | 1581 | - | 44,52,52 | 1.55 | 8 (18%) | 51,80,80 | 1.75 | 5 (9%) |
| 3 | OXL | M | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | N | 1581 | - | 44,52,52 | 1.70 | 9 (20%) | 51,80,80 | 1.79 | 4 (7%) |
| 3 | OXL | N | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | O | 1581 | - | 44,52,52 | 1.62 | 9 (20%) | 51,80,80 | 1.82 | 4 (7%) |
| 3 | OXL | O | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |
| 2 | NAP | P | 1581 | - | 44,52,52 | 1.56 | 10 (22%) | 51,80,80 | 1.76 | 5 (9%) |
| 3 | OXL | P | 1582 | 4 | 0,5,5 | 0.00 | - | 0,6,6 | 0.00 | - |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 2 | NAP | A | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | A | 1583 | 4 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | B | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | B | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | C | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | C | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | D | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | D | 1582 | 4,6 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | E | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | E | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | F | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | F | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | G | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | G | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | H | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | H | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | I | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | I | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 2 | NAP | J | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | J | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | K | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | K | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | L | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | L | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | M | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | M | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | N | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | N | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | O | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | O | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |
| 2 | NAP | P | 1581 | - | - | 0/27/67/67 | 0/5/5/5 |
| 3 | OXL | P | 1582 | 4 | - | 0/0/4/4 | 0/0/0/0 |

All (142) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | D | 1581 | NAP | C5A-C4A | -3.46 | 1.32 | 1.40 |
| 2 | J | 1581 | NAP | C5A-C4A | -3.34 | 1.33 | 1.40 |
| 2 | P | 1581 | NAP | C5A-C4A | -3.31 | 1.33 | 1.40 |
| 2 | F | 1581 | NAP | C5A-C4A | -3.30 | 1.33 | 1.40 |
| 2 | F | 1581 | NAP | C2D-C1D | -3.24 | 1.48 | 1.53 |
| 2 | L | 1581 | NAP | C5A-C4A | -3.22 | 1.33 | 1.40 |
| 2 | G | 1581 | NAP | C5A-C4A | -3.18 | 1.33 | 1.40 |
| 2 | I | 1581 | NAP | C5A-C4A | -3.11 | 1.33 | 1.40 |
| 2 | H | 1581 | NAP | C5A-C4A | -3.11 | 1.33 | 1.40 |
| 2 | K | 1581 | NAP | C5A-C4A | -3.05 | 1.33 | 1.40 |
| 2 | A | 1581 | NAP | C5A-C4A | -3.04 | 1.33 | 1.40 |
| 2 | C | 1581 | NAP | C5A-C4A | -3.02 | 1.33 | 1.40 |
| 2 | B | 1581 | NAP | C5A-C4A | -3.01 | 1.33 | 1.40 |
| 2 | E | 1581 | NAP | C5A-C4A | -3.00 | 1.33 | 1.40 |
| 2 | O | 1581 | NAP | C5A-C4A | -2.99 | 1.33 | 1.40 |
| 2 | N | 1581 | NAP | C5A-C4A | -2.95 | 1.33 | 1.40 |
| 2 | D | 1581 | NAP | C2D-C1D | -2.95 | 1.49 | 1.53 |
| 2 | M | 1581 | NAP | C5A-C4A | -2.79 | 1.34 | 1.40 |
| 2 | C | 1581 | NAP | C2D-C1D | -2.76 | 1.49 | 1.53 |
| 2 | P | 1581 | NAP | C5A-N7A | -2.47 | 1.31 | 1.39 |
| 2 | E | 1581 | NAP | C5A-N7A | -2.40 | 1.31 | 1.39 |
| 2 | M | 1581 | NAP | C5A-N7A | -2.39 | 1.31 | 1.39 |
| 2 | L | 1581 | NAP | C2D-C1D | -2.37 | 1.49 | 1.53 |
| 2 | O | 1581 | NAP | C3B-C2B | -2.36 | 1.47 | 1.53 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2 | D | 1581 | NAP | C5A-N7A | -2.35 | 1.31 | 1.39 |
| 2 | L | 1581 | NAP | C5A-N7A | -2.34 | 1.31 | 1.39 |
| 2 | O | 1581 | NAP | C5A-N7A | -2.33 | 1.31 | 1.39 |
| 2 | A | 1581 | NAP | C5A-N7A | -2.30 | 1.31 | 1.39 |
| 2 | P | 1581 | NAP | C2D-C1D | -2.29 | 1.50 | 1.53 |
| 2 | K | 1581 | NAP | C5A-N7A | -2.25 | 1.31 | 1.39 |
| 2 | N | 1581 | NAP | C5A-N7A | -2.23 | 1.31 | 1.39 |
| 2 | J | 1581 | NAP | C5A-N7A | -2.20 | 1.32 | 1.39 |
| 2 | H | 1581 | NAP | C5A-N7A | -2.19 | 1.32 | 1.39 |
| 2 | I | 1581 | NAP | C5A-N7A | -2.12 | 1.32 | 1.39 |
| 2 | B | 1581 | NAP | C5A-N7A | -2.10 | 1.32 | 1.39 |
| 2 | F | 1581 | NAP | C5A-N7A | -2.02 | 1.32 | 1.39 |
| 2 | B | 1581 | NAP | O4D-C4D | 2.00 | 1.49 | 1.45 |
| 2 | P | 1581 | NAP | C4N-C3N | 2.01 | 1.42 | 1.39 |
| 2 | H | 1581 | NAP | C2A-N1A | 2.02 | 1.37 | 1.33 |
| 2 | B | 1581 | NAP | C4N-C3N | 2.03 | 1.42 | 1.39 |
| 2 | E | 1581 | NAP | P2B-O2B | 2.03 | 1.63 | 1.59 |
| 2 | I | 1581 | NAP | O4D-C4D | 2.07 | 1.49 | 1.45 |
| 2 | N | 1581 | NAP | C2A-N1A | 2.09 | 1.37 | 1.33 |
| 2 | A | 1581 | NAP | C2A-N1A | 2.11 | 1.37 | 1.33 |
| 2 | N | 1581 | NAP | C5N-C4N | 2.12 | 1.42 | 1.38 |
| 2 | B | 1581 | NAP | C2A-N1A | 2.12 | 1.37 | 1.33 |
| 2 | J | 1581 | NAP | C2A-N1A | 2.18 | 1.38 | 1.33 |
| 2 | I | 1581 | NAP | C5N-C4N | 2.19 | 1.43 | 1.38 |
| 2 | O | 1581 | NAP | O4D-C4D | 2.20 | 1.50 | 1.45 |
| 2 | L | 1581 | NAP | C4N-C3N | 2.20 | 1.42 | 1.39 |
| 2 | I | 1581 | NAP | C2A-N1A | 2.20 | 1.38 | 1.33 |
| 2 | D | 1581 | NAP | C2A-N1A | 2.24 | 1.38 | 1.33 |
| 2 | P | 1581 | NAP | C5N-C4N | 2.26 | 1.43 | 1.38 |
| 2 | L | 1581 | NAP | C5N-C4N | 2.26 | 1.43 | 1.38 |
| 2 | A | 1581 | NAP | C4N-C3N | 2.27 | 1.43 | 1.39 |
| 2 | K | 1581 | NAP | C4N-C3N | 2.32 | 1.43 | 1.39 |
| 2 | M | 1581 | NAP | C2A-N1A | 2.33 | 1.38 | 1.33 |
| 2 | H | 1581 | NAP | O4D-C4D | 2.33 | 1.50 | 1.45 |
| 2 | L | 1581 | NAP | C2A-N1A | 2.33 | 1.38 | 1.33 |
| 2 | G | 1581 | NAP | C3N-C7N | 2.34 | 1.54 | 1.50 |
| 2 | A | 1581 | NAP | P2B-O2B | 2.34 | 1.63 | 1.59 |
| 2 | E | 1581 | NAP | C2A-N1A | 2.37 | 1.38 | 1.33 |
| 2 | F | 1581 | NAP | O4D-C1D | 2.40 | 1.44 | 1.41 |
| 2 | P | 1581 | NAP | O4D-C1D | 2.43 | 1.44 | 1.41 |
| 2 | O | 1581 | NAP | C3N-C7N | 2.45 | 1.54 | 1.50 |
| 2 | I | 1581 | NAP | C4N-C3N | 2.47 | 1.43 | 1.39 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2 | N | 1581 | NAP | C3N-C7N | 2.48 | 1.54 | 1.50 |
| 2 | B | 1581 | NAP | O4D-C1D | 2.52 | 1.44 | 1.41 |
| 2 | M | 1581 | NAP | O4D-C1D | 2.55 | 1.44 | 1.41 |
| 2 | P | 1581 | NAP | C3N-C7N | 2.59 | 1.54 | 1.50 |
| 2 | H | 1581 | NAP | C3N-C7N | 2.60 | 1.54 | 1.50 |
| 2 | J | 1581 | NAP | C3N-C7N | 2.62 | 1.54 | 1.50 |
| 2 | D | 1581 | NAP | C3N-C7N | 2.71 | 1.54 | 1.50 |
| 2 | M | 1581 | NAP | C3N-C7N | 2.78 | 1.54 | 1.50 |
| 2 | B | 1581 | NAP | C3N-C7N | 2.81 | 1.54 | 1.50 |
| 2 | O | 1581 | NAP | C6N-N1N | 2.90 | 1.43 | 1.35 |
| 2 | M | 1581 | NAP | C2A-N3A | 2.96 | 1.37 | 1.32 |
| 2 | O | 1581 | NAP | O4B-C1B | 2.99 | 1.45 | 1.41 |
| 2 | I | 1581 | NAP | C2A-N3A | 3.00 | 1.37 | 1.32 |
| 2 | J | 1581 | NAP | O4B-C1B | 3.01 | 1.45 | 1.41 |
| 2 | O | 1581 | NAP | C2A-N3A | 3.01 | 1.37 | 1.32 |
| 2 | C | 1581 | NAP | C2A-N3A | 3.03 | 1.37 | 1.32 |
| 2 | F | 1581 | NAP | C2A-N3A | 3.05 | 1.37 | 1.32 |
| 2 | D | 1581 | NAP | C2A-N3A | 3.07 | 1.37 | 1.32 |
| 2 | F | 1581 | NAP | O4B-C1B | 3.08 | 1.45 | 1.41 |
| 2 | P | 1581 | NAP | O4B-C1B | 3.09 | 1.45 | 1.41 |
| 2 | J | 1581 | NAP | C2A-N3A | 3.10 | 1.37 | 1.32 |
| 2 | L | 1581 | NAP | O4D-C1D | 3.11 | 1.45 | 1.41 |
| 2 | D | 1581 | NAP | O4D-C1D | 3.15 | 1.45 | 1.41 |
| 2 | D | 1581 | NAP | C6N-N1N | 3.16 | 1.43 | 1.35 |
| 2 | K | 1581 | NAP | C2A-N3A | 3.18 | 1.37 | 1.32 |
| 2 | C | 1581 | NAP | C6N-N1N | 3.19 | 1.43 | 1.35 |
| 2 | F | 1581 | NAP | C3N-C7N | 3.20 | 1.55 | 1.50 |
| 2 | A | 1581 | NAP | C2A-N3A | 3.22 | 1.37 | 1.32 |
| 2 | A | 1581 | NAP | C3N-C7N | 3.23 | 1.55 | 1.50 |
| 2 | G | 1581 | NAP | C2A-N3A | 3.23 | 1.37 | 1.32 |
| 2 | H | 1581 | NAP | C6N-N1N | 3.25 | 1.43 | 1.35 |
| 2 | I | 1581 | NAP | O4D-C1D | 3.25 | 1.45 | 1.41 |
| 2 | N | 1581 | NAP | O4D-C1D | 3.30 | 1.45 | 1.41 |
| 2 | E | 1581 | NAP | O4B-C1B | 3.31 | 1.45 | 1.41 |
| 2 | P | 1581 | NAP | C2A-N3A | 3.31 | 1.37 | 1.32 |
| 2 | L | 1581 | NAP | C2A-N3A | 3.35 | 1.37 | 1.32 |
| 2 | M | 1581 | NAP | C6N-N1N | 3.38 | 1.44 | 1.35 |
| 2 | K | 1581 | NAP | O4D-C1D | 3.39 | 1.46 | 1.41 |
| 2 | I | 1581 | NAP | O4B-C1B | 3.41 | 1.46 | 1.41 |
| 2 | G | 1581 | NAP | C6N-N1N | 3.42 | 1.44 | 1.35 |
| 2 | E | 1581 | NAP | C6N-N1N | 3.44 | 1.44 | 1.35 |
| 2 | J | 1581 | NAP | C6N-N1N | 3.47 | 1.44 | 1.35 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2 | B | 1581 | NAP | C6N-N1N | 3.51 | 1.44 | 1.35 |
| 2 | B | 1581 | NAP | C2A-N3A | 3.52 | 1.38 | 1.32 |
| 2 | E | 1581 | NAP | C2A-N3A | 3.52 | 1.38 | 1.32 |
| 2 | L | 1581 | NAP | C6N-N1N | 3.52 | 1.44 | 1.35 |
| 2 | B | 1581 | NAP | O4B-C1B | 3.54 | 1.46 | 1.41 |
| 2 | L | 1581 | NAP | C3N-C7N | 3.57 | 1.56 | 1.50 |
| 2 | H | 1581 | NAP | C2A-N3A | 3.58 | 1.38 | 1.32 |
| 2 | G | 1581 | NAP | O4B-C1B | 3.58 | 1.46 | 1.41 |
| 2 | P | 1581 | NAP | C6N-N1N | 3.60 | 1.44 | 1.35 |
| 2 | A | 1581 | NAP | C6N-N1N | 3.60 | 1.44 | 1.35 |
| 2 | K | 1581 | NAP | C3N-C7N | 3.61 | 1.56 | 1.50 |
| 2 | E | 1581 | NAP | C3N-C7N | 3.61 | 1.56 | 1.50 |
| 2 | K | 1581 | NAP | C6N-N1N | 3.61 | 1.44 | 1.35 |
| 2 | I | 1581 | NAP | C3N-C7N | 3.65 | 1.56 | 1.50 |
| 2 | M | 1581 | NAP | O4B-C1B | 3.66 | 1.46 | 1.41 |
| 2 | A | 1581 | NAP | O4D-C1D | 3.66 | 1.46 | 1.41 |
| 2 | N | 1581 | NAP | C6N-N1N | 3.69 | 1.45 | 1.35 |
| 2 | F | 1581 | NAP | C6N-N1N | 3.69 | 1.45 | 1.35 |
| 2 | C | 1581 | NAP | O4D-C1D | 3.70 | 1.46 | 1.41 |
| 2 | C | 1581 | NAP | C3N-C7N | 3.70 | 1.56 | 1.50 |
| 2 | N | 1581 | NAP | O4B-C1B | 3.70 | 1.46 | 1.41 |
| 2 | C | 1581 | NAP | O4B-C1B | 3.75 | 1.46 | 1.41 |
| 2 | H | 1581 | NAP | O4B-C1B | 3.77 | 1.46 | 1.41 |
| 2 | E | 1581 | NAP | O4D-C1D | 3.80 | 1.46 | 1.41 |
| 2 | G | 1581 | NAP | O4D-C1D | 3.83 | 1.46 | 1.41 |
| 2 | D | 1581 | NAP | O4B-C1B | 3.85 | 1.46 | 1.41 |
| 2 | N | 1581 | NAP | C2A-N3A | 3.99 | 1.38 | 1.32 |
| 2 | I | 1581 | NAP | C6N-N1N | 4.00 | 1.45 | 1.35 |
| 2 | J | 1581 | NAP | O4D-C1D | 4.01 | 1.46 | 1.41 |
| 2 | H | 1581 | NAP | O4D-C1D | 4.29 | 1.47 | 1.41 |
| 2 | O | 1581 | NAP | O4D-C1D | 4.43 | 1.47 | 1.41 |
| 2 | L | 1581 | NAP | O4B-C1B | 4.49 | 1.47 | 1.41 |
| 2 | A | 1581 | NAP | O4B-C1B | 4.49 | 1.47 | 1.41 |
| 2 | K | 1581 | NAP | O4B-C1B | 4.72 | 1.47 | 1.41 |

All (67) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 2 | D | 1581 | NAP | N3A-C2A-N1A | -10.03 | 120.13 | 128.86 |
| 2 | J | 1581 | NAP | N3A-C2A-N1A | -9.72 | 120.39 | 128.86 |
| 2 | G | 1581 | NAP | N3A-C2A-N1A | -9.68 | 120.43 | 128.86 |
| 2 | L | 1581 | NAP | N3A-C2A-N1A | -9.63 | 120.47 | 128.86 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | H | 1581 | NAP | N3A-C2A-N1A | -9.59 | 120.50 | 128.86 |
| 2 | O | 1581 | NAP | N3A-C2A-N1A | -9.54 | 120.55 | 128.86 |
| 2 | A | 1581 | NAP | N3A-C2A-N1A | -9.52 | 120.57 | 128.86 |
| 2 | E | 1581 | NAP | N3A-C2A-N1A | -9.50 | 120.59 | 128.86 |
| 2 | F | 1581 | NAP | N3A-C2A-N1A | -9.49 | 120.59 | 128.86 |
| 2 | K | 1581 | NAP | N3A-C2A-N1A | -9.43 | 120.64 | 128.86 |
| 2 | I | 1581 | NAP | N3A-C2A-N1A | -9.41 | 120.66 | 128.86 |
| 2 | P | 1581 | NAP | N3A-C2A-N1A | -9.40 | 120.67 | 128.86 |
| 2 | N | 1581 | NAP | N3A-C2A-N1A | -9.38 | 120.69 | 128.86 |
| 2 | M | 1581 | NAP | N3A-C2A-N1A | -9.21 | 120.84 | 128.86 |
| 2 | B | 1581 | NAP | N3A-C2A-N1A | -9.16 | 120.88 | 128.86 |
| 2 | C | 1581 | NAP | N3A-C2A-N1A | -9.13 | 120.91 | 128.86 |
| 2 | N | 1581 | NAP | C4B-O4B-C1B | -3.96 | 105.55 | 109.77 |
| 2 | I | 1581 | NAP | C4B-O4B-C1B | -3.95 | 105.56 | 109.77 |
| 2 | J | 1581 | NAP | C4B-O4B-C1B | -3.89 | 105.63 | 109.77 |
| 2 | L | 1581 | NAP | C4B-O4B-C1B | -3.84 | 105.68 | 109.77 |
| 2 | K | 1581 | NAP | C4B-O4B-C1B | -3.84 | 105.69 | 109.77 |
| 2 | C | 1581 | NAP | C4B-O4B-C1B | -3.83 | 105.69 | 109.77 |
| 2 | O | 1581 | NAP | C4B-O4B-C1B | -3.65 | 105.89 | 109.77 |
| 2 | B | 1581 | NAP | C4B-O4B-C1B | -3.59 | 105.95 | 109.77 |
| 2 | D | 1581 | NAP | C4B-O4B-C1B | -3.49 | 106.05 | 109.77 |
| 2 | P | 1581 | NAP | C4B-O4B-C1B | -3.43 | 106.12 | 109.77 |
| 2 | G | 1581 | NAP | C4B-O4B-C1B | -3.38 | 106.17 | 109.77 |
| 2 | F | 1581 | NAP | C4B-O4B-C1B | -3.18 | 106.38 | 109.77 |
| 2 | A | 1581 | NAP | C4B-O4B-C1B | -3.17 | 106.39 | 109.77 |
| 2 | M | 1581 | NAP | C4B-O4B-C1B | -3.17 | 106.40 | 109.77 |
| 2 | O | 1581 | NAP | C4D-O4D-C1D | -3.16 | 106.41 | 109.77 |
| 2 | E | 1581 | NAP | C4B-O4B-C1B | -3.14 | 106.43 | 109.77 |
| 2 | H | 1581 | NAP | C4D-O4D-C1D | -3.10 | 106.47 | 109.77 |
| 2 | I | 1581 | NAP | C4D-O4D-C1D | -2.83 | 106.75 | 109.77 |
| 2 | F | 1581 | NAP | C4D-O4D-C1D | -2.73 | 106.87 | 109.77 |
| 2 | N | 1581 | NAP | C4D-O4D-C1D | -2.54 | 107.07 | 109.77 |
| 2 | J | 1581 | NAP | C4D-O4D-C1D | -2.49 | 107.11 | 109.77 |
| 2 | H | 1581 | NAP | C4B-O4B-C1B | -2.45 | 107.16 | 109.77 |
| 2 | B | 1581 | NAP | C4D-O4D-C1D | -2.40 | 107.21 | 109.77 |
| 2 | D | 1581 | NAP | C4D-O4D-C1D | -2.35 | 107.27 | 109.77 |
| 2 | C | 1581 | NAP | C3N-C7N-N7N | -2.29 | 115.16 | 117.77 |
| 2 | E | 1581 | NAP | C3N-C7N-N7N | -2.23 | 115.22 | 117.77 |
| 2 | M | 1581 | NAP | C4D-O4D-C1D | -2.23 | 107.40 | 109.77 |
| 2 | K | 1581 | NAP | C3N-C7N-N7N | -2.20 | 115.26 | 117.77 |
| 2 | P | 1581 | NAP | C3N-C7N-N7N | -2.20 | 115.27 | 117.77 |
| 2 | K | 1581 | NAP | C4D-O4D-C1D | -2.18 | 107.45 | 109.77 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2 | P | 1581 | NAP | C4D-O4D-C1D | -2.17 | 107.46 | 109.77 |
| 2 | H | 1581 | NAP | C3N-C7N-N7N | -2.12 | 115.35 | 117.77 |
| 2 | M | 1581 | NAP | C3N-C7N-N7N | -2.08 | 115.40 | 117.77 |
| 2 | F | 1581 | NAP | C3N-C7N-N7N | -2.04 | 115.45 | 117.77 |
| 2 | G | 1581 | NAP | C3N-C7N-N7N | -2.03 | 115.45 | 117.77 |
| 2 | H | 1581 | NAP | C4A-C5A-N7A | 4.27 | 113.53 | 109.41 |
| 2 | B | 1581 | NAP | C4A-C5A-N7A | 4.27 | 113.54 | 109.41 |
| 2 | M | 1581 | NAP | C4A-C5A-N7A | 4.28 | 113.54 | 109.41 |
| 2 | C | 1581 | NAP | C4A-C5A-N7A | 4.28 | 113.54 | 109.41 |
| 2 | L | 1581 | NAP | C4A-C5A-N7A | 4.32 | 113.58 | 109.41 |
| 2 | N | 1581 | NAP | C4A-C5A-N7A | 4.34 | 113.61 | 109.41 |
| 2 | F | 1581 | NAP | C4A-C5A-N7A | 4.35 | 113.61 | 109.41 |
| 2 | P | 1581 | NAP | C4A-C5A-N7A | 4.36 | 113.62 | 109.41 |
| 2 | J | 1581 | NAP | C4A-C5A-N7A | 4.38 | 113.64 | 109.41 |
| 2 | I | 1581 | NAP | C4A-C5A-N7A | 4.38 | 113.64 | 109.41 |
| 2 | K | 1581 | NAP | C4A-C5A-N7A | 4.48 | 113.73 | 109.41 |
| 2 | D | 1581 | NAP | C4A-C5A-N7A | 4.50 | 113.76 | 109.41 |
| 2 | G | 1581 | NAP | C4A-C5A-N7A | 4.50 | 113.76 | 109.41 |
| 2 | E | 1581 | NAP | C4A-C5A-N7A | 4.51 | 113.77 | 109.41 |
| 2 | O | 1581 | NAP | C4A-C5A-N7A | 4.58 | 113.84 | 109.41 |
| 2 | A | 1581 | NAP | C4A-C5A-N7A | 4.63 | 113.88 | 109.41 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

29 monomers are involved in 65 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | A | 1581 | NAP | 4 | 0 |
| 3 | A | 1583 | OXL | 1 | 0 |
| 2 | B | 1581 | NAP | 4 | 0 |
| 3 | B | 1582 | OXL | 1 | 0 |
| 2 | C | 1581 | NAP | 2 | 0 |
| 3 | C | 1582 | OXL | 3 | 0 |
| 2 | D | 1581 | NAP | 2 | 0 |
| 3 | D | 1582 | OXL | 2 | 0 |
| 2 | E | 1581 | NAP | 3 | 0 |
| 3 | E | 1582 | OXL | 1 | 0 |
| 2 | F | 1581 | NAP | 2 | 0 |
| 3 | F | 1582 | OXL | 1 | 0 |
| 2 | G | 1581 | NAP | 3 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3 | G | 1582 | OXL | 1 | 0 |
| 2 | H | 1581 | NAP | 3 | 0 |
| 3 | H | 1582 | OXL | 1 | 0 |
| 2 | I | 1581 | NAP | 3 | 0 |
| 2 | J | 1581 | NAP | 4 | 0 |
| 3 | J | 1582 | OXL | 1 | 0 |
| 2 | K | 1581 | NAP | 5 | 0 |
| 3 | K | 1582 | OXL | 1 | 0 |
| 2 | L | 1581 | NAP | 5 | 0 |
| 3 | L | 1582 | OXL | 1 | 0 |
| 2 | M | 1581 | NAP | 3 | 0 |
| 2 | N | 1581 | NAP | 3 | 0 |
| 3 | N | 1582 | OXL | 1 | 0 |
| 2 | O | 1581 | NAP | 2 | 0 |
| 2 | P | 1581 | NAP | 1 | 0 |
| 3 | P | 1582 | OXL | 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.