



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:05 PM BST

PDB ID : 3HQQ
Title : Crystal structure of Leishmania mexicana pyruvate kinase (LmPYK) in complex with Fructose 2,6 biphosphate
Authors : Morgan, H.P.; Walkinshaw, M.D.
Deposited on : 2009-06-08
Resolution : 5.07 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

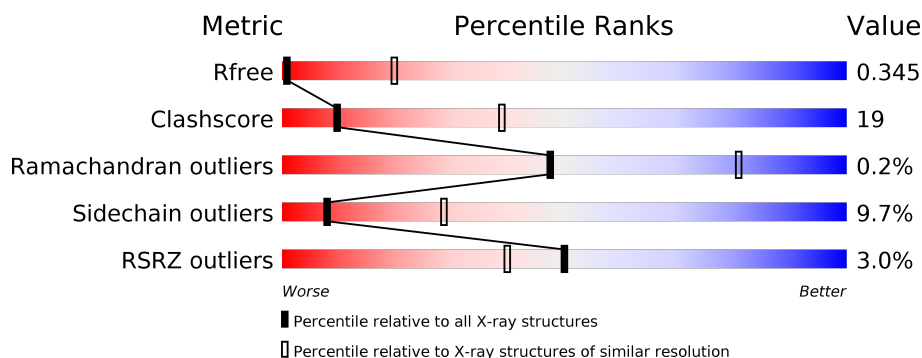
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.07 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1144 (6.34-3.80) |
| Clashscore | 141614 | 1006 (6.34-3.82) |
| Ramachandran outliers | 138981 | 1150 (6.34-3.80) |
| Sidechain outliers | 138945 | 1126 (6.34-3.80) |
| RSRZ outliers | 127900 | 1012 (6.34-3.72) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 499 | <div> <div>6%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div></div> </div> </div> |
| 1 | B | 499 | <div> <div>3%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div></div> </div> </div> |
| 1 | C | 499 | <div> <div>2%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>5%</div> </div> </div> |
| 1 | D | 499 | <div> <div>4%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div></div> </div> </div> |
| 1 | E | 499 | <div> <div>3%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div></div> </div> </div> |
| 1 | F | 499 | <div> <div>3%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div></div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | G | 499 | |
| 1 | H | 499 | |
| 1 | I | 499 | |
| 1 | J | 499 | |
| 1 | K | 499 | |
| 1 | L | 499 | |
| 1 | M | 499 | |
| 1 | N | 499 | |
| 1 | O | 499 | |
| 1 | P | 499 | |
| 1 | Q | 499 | |
| 1 | R | 499 | |
| 1 | S | 499 | |
| 1 | T | 499 | |
| 1 | U | 499 | |
| 1 | V | 499 | |
| 1 | W | 499 | |
| 1 | X | 499 | |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 91656 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 Pyruvate kinase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | B | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | C | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | D | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | E | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | F | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | G | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | H | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | I | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | J | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | K | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | L | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | M | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | N | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | O | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | P | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | Q | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | R | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | S | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | T | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | U | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | V | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | W | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |
| 1 | X | 498 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3799 | 2368 | 670 | 735 | 26 | | | |

There are 96 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| A | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| A | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| A | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| B | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| B | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| B | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| B | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| C | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| C | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| C | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| C | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| D | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| D | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| D | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| D | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| E | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| E | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| E | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| E | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| F | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| F | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| F | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |

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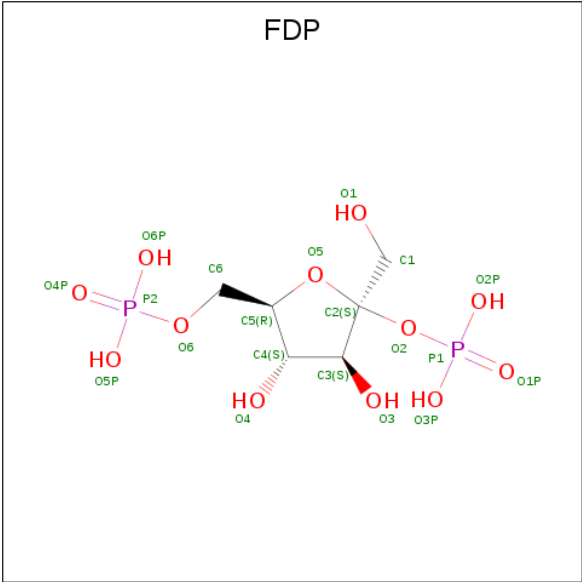
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| F | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| G | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| G | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| G | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| G | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| H | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| H | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| H | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| H | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| I | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| I | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| I | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| I | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| J | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| J | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| J | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| J | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| K | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| K | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| K | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| K | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| L | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| L | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| L | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| L | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| M | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| M | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| M | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| M | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| N | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| N | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| N | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| N | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| O | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| O | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| O | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| O | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| P | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| P | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| P | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| P | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| Q | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| Q | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| Q | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| Q | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| R | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| R | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| R | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| R | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| S | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| S | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| S | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| S | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| T | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| T | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| T | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| T | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| U | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| U | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| U | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| U | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| V | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| V | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| V | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| V | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| W | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| W | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| W | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| W | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| X | 382 | SER | GLY | SEE REMARK 999 | UNP Q27686 |
| X | 389 | TYR | SER | SEE REMARK 999 | UNP Q27686 |
| X | 404 | ARG | ALA | SEE REMARK 999 | UNP Q27686 |
| X | 405 | SER | GLY | SEE REMARK 999 | UNP Q27686 |

- Molecule 2 is 2,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FDP) (formula: $C_6H_{14}O_{12}P_2$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 2 | A | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | B | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | C | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | E | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | F | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | G | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | H | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | I | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | J | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | K | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | L | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | M | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | N | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |

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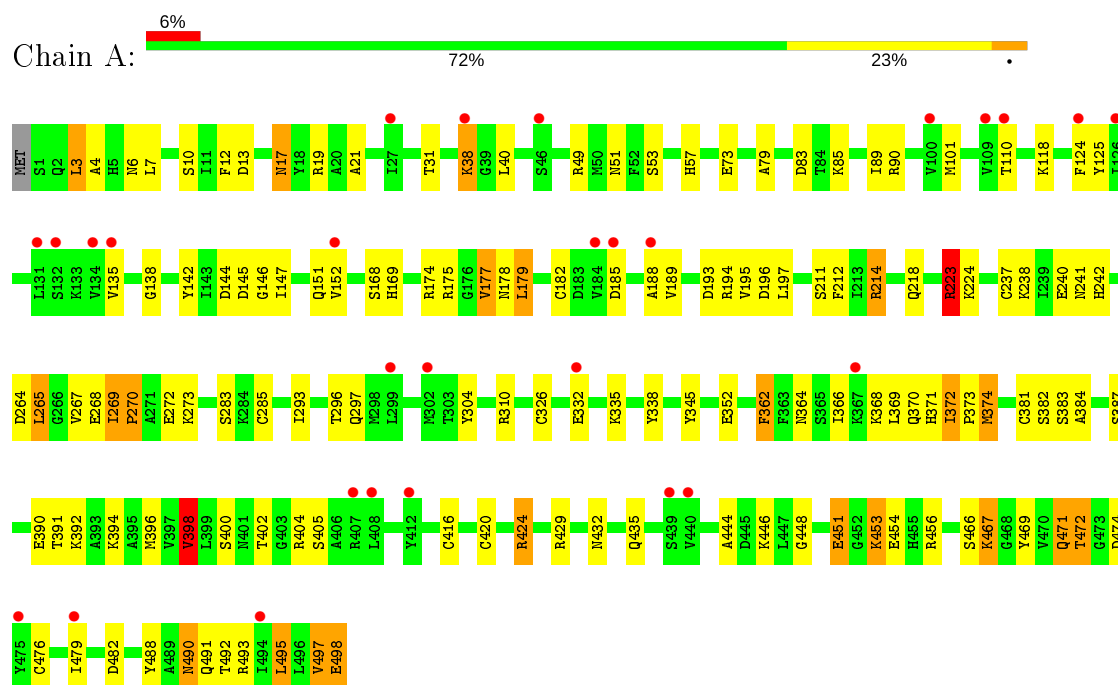
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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---------|---------|
| 2 | O | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | P | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | Q | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | R | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | S | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | T | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | U | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | V | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | W | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |
| 2 | X | 1 | Total | C | O | P | 0 | 0 |
| | | | 20 | 6 | 12 | 2 | | |

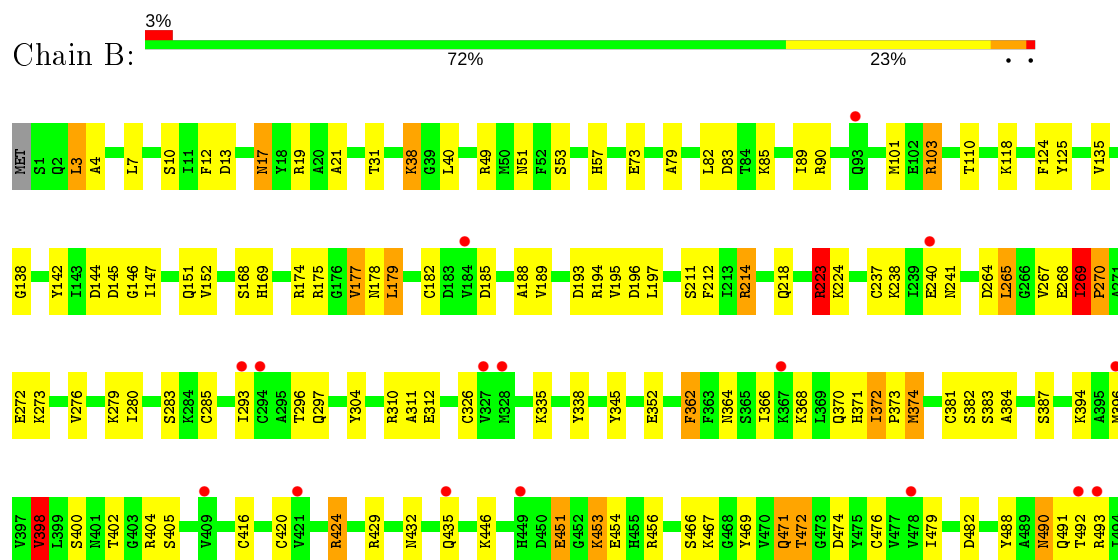
3 Residue-property plots [i](#)

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

• Molecule 1: Pyruvate kinase

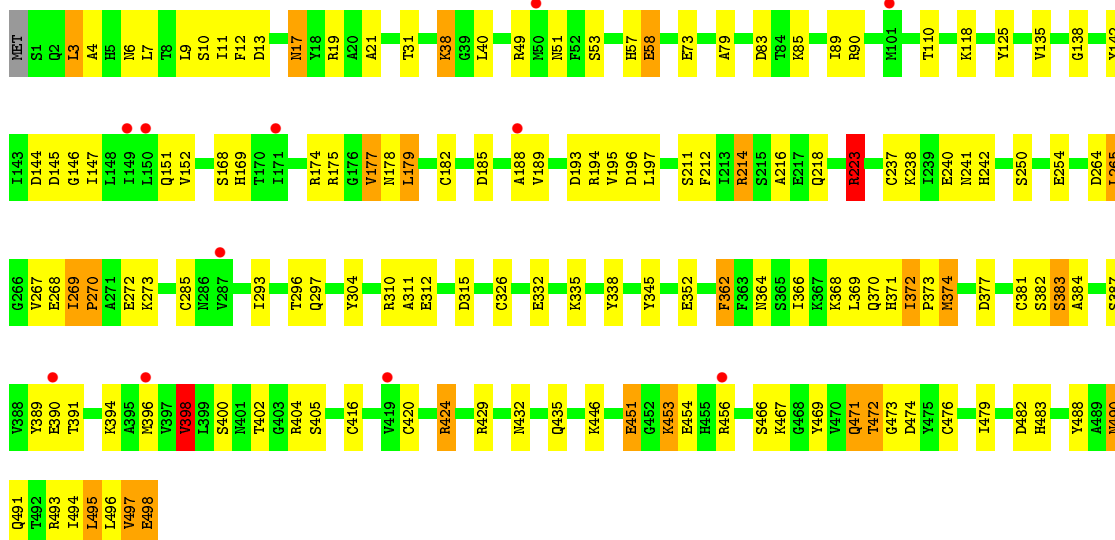


• Molecule 1: Pyruvate kinase

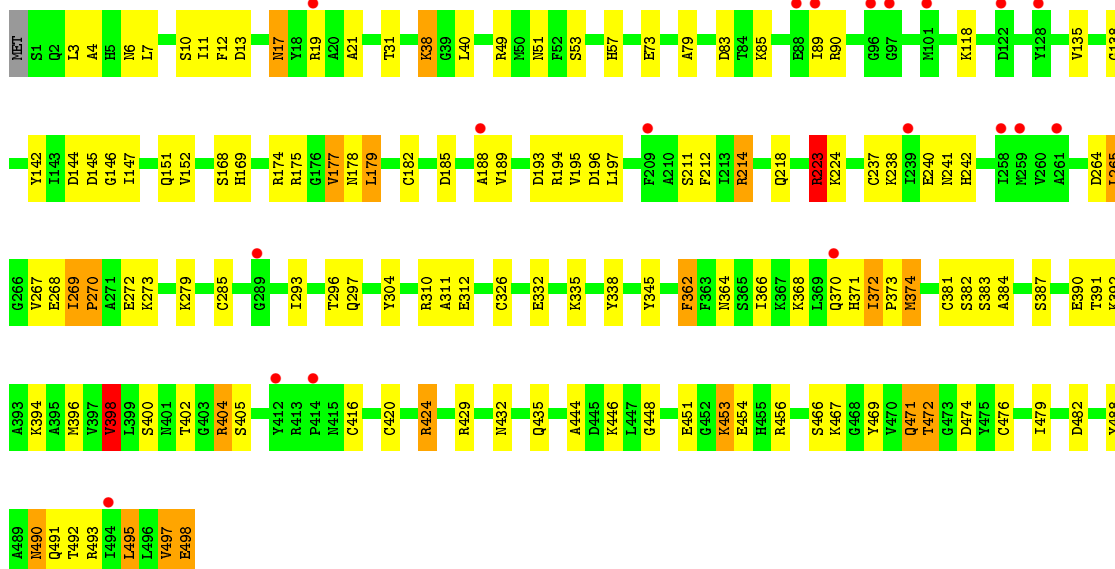


L495
L496
V497
E498

• Molecule 1: Pyruvate kinase

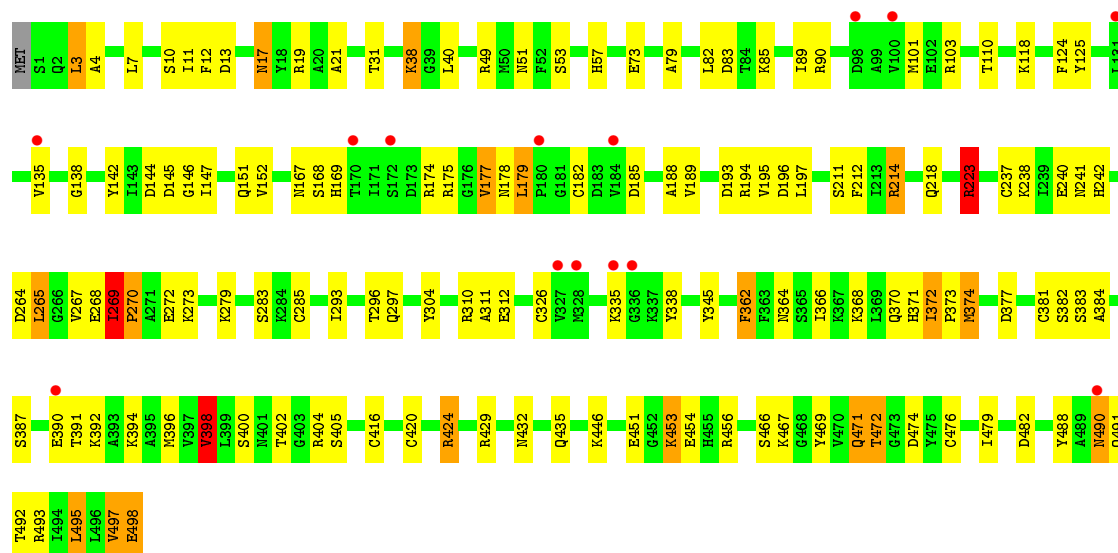


• Molecule 1: Pyruvate kinase

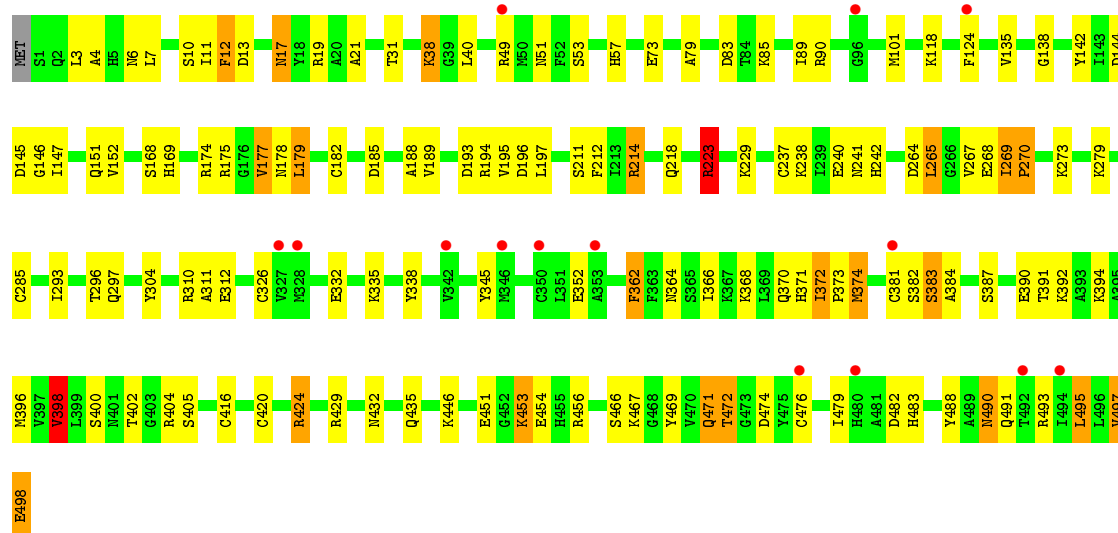


• Molecule 1: Pyruvate kinase

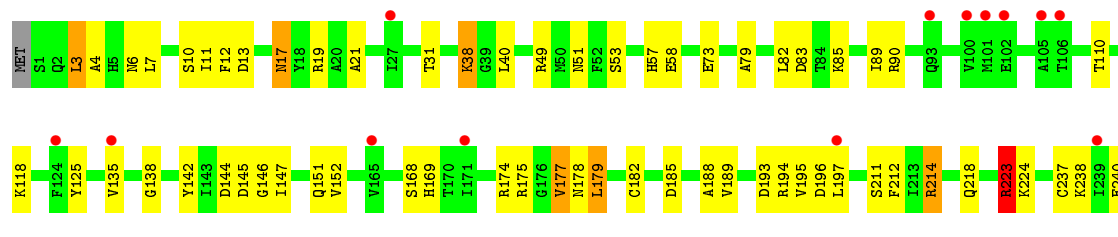
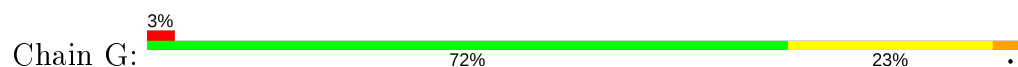


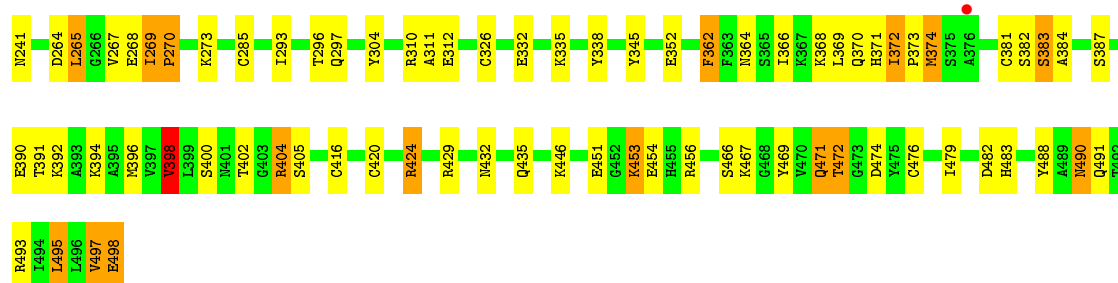


• Molecule 1: Pyruvate kinase

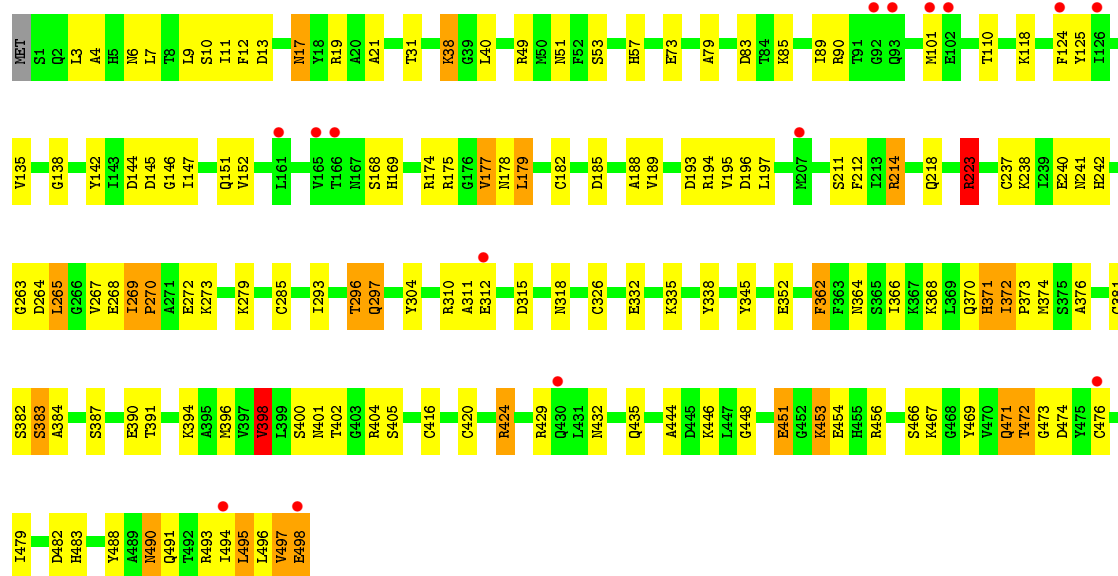


• Molecule 1: Pyruvate kinase

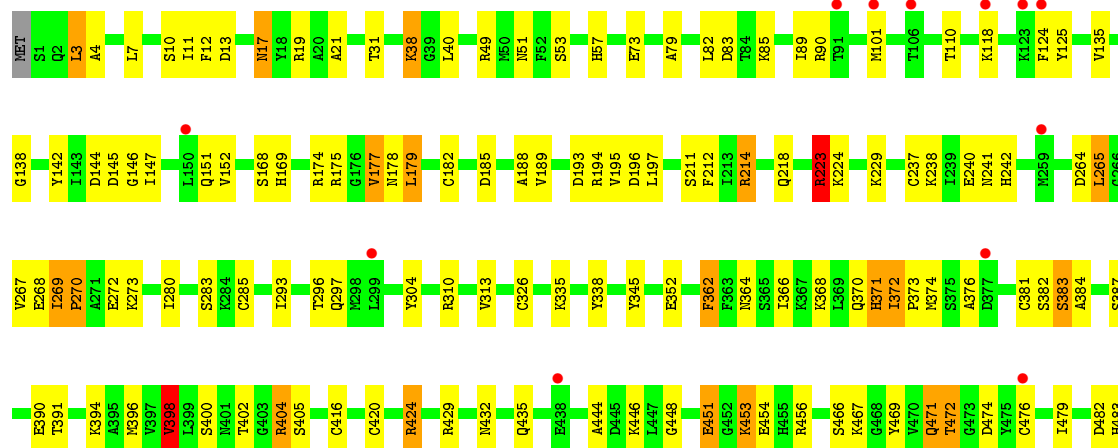




• Molecule 1: Pyruvate kinase

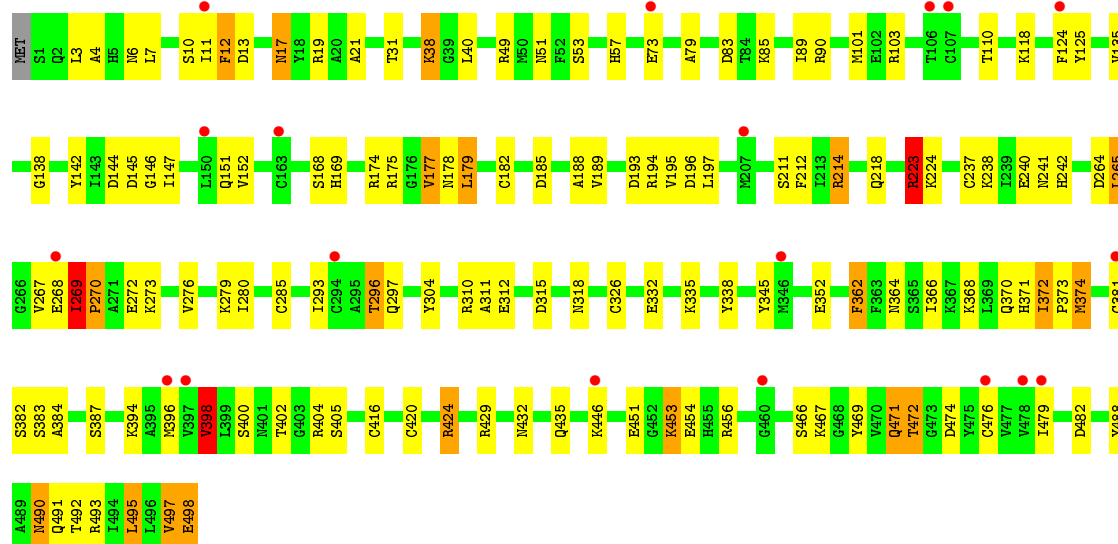


• Molecule 1: Pyruvate kinase

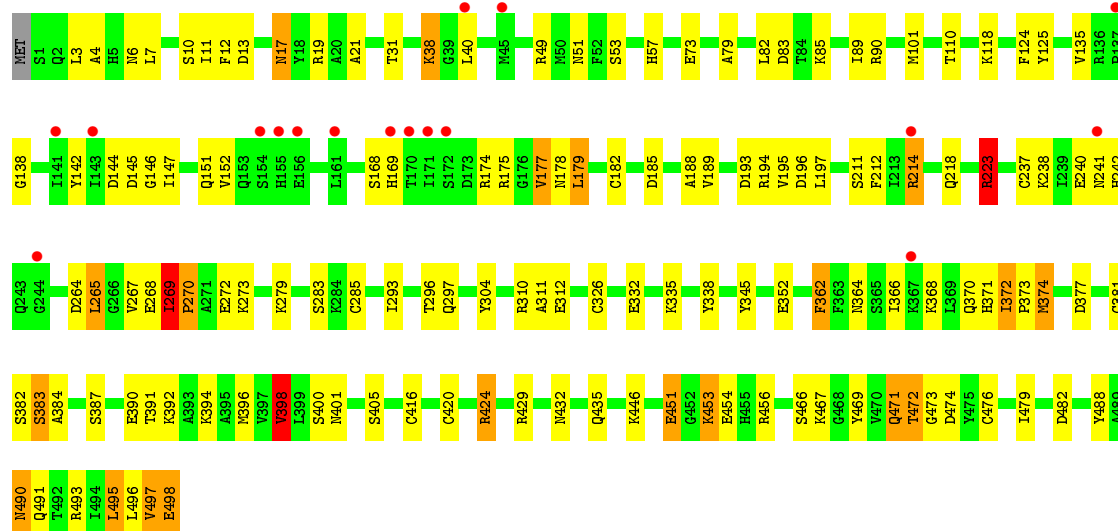




• Molecule 1: Pyruvate kinase

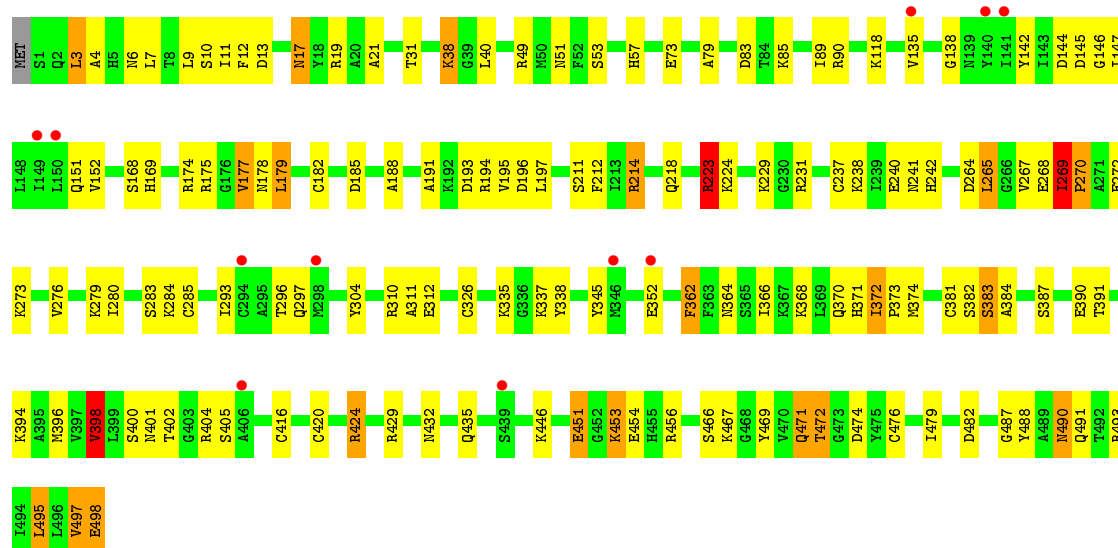


• Molecule 1: Pyruvate kinase

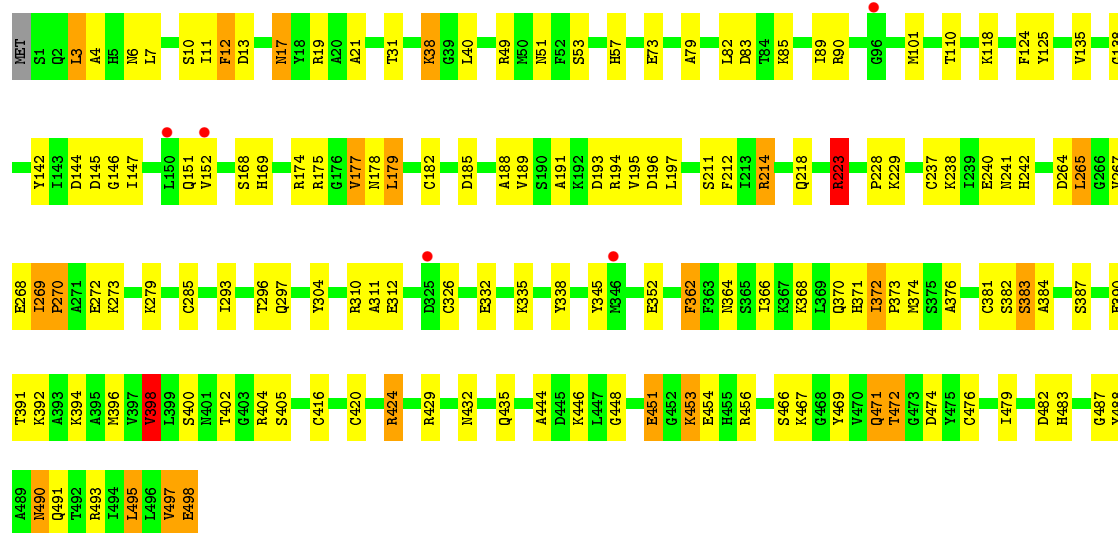


• Molecule 1: Pyruvate kinase

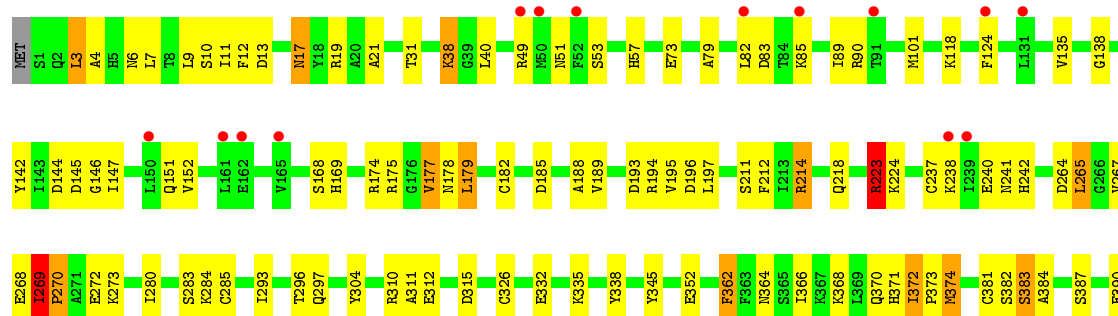


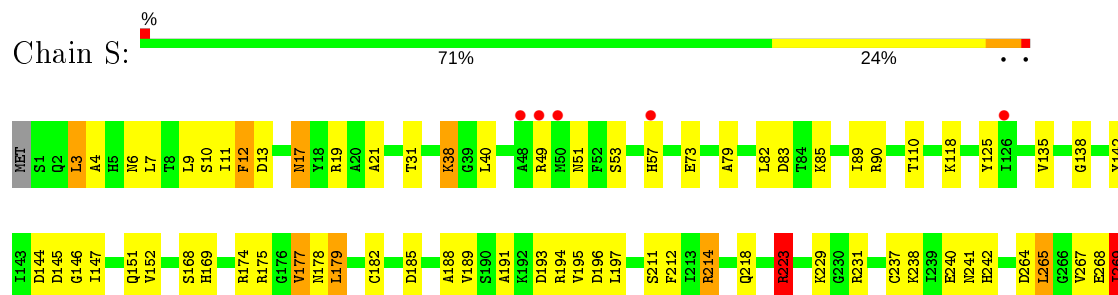
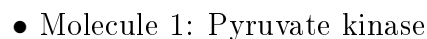
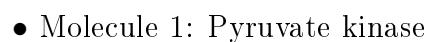


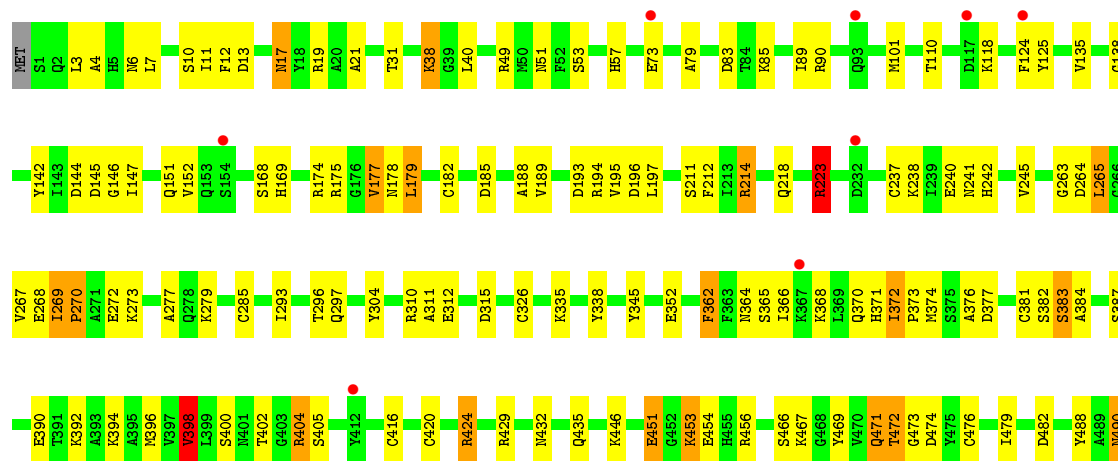
• Molecule 1: Pyruvate kinase

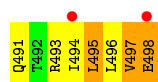


• Molecule 1: Pyruvate kinase

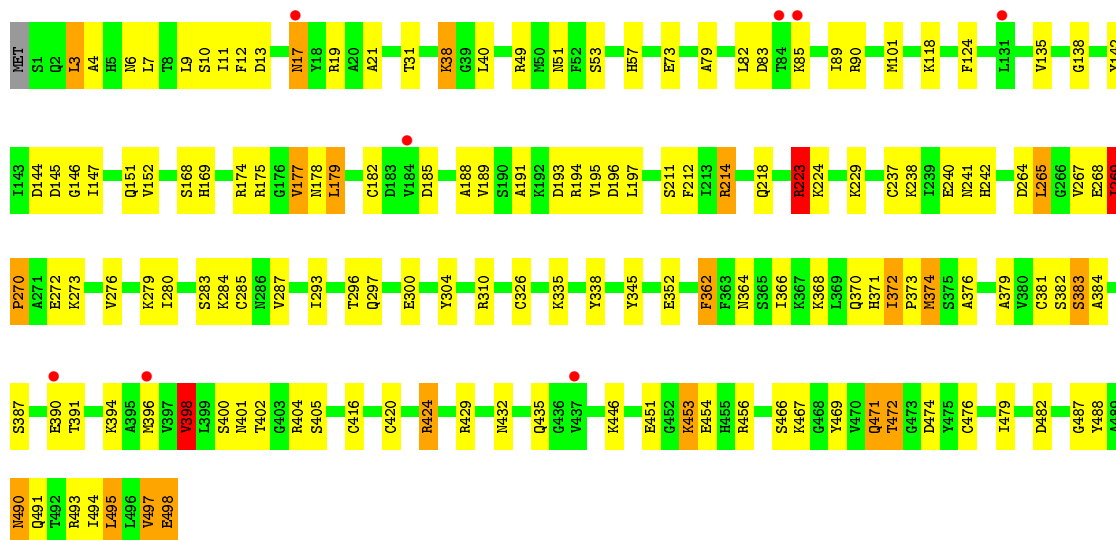




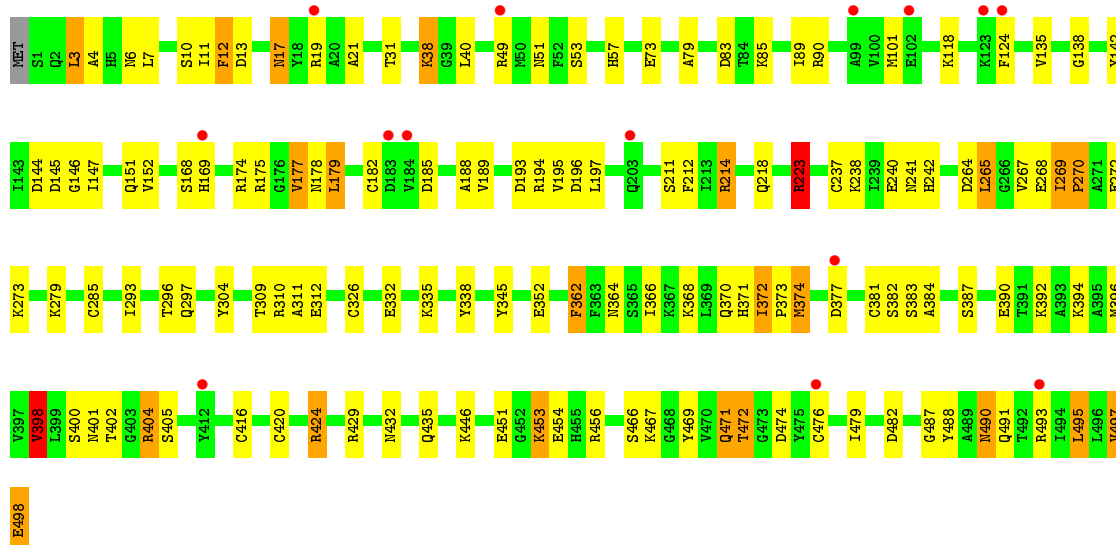
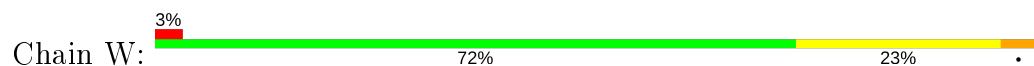




• Molecule 1: Pyruvate kinase

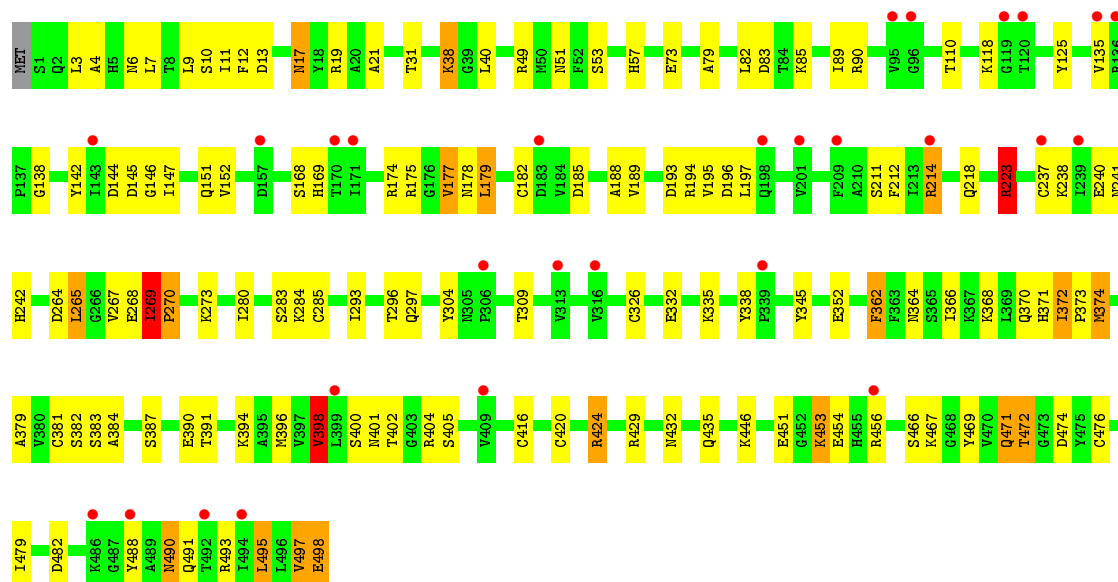


• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | C 2 2 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 243.84Å 254.69Å 892.49Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 39.81 – 5.07 39.81 – 5.07 | Depositor EDS |
| % Data completeness (in resolution range) | 100.0 (39.81-5.07) 86.3 (39.81-5.07) | Depositor EDS |
| R_{merge} | 0.19 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.42 (at 5.09Å) | Xtriage |
| Refinement program | REFMAC 5.5.0066 | Depositor |
| R, R_{free} | 0.353 , 0.357 0.343 , 0.345 | Depositor DCC |
| R_{free} test set | 5652 reflections (5.01%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 131.8 | Xtriage |
| Anisotropy | 0.034 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.31 , 28.7 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$ | Xtriage |
| Estimated twinning fraction | 0.118 for -k,-h,-l | Xtriage |
| F_o, F_c correlation | 0.76 | EDS |
| Total number of atoms | 91656 | wwPDB-VP |
| Average B, all atoms (Å ²) | 24.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 | 1.44 | 12/3856 (0.3%) | 0.85 | 7/5220 (0.1%) |
| 1 | B | 1.44 | 10/3856 (0.3%) | 0.85 | 8/5220 (0.2%) |
| 1 | C | 1.44 | 11/3856 (0.3%) | 0.85 | 7/5220 (0.1%) |
| 1 | D | 1.44 | 12/3856 (0.3%) | 0.85 | 7/5220 (0.1%) |
| 1 | E | 1.44 | 10/3856 (0.3%) | 0.85 | 8/5220 (0.2%) |
| 1 | F | 1.44 | 11/3856 (0.3%) | 0.85 | 7/5220 (0.1%) |
| 1 | G | 1.44 | 13/3856 (0.3%) | 0.85 | 8/5220 (0.2%) |
| 1 | H | 1.44 | 12/3856 (0.3%) | 0.85 | 7/5220 (0.1%) |
| 1 | I | 1.44 | 10/3856 (0.3%) | 0.85 | 8/5220 (0.2%) |
| 1 | J | 1.44 | 11/3856 (0.3%) | 0.85 | 7/5220 (0.1%) |
| 1 | K | 1.44 | 11/3856 (0.3%) | 0.85 | 8/5220 (0.2%) |
| 1 | L | 1.44 | 10/3856 (0.3%) | 0.85 | 7/5220 (0.1%) |
| 1 | M | 1.44 | 11/3856 (0.3%) | 0.85 | 8/5220 (0.2%) |
| 1 | N | 1.44 | 11/3856 (0.3%) | 0.85 | 8/5220 (0.2%) |
| 1 | O | 1.44 | 11/3856 (0.3%) | 0.85 | 8/5220 (0.2%) |
| 1 | P | 1.44 | 11/3856 (0.3%) | 0.85 | 8/5220 (0.2%) |
| 1 | Q | 1.44 | 11/3856 (0.3%) | 0.85 | 8/5220 (0.2%) |
| 1 | R | 1.44 | 10/3856 (0.3%) | 0.85 | 7/5220 (0.1%) |
| 1 | S | 1.44 | 11/3856 (0.3%) | 0.85 | 8/5220 (0.2%) |
| 1 | T | 1.44 | 11/3856 (0.3%) | 0.85 | 7/5220 (0.1%) |
| 1 | U | 1.44 | 10/3856 (0.3%) | 0.85 | 7/5220 (0.1%) |
| 1 | V | 1.44 | 11/3856 (0.3%) | 0.85 | 8/5220 (0.2%) |
| 1 | W | 1.44 | 12/3856 (0.3%) | 0.85 | 7/5220 (0.1%) |
| 1 | X | 1.44 | 13/3856 (0.3%) | 0.85 | 8/5220 (0.2%) |
| All | All | 1.44 | 266/92544 (0.3%) | 0.85 | 181/125280 (0.1%) |

All (266) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | L | 476 | CYS | CB-SG | -7.67 | 1.69 | 1.82 |
| 1 | R | 476 | CYS | CB-SG | -7.64 | 1.69 | 1.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | J | 476 | CYS | CB-SG | -7.64 | 1.69 | 1.82 |
| 1 | D | 476 | CYS | CB-SG | -7.63 | 1.69 | 1.82 |
| 1 | E | 476 | CYS | CB-SG | -7.62 | 1.69 | 1.82 |
| 1 | Q | 476 | CYS | CB-SG | -7.61 | 1.69 | 1.82 |
| 1 | W | 476 | CYS | CB-SG | -7.61 | 1.69 | 1.82 |
| 1 | H | 476 | CYS | CB-SG | -7.60 | 1.69 | 1.82 |
| 1 | V | 476 | CYS | CB-SG | -7.60 | 1.69 | 1.82 |
| 1 | I | 476 | CYS | CB-SG | -7.60 | 1.69 | 1.82 |
| 1 | U | 476 | CYS | CB-SG | -7.60 | 1.69 | 1.82 |
| 1 | G | 476 | CYS | CB-SG | -7.59 | 1.69 | 1.82 |
| 1 | O | 476 | CYS | CB-SG | -7.59 | 1.69 | 1.82 |
| 1 | N | 476 | CYS | CB-SG | -7.59 | 1.69 | 1.82 |
| 1 | T | 476 | CYS | CB-SG | -7.58 | 1.69 | 1.82 |
| 1 | P | 476 | CYS | CB-SG | -7.58 | 1.69 | 1.82 |
| 1 | M | 476 | CYS | CB-SG | -7.57 | 1.69 | 1.82 |
| 1 | S | 476 | CYS | CB-SG | -7.57 | 1.69 | 1.82 |
| 1 | K | 476 | CYS | CB-SG | -7.56 | 1.69 | 1.82 |
| 1 | F | 476 | CYS | CB-SG | -7.55 | 1.69 | 1.82 |
| 1 | X | 476 | CYS | CB-SG | -7.54 | 1.69 | 1.82 |
| 1 | A | 476 | CYS | CB-SG | -7.53 | 1.69 | 1.82 |
| 1 | C | 476 | CYS | CB-SG | -7.52 | 1.69 | 1.82 |
| 1 | B | 476 | CYS | CB-SG | -7.51 | 1.69 | 1.82 |
| 1 | S | 416 | CYS | CB-SG | -7.26 | 1.70 | 1.82 |
| 1 | Q | 416 | CYS | CB-SG | -7.25 | 1.70 | 1.82 |
| 1 | W | 416 | CYS | CB-SG | -7.23 | 1.70 | 1.82 |
| 1 | G | 416 | CYS | CB-SG | -7.23 | 1.70 | 1.82 |
| 1 | H | 416 | CYS | CB-SG | -7.23 | 1.70 | 1.82 |
| 1 | N | 416 | CYS | CB-SG | -7.22 | 1.70 | 1.82 |
| 1 | D | 416 | CYS | CB-SG | -7.21 | 1.70 | 1.82 |
| 1 | R | 416 | CYS | CB-SG | -7.21 | 1.70 | 1.82 |
| 1 | O | 416 | CYS | CB-SG | -7.20 | 1.70 | 1.82 |
| 1 | U | 416 | CYS | CB-SG | -7.20 | 1.70 | 1.82 |
| 1 | L | 416 | CYS | CB-SG | -7.20 | 1.70 | 1.82 |
| 1 | B | 416 | CYS | CB-SG | -7.18 | 1.70 | 1.82 |
| 1 | V | 416 | CYS | CB-SG | -7.18 | 1.70 | 1.82 |
| 1 | C | 416 | CYS | CB-SG | -7.18 | 1.70 | 1.82 |
| 1 | T | 416 | CYS | CB-SG | -7.17 | 1.70 | 1.82 |
| 1 | X | 416 | CYS | CB-SG | -7.17 | 1.70 | 1.82 |
| 1 | I | 416 | CYS | CB-SG | -7.16 | 1.70 | 1.82 |
| 1 | P | 416 | CYS | CB-SG | -7.16 | 1.70 | 1.82 |
| 1 | E | 416 | CYS | CB-SG | -7.16 | 1.70 | 1.82 |
| 1 | F | 416 | CYS | CB-SG | -7.15 | 1.70 | 1.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 416 | CYS | CB-SG | -7.14 | 1.70 | 1.82 |
| 1 | J | 416 | CYS | CB-SG | -7.14 | 1.70 | 1.82 |
| 1 | M | 416 | CYS | CB-SG | -7.13 | 1.70 | 1.82 |
| 1 | K | 416 | CYS | CB-SG | -7.12 | 1.70 | 1.82 |
| 1 | H | 469 | TYR | CD2-CE2 | -5.82 | 1.30 | 1.39 |
| 1 | K | 469 | TYR | CD2-CE2 | -5.82 | 1.30 | 1.39 |
| 1 | F | 469 | TYR | CD2-CE2 | -5.79 | 1.30 | 1.39 |
| 1 | P | 469 | TYR | CD2-CE2 | -5.78 | 1.30 | 1.39 |
| 1 | N | 469 | TYR | CD2-CE2 | -5.78 | 1.30 | 1.39 |
| 1 | U | 469 | TYR | CD2-CE2 | -5.78 | 1.30 | 1.39 |
| 1 | O | 469 | TYR | CD2-CE2 | -5.77 | 1.30 | 1.39 |
| 1 | X | 469 | TYR | CD2-CE2 | -5.77 | 1.30 | 1.39 |
| 1 | V | 469 | TYR | CD2-CE2 | -5.77 | 1.30 | 1.39 |
| 1 | M | 469 | TYR | CD2-CE2 | -5.76 | 1.30 | 1.39 |
| 1 | L | 469 | TYR | CD2-CE2 | -5.76 | 1.30 | 1.39 |
| 1 | R | 469 | TYR | CD2-CE2 | -5.75 | 1.30 | 1.39 |
| 1 | S | 469 | TYR | CD2-CE2 | -5.75 | 1.30 | 1.39 |
| 1 | J | 469 | TYR | CD2-CE2 | -5.74 | 1.30 | 1.39 |
| 1 | D | 469 | TYR | CD2-CE2 | -5.74 | 1.30 | 1.39 |
| 1 | A | 469 | TYR | CD2-CE2 | -5.73 | 1.30 | 1.39 |
| 1 | T | 469 | TYR | CD2-CE2 | -5.73 | 1.30 | 1.39 |
| 1 | W | 469 | TYR | CD2-CE2 | -5.72 | 1.30 | 1.39 |
| 1 | C | 469 | TYR | CD2-CE2 | -5.71 | 1.30 | 1.39 |
| 1 | E | 469 | TYR | CD2-CE2 | -5.70 | 1.30 | 1.39 |
| 1 | I | 469 | TYR | CD2-CE2 | -5.69 | 1.30 | 1.39 |
| 1 | B | 469 | TYR | CD2-CE2 | -5.69 | 1.30 | 1.39 |
| 1 | G | 469 | TYR | CD2-CE2 | -5.69 | 1.30 | 1.39 |
| 1 | Q | 469 | TYR | CD2-CE2 | -5.69 | 1.30 | 1.39 |
| 1 | Q | 420 | CYS | CB-SG | -5.65 | 1.72 | 1.81 |
| 1 | J | 420 | CYS | CB-SG | -5.64 | 1.72 | 1.81 |
| 1 | S | 420 | CYS | CB-SG | -5.64 | 1.72 | 1.81 |
| 1 | E | 420 | CYS | CB-SG | -5.62 | 1.72 | 1.81 |
| 1 | N | 420 | CYS | CB-SG | -5.62 | 1.72 | 1.81 |
| 1 | H | 420 | CYS | CB-SG | -5.61 | 1.72 | 1.81 |
| 1 | C | 420 | CYS | CB-SG | -5.60 | 1.72 | 1.81 |
| 1 | L | 420 | CYS | CB-SG | -5.60 | 1.72 | 1.81 |
| 1 | U | 420 | CYS | CB-SG | -5.60 | 1.72 | 1.81 |
| 1 | X | 420 | CYS | CB-SG | -5.60 | 1.72 | 1.81 |
| 1 | F | 420 | CYS | CB-SG | -5.59 | 1.72 | 1.81 |
| 1 | B | 381 | CYS | CB-SG | -5.59 | 1.72 | 1.81 |
| 1 | V | 420 | CYS | CB-SG | -5.59 | 1.72 | 1.81 |
| 1 | G | 420 | CYS | CB-SG | -5.59 | 1.72 | 1.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | A | 420 | CYS | CB-SG | -5.57 | 1.72 | 1.81 |
| 1 | D | 420 | CYS | CB-SG | -5.57 | 1.72 | 1.81 |
| 1 | I | 420 | CYS | CB-SG | -5.57 | 1.72 | 1.81 |
| 1 | K | 420 | CYS | CB-SG | -5.57 | 1.72 | 1.81 |
| 1 | M | 420 | CYS | CB-SG | -5.57 | 1.72 | 1.81 |
| 1 | I | 381 | CYS | CB-SG | -5.56 | 1.72 | 1.81 |
| 1 | N | 381 | CYS | CB-SG | -5.56 | 1.72 | 1.81 |
| 1 | D | 381 | CYS | CB-SG | -5.56 | 1.72 | 1.81 |
| 1 | W | 420 | CYS | CB-SG | -5.55 | 1.72 | 1.81 |
| 1 | M | 381 | CYS | CB-SG | -5.55 | 1.72 | 1.81 |
| 1 | R | 381 | CYS | CB-SG | -5.55 | 1.72 | 1.81 |
| 1 | R | 420 | CYS | CB-SG | -5.55 | 1.72 | 1.81 |
| 1 | P | 420 | CYS | CB-SG | -5.54 | 1.72 | 1.81 |
| 1 | C | 381 | CYS | CB-SG | -5.53 | 1.72 | 1.81 |
| 1 | T | 420 | CYS | CB-SG | -5.53 | 1.72 | 1.81 |
| 1 | F | 381 | CYS | CB-SG | -5.52 | 1.72 | 1.81 |
| 1 | O | 420 | CYS | CB-SG | -5.52 | 1.72 | 1.81 |
| 1 | X | 381 | CYS | CB-SG | -5.52 | 1.72 | 1.81 |
| 1 | V | 381 | CYS | CB-SG | -5.52 | 1.72 | 1.81 |
| 1 | B | 420 | CYS | CB-SG | -5.52 | 1.72 | 1.81 |
| 1 | W | 381 | CYS | CB-SG | -5.52 | 1.72 | 1.81 |
| 1 | K | 381 | CYS | CB-SG | -5.51 | 1.72 | 1.81 |
| 1 | Q | 381 | CYS | CB-SG | -5.51 | 1.72 | 1.81 |
| 1 | S | 381 | CYS | CB-SG | -5.51 | 1.72 | 1.81 |
| 1 | O | 381 | CYS | CB-SG | -5.50 | 1.72 | 1.81 |
| 1 | L | 381 | CYS | CB-SG | -5.49 | 1.72 | 1.81 |
| 1 | E | 381 | CYS | CB-SG | -5.49 | 1.72 | 1.81 |
| 1 | H | 381 | CYS | CB-SG | -5.48 | 1.72 | 1.81 |
| 1 | J | 381 | CYS | CB-SG | -5.48 | 1.72 | 1.81 |
| 1 | U | 381 | CYS | CB-SG | -5.48 | 1.72 | 1.81 |
| 1 | A | 381 | CYS | CB-SG | -5.48 | 1.72 | 1.81 |
| 1 | P | 381 | CYS | CB-SG | -5.46 | 1.73 | 1.81 |
| 1 | T | 381 | CYS | CB-SG | -5.46 | 1.73 | 1.81 |
| 1 | C | 237 | CYS | CB-SG | -5.46 | 1.73 | 1.81 |
| 1 | G | 381 | CYS | CB-SG | -5.43 | 1.73 | 1.81 |
| 1 | B | 237 | CYS | CB-SG | -5.43 | 1.73 | 1.81 |
| 1 | F | 237 | CYS | CB-SG | -5.42 | 1.73 | 1.81 |
| 1 | H | 237 | CYS | CB-SG | -5.42 | 1.73 | 1.81 |
| 1 | Q | 237 | CYS | CB-SG | -5.41 | 1.73 | 1.81 |
| 1 | I | 237 | CYS | CB-SG | -5.40 | 1.73 | 1.81 |
| 1 | U | 237 | CYS | CB-SG | -5.40 | 1.73 | 1.81 |
| 1 | N | 237 | CYS | CB-SG | -5.40 | 1.73 | 1.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | W | 237 | CYS | CB-SG | -5.39 | 1.73 | 1.81 |
| 1 | J | 237 | CYS | CB-SG | -5.38 | 1.73 | 1.81 |
| 1 | K | 237 | CYS | CB-SG | -5.38 | 1.73 | 1.81 |
| 1 | O | 469 | TYR | CD1-CE1 | -5.37 | 1.31 | 1.39 |
| 1 | P | 237 | CYS | CB-SG | -5.37 | 1.73 | 1.81 |
| 1 | G | 237 | CYS | CB-SG | -5.36 | 1.73 | 1.81 |
| 1 | L | 237 | CYS | CB-SG | -5.35 | 1.73 | 1.81 |
| 1 | D | 237 | CYS | CB-SG | -5.34 | 1.73 | 1.81 |
| 1 | S | 237 | CYS | CB-SG | -5.34 | 1.73 | 1.81 |
| 1 | I | 469 | TYR | CD1-CE1 | -5.34 | 1.31 | 1.39 |
| 1 | B | 469 | TYR | CD1-CE1 | -5.34 | 1.31 | 1.39 |
| 1 | X | 237 | CYS | CB-SG | -5.34 | 1.73 | 1.81 |
| 1 | A | 237 | CYS | CB-SG | -5.33 | 1.73 | 1.81 |
| 1 | M | 469 | TYR | CD1-CE1 | -5.33 | 1.31 | 1.39 |
| 1 | G | 469 | TYR | CD1-CE1 | -5.33 | 1.31 | 1.39 |
| 1 | W | 469 | TYR | CD1-CE1 | -5.33 | 1.31 | 1.39 |
| 1 | M | 237 | CYS | CB-SG | -5.32 | 1.73 | 1.81 |
| 1 | T | 237 | CYS | CB-SG | -5.32 | 1.73 | 1.81 |
| 1 | L | 469 | TYR | CD1-CE1 | -5.32 | 1.31 | 1.39 |
| 1 | R | 237 | CYS | CB-SG | -5.32 | 1.73 | 1.81 |
| 1 | E | 237 | CYS | CB-SG | -5.32 | 1.73 | 1.81 |
| 1 | V | 237 | CYS | CB-SG | -5.31 | 1.73 | 1.81 |
| 1 | O | 237 | CYS | CB-SG | -5.31 | 1.73 | 1.81 |
| 1 | N | 469 | TYR | CD1-CE1 | -5.31 | 1.31 | 1.39 |
| 1 | S | 469 | TYR | CD1-CE1 | -5.30 | 1.31 | 1.39 |
| 1 | F | 469 | TYR | CD1-CE1 | -5.30 | 1.31 | 1.39 |
| 1 | V | 469 | TYR | CD1-CE1 | -5.30 | 1.31 | 1.39 |
| 1 | J | 469 | TYR | CD1-CE1 | -5.29 | 1.31 | 1.39 |
| 1 | Q | 469 | TYR | CD1-CE1 | -5.29 | 1.31 | 1.39 |
| 1 | P | 469 | TYR | CD1-CE1 | -5.29 | 1.31 | 1.39 |
| 1 | X | 469 | TYR | CD1-CE1 | -5.29 | 1.31 | 1.39 |
| 1 | E | 469 | TYR | CD1-CE1 | -5.29 | 1.31 | 1.39 |
| 1 | K | 469 | TYR | CD1-CE1 | -5.29 | 1.31 | 1.39 |
| 1 | U | 469 | TYR | CD1-CE1 | -5.28 | 1.31 | 1.39 |
| 1 | D | 469 | TYR | CD1-CE1 | -5.28 | 1.31 | 1.39 |
| 1 | R | 469 | TYR | CD1-CE1 | -5.27 | 1.31 | 1.39 |
| 1 | H | 469 | TYR | CD1-CE1 | -5.27 | 1.31 | 1.39 |
| 1 | T | 469 | TYR | CD1-CE1 | -5.27 | 1.31 | 1.39 |
| 1 | C | 469 | TYR | CD1-CE1 | -5.26 | 1.31 | 1.39 |
| 1 | V | 285 | CYS | CB-SG | -5.25 | 1.73 | 1.81 |
| 1 | G | 285 | CYS | CB-SG | -5.25 | 1.73 | 1.81 |
| 1 | H | 338 | TYR | CD2-CE2 | -5.24 | 1.31 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | A | 469 | TYR | CD1-CE1 | -5.24 | 1.31 | 1.39 |
| 1 | D | 338 | TYR | CD2-CE2 | -5.24 | 1.31 | 1.39 |
| 1 | J | 285 | CYS | CB-SG | -5.23 | 1.73 | 1.81 |
| 1 | O | 285 | CYS | CB-SG | -5.23 | 1.73 | 1.81 |
| 1 | B | 338 | TYR | CD2-CE2 | -5.22 | 1.31 | 1.39 |
| 1 | B | 488 | TYR | CD2-CE2 | -5.22 | 1.31 | 1.39 |
| 1 | F | 338 | TYR | CD2-CE2 | -5.22 | 1.31 | 1.39 |
| 1 | N | 488 | TYR | CD2-CE2 | -5.22 | 1.31 | 1.39 |
| 1 | A | 488 | TYR | CD2-CE2 | -5.22 | 1.31 | 1.39 |
| 1 | F | 285 | CYS | CB-SG | -5.22 | 1.73 | 1.81 |
| 1 | O | 488 | TYR | CD2-CE2 | -5.22 | 1.31 | 1.39 |
| 1 | N | 285 | CYS | CB-SG | -5.22 | 1.73 | 1.81 |
| 1 | R | 285 | CYS | CB-SG | -5.22 | 1.73 | 1.81 |
| 1 | W | 338 | TYR | CD2-CE2 | -5.21 | 1.31 | 1.39 |
| 1 | X | 285 | CYS | CB-SG | -5.21 | 1.73 | 1.81 |
| 1 | B | 285 | CYS | CB-SG | -5.20 | 1.73 | 1.81 |
| 1 | C | 285 | CYS | CB-SG | -5.20 | 1.73 | 1.81 |
| 1 | C | 488 | TYR | CD2-CE2 | -5.20 | 1.31 | 1.39 |
| 1 | F | 488 | TYR | CD2-CE2 | -5.20 | 1.31 | 1.39 |
| 1 | P | 285 | CYS | CB-SG | -5.20 | 1.73 | 1.81 |
| 1 | E | 338 | TYR | CD2-CE2 | -5.20 | 1.31 | 1.39 |
| 1 | I | 285 | CYS | CB-SG | -5.20 | 1.73 | 1.81 |
| 1 | T | 285 | CYS | CB-SG | -5.20 | 1.73 | 1.81 |
| 1 | G | 488 | TYR | CD2-CE2 | -5.19 | 1.31 | 1.39 |
| 1 | S | 338 | TYR | CD2-CE2 | -5.19 | 1.31 | 1.39 |
| 1 | D | 488 | TYR | CD2-CE2 | -5.19 | 1.31 | 1.39 |
| 1 | U | 338 | TYR | CD2-CE2 | -5.19 | 1.31 | 1.39 |
| 1 | H | 285 | CYS | CB-SG | -5.18 | 1.73 | 1.81 |
| 1 | Q | 488 | TYR | CD2-CE2 | -5.18 | 1.31 | 1.39 |
| 1 | K | 338 | TYR | CD2-CE2 | -5.18 | 1.31 | 1.39 |
| 1 | V | 488 | TYR | CD2-CE2 | -5.18 | 1.31 | 1.39 |
| 1 | W | 488 | TYR | CD2-CE2 | -5.18 | 1.31 | 1.39 |
| 1 | D | 285 | CYS | CB-SG | -5.18 | 1.73 | 1.81 |
| 1 | U | 285 | CYS | CB-SG | -5.17 | 1.73 | 1.81 |
| 1 | A | 338 | TYR | CD2-CE2 | -5.17 | 1.31 | 1.39 |
| 1 | I | 338 | TYR | CD2-CE2 | -5.17 | 1.31 | 1.39 |
| 1 | G | 338 | TYR | CD2-CE2 | -5.17 | 1.31 | 1.39 |
| 1 | J | 488 | TYR | CD2-CE2 | -5.17 | 1.31 | 1.39 |
| 1 | Q | 285 | CYS | CB-SG | -5.17 | 1.73 | 1.81 |
| 1 | C | 338 | TYR | CD2-CE2 | -5.17 | 1.31 | 1.39 |
| 1 | J | 338 | TYR | CD2-CE2 | -5.17 | 1.31 | 1.39 |
| 1 | L | 338 | TYR | CD2-CE2 | -5.17 | 1.31 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | M | 285 | CYS | CB-SG | -5.17 | 1.73 | 1.81 |
| 1 | R | 488 | TYR | CD2-CE2 | -5.17 | 1.31 | 1.39 |
| 1 | L | 488 | TYR | CD2-CE2 | -5.16 | 1.31 | 1.39 |
| 1 | P | 338 | TYR | CD2-CE2 | -5.16 | 1.31 | 1.39 |
| 1 | E | 285 | CYS | CB-SG | -5.16 | 1.73 | 1.81 |
| 1 | N | 338 | TYR | CD2-CE2 | -5.16 | 1.31 | 1.39 |
| 1 | S | 488 | TYR | CD2-CE2 | -5.16 | 1.31 | 1.39 |
| 1 | T | 488 | TYR | CD2-CE2 | -5.16 | 1.31 | 1.39 |
| 1 | V | 338 | TYR | CD2-CE2 | -5.16 | 1.31 | 1.39 |
| 1 | S | 285 | CYS | CB-SG | -5.15 | 1.73 | 1.81 |
| 1 | U | 488 | TYR | CD2-CE2 | -5.15 | 1.31 | 1.39 |
| 1 | K | 285 | CYS | CB-SG | -5.15 | 1.73 | 1.81 |
| 1 | T | 338 | TYR | CD2-CE2 | -5.15 | 1.31 | 1.39 |
| 1 | L | 285 | CYS | CB-SG | -5.15 | 1.73 | 1.81 |
| 1 | R | 338 | TYR | CD2-CE2 | -5.15 | 1.31 | 1.39 |
| 1 | X | 488 | TYR | CD2-CE2 | -5.14 | 1.31 | 1.39 |
| 1 | A | 285 | CYS | CB-SG | -5.14 | 1.73 | 1.81 |
| 1 | Q | 338 | TYR | CD2-CE2 | -5.14 | 1.31 | 1.39 |
| 1 | W | 285 | CYS | CB-SG | -5.14 | 1.73 | 1.81 |
| 1 | O | 338 | TYR | CD2-CE2 | -5.13 | 1.31 | 1.39 |
| 1 | X | 338 | TYR | CD2-CE2 | -5.13 | 1.31 | 1.39 |
| 1 | E | 488 | TYR | CD2-CE2 | -5.13 | 1.31 | 1.39 |
| 1 | K | 488 | TYR | CD2-CE2 | -5.13 | 1.31 | 1.39 |
| 1 | I | 488 | TYR | CD2-CE2 | -5.13 | 1.31 | 1.39 |
| 1 | P | 488 | TYR | CD2-CE2 | -5.11 | 1.31 | 1.39 |
| 1 | O | 332 | GLU | CD-OE1 | -5.11 | 1.20 | 1.25 |
| 1 | H | 488 | TYR | CD2-CE2 | -5.10 | 1.31 | 1.39 |
| 1 | M | 488 | TYR | CD2-CE2 | -5.10 | 1.31 | 1.39 |
| 1 | M | 338 | TYR | CD2-CE2 | -5.08 | 1.31 | 1.39 |
| 1 | D | 338 | TYR | CD1-CE1 | -5.08 | 1.31 | 1.39 |
| 1 | G | 332 | GLU | CD-OE1 | -5.07 | 1.20 | 1.25 |
| 1 | W | 332 | GLU | CD-OE1 | -5.07 | 1.20 | 1.25 |
| 1 | X | 332 | GLU | CD-OE1 | -5.05 | 1.20 | 1.25 |
| 1 | N | 332 | GLU | CD-OE1 | -5.05 | 1.20 | 1.25 |
| 1 | X | 488 | TYR | CD1-CE1 | -5.05 | 1.31 | 1.39 |
| 1 | G | 488 | TYR | CD1-CE1 | -5.05 | 1.31 | 1.39 |
| 1 | G | 338 | TYR | CD1-CE1 | -5.05 | 1.31 | 1.39 |
| 1 | P | 338 | TYR | CD1-CE1 | -5.04 | 1.31 | 1.39 |
| 1 | T | 338 | TYR | CD1-CE1 | -5.04 | 1.31 | 1.39 |
| 1 | A | 332 | GLU | CD-OE1 | -5.03 | 1.20 | 1.25 |
| 1 | H | 488 | TYR | CD1-CE1 | -5.03 | 1.31 | 1.39 |
| 1 | D | 332 | GLU | CD-OE1 | -5.03 | 1.20 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | C | 332 | GLU | CD-OE1 | -5.03 | 1.20 | 1.25 |
| 1 | K | 332 | GLU | CD-OE1 | -5.02 | 1.20 | 1.25 |
| 1 | J | 332 | GLU | CD-OE1 | -5.02 | 1.20 | 1.25 |
| 1 | F | 332 | GLU | CD-OE1 | -5.02 | 1.20 | 1.25 |
| 1 | W | 338 | TYR | CD1-CE1 | -5.01 | 1.31 | 1.39 |
| 1 | X | 338 | TYR | CD1-CE1 | -5.01 | 1.31 | 1.39 |
| 1 | S | 338 | TYR | CD1-CE1 | -5.01 | 1.31 | 1.39 |
| 1 | H | 332 | GLU | CD-OE1 | -5.01 | 1.20 | 1.25 |
| 1 | Q | 332 | GLU | CD-OE1 | -5.01 | 1.20 | 1.25 |
| 1 | A | 488 | TYR | CD1-CE1 | -5.00 | 1.31 | 1.39 |
| 1 | V | 488 | TYR | CD1-CE1 | -5.00 | 1.31 | 1.39 |
| 1 | M | 332 | GLU | CD-OE1 | -5.00 | 1.20 | 1.25 |

All (181) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | V | 270 | PRO | O-C-N | 7.21 | 134.24 | 122.70 |
| 1 | K | 270 | PRO | O-C-N | 7.19 | 134.21 | 122.70 |
| 1 | P | 270 | PRO | O-C-N | 7.17 | 134.18 | 122.70 |
| 1 | I | 270 | PRO | O-C-N | 7.17 | 134.17 | 122.70 |
| 1 | C | 270 | PRO | O-C-N | 7.16 | 134.16 | 122.70 |
| 1 | O | 270 | PRO | O-C-N | 7.16 | 134.16 | 122.70 |
| 1 | E | 270 | PRO | O-C-N | 7.15 | 134.14 | 122.70 |
| 1 | H | 270 | PRO | O-C-N | 7.15 | 134.14 | 122.70 |
| 1 | U | 270 | PRO | O-C-N | 7.15 | 134.14 | 122.70 |
| 1 | M | 270 | PRO | O-C-N | 7.15 | 134.14 | 122.70 |
| 1 | L | 270 | PRO | O-C-N | 7.15 | 134.14 | 122.70 |
| 1 | T | 270 | PRO | O-C-N | 7.15 | 134.14 | 122.70 |
| 1 | A | 270 | PRO | O-C-N | 7.14 | 134.13 | 122.70 |
| 1 | B | 270 | PRO | O-C-N | 7.14 | 134.13 | 122.70 |
| 1 | G | 270 | PRO | O-C-N | 7.14 | 134.12 | 122.70 |
| 1 | W | 270 | PRO | O-C-N | 7.14 | 134.12 | 122.70 |
| 1 | R | 270 | PRO | O-C-N | 7.13 | 134.11 | 122.70 |
| 1 | Q | 270 | PRO | O-C-N | 7.13 | 134.11 | 122.70 |
| 1 | X | 270 | PRO | O-C-N | 7.13 | 134.11 | 122.70 |
| 1 | S | 270 | PRO | O-C-N | 7.13 | 134.10 | 122.70 |
| 1 | J | 270 | PRO | O-C-N | 7.10 | 134.07 | 122.70 |
| 1 | F | 270 | PRO | O-C-N | 7.10 | 134.06 | 122.70 |
| 1 | N | 270 | PRO | O-C-N | 7.10 | 134.06 | 122.70 |
| 1 | D | 270 | PRO | O-C-N | 7.07 | 134.01 | 122.70 |
| 1 | I | 398 | VAL | CB-CA-C | -7.07 | 97.98 | 111.40 |
| 1 | T | 398 | VAL | CB-CA-C | -7.05 | 98.00 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | C | 398 | VAL | CB-CA-C | -7.05 | 98.00 | 111.40 |
| 1 | G | 398 | VAL | CB-CA-C | -7.05 | 98.01 | 111.40 |
| 1 | B | 398 | VAL | CB-CA-C | -7.04 | 98.02 | 111.40 |
| 1 | V | 398 | VAL | CB-CA-C | -7.04 | 98.01 | 111.40 |
| 1 | E | 398 | VAL | CB-CA-C | -7.04 | 98.02 | 111.40 |
| 1 | L | 398 | VAL | CB-CA-C | -7.04 | 98.03 | 111.40 |
| 1 | W | 398 | VAL | CB-CA-C | -7.03 | 98.04 | 111.40 |
| 1 | J | 398 | VAL | CB-CA-C | -7.03 | 98.04 | 111.40 |
| 1 | X | 398 | VAL | CB-CA-C | -7.03 | 98.04 | 111.40 |
| 1 | Q | 398 | VAL | CB-CA-C | -7.02 | 98.06 | 111.40 |
| 1 | A | 398 | VAL | CB-CA-C | -7.02 | 98.06 | 111.40 |
| 1 | F | 398 | VAL | CB-CA-C | -7.02 | 98.06 | 111.40 |
| 1 | H | 398 | VAL | CB-CA-C | -7.02 | 98.06 | 111.40 |
| 1 | R | 398 | VAL | CB-CA-C | -7.02 | 98.07 | 111.40 |
| 1 | S | 398 | VAL | CB-CA-C | -7.01 | 98.08 | 111.40 |
| 1 | M | 398 | VAL | CB-CA-C | -7.01 | 98.08 | 111.40 |
| 1 | O | 398 | VAL | CB-CA-C | -7.01 | 98.08 | 111.40 |
| 1 | K | 398 | VAL | CB-CA-C | -7.00 | 98.09 | 111.40 |
| 1 | U | 398 | VAL | CB-CA-C | -7.00 | 98.09 | 111.40 |
| 1 | D | 398 | VAL | CB-CA-C | -7.00 | 98.09 | 111.40 |
| 1 | N | 398 | VAL | CB-CA-C | -6.99 | 98.12 | 111.40 |
| 1 | P | 398 | VAL | CB-CA-C | -6.98 | 98.14 | 111.40 |
| 1 | B | 223 | ARG | NE-CZ-NH1 | 6.72 | 123.66 | 120.30 |
| 1 | H | 223 | ARG | NE-CZ-NH1 | 6.60 | 123.60 | 120.30 |
| 1 | D | 223 | ARG | NE-CZ-NH1 | 6.59 | 123.60 | 120.30 |
| 1 | A | 223 | ARG | NE-CZ-NH1 | 6.56 | 123.58 | 120.30 |
| 1 | R | 223 | ARG | NE-CZ-NH1 | 6.55 | 123.58 | 120.30 |
| 1 | C | 223 | ARG | NE-CZ-NH1 | 6.55 | 123.58 | 120.30 |
| 1 | X | 223 | ARG | NE-CZ-NH1 | 6.55 | 123.57 | 120.30 |
| 1 | Q | 223 | ARG | NE-CZ-NH1 | 6.54 | 123.57 | 120.30 |
| 1 | N | 223 | ARG | NE-CZ-NH1 | 6.54 | 123.57 | 120.30 |
| 1 | S | 223 | ARG | NE-CZ-NH1 | 6.52 | 123.56 | 120.30 |
| 1 | E | 223 | ARG | NE-CZ-NH1 | 6.51 | 123.56 | 120.30 |
| 1 | G | 223 | ARG | NE-CZ-NH1 | 6.49 | 123.55 | 120.30 |
| 1 | W | 223 | ARG | NE-CZ-NH1 | 6.49 | 123.54 | 120.30 |
| 1 | O | 223 | ARG | NE-CZ-NH1 | 6.45 | 123.53 | 120.30 |
| 1 | F | 223 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |
| 1 | K | 223 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |
| 1 | T | 223 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |
| 1 | U | 223 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |
| 1 | L | 223 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |
| 1 | I | 223 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | J | 223 | ARG | NE-CZ-NH1 | 6.43 | 123.52 | 120.30 |
| 1 | M | 223 | ARG | NE-CZ-NH1 | 6.43 | 123.52 | 120.30 |
| 1 | V | 223 | ARG | NE-CZ-NH1 | 6.42 | 123.51 | 120.30 |
| 1 | P | 223 | ARG | NE-CZ-NH1 | 6.41 | 123.50 | 120.30 |
| 1 | V | 495 | LEU | CA-CB-CG | 6.33 | 129.86 | 115.30 |
| 1 | O | 495 | LEU | CA-CB-CG | 6.33 | 129.86 | 115.30 |
| 1 | E | 495 | LEU | CA-CB-CG | 6.32 | 129.84 | 115.30 |
| 1 | I | 495 | LEU | CA-CB-CG | 6.32 | 129.84 | 115.30 |
| 1 | L | 495 | LEU | CA-CB-CG | 6.32 | 129.83 | 115.30 |
| 1 | R | 495 | LEU | CA-CB-CG | 6.32 | 129.83 | 115.30 |
| 1 | W | 495 | LEU | CA-CB-CG | 6.32 | 129.83 | 115.30 |
| 1 | X | 495 | LEU | CA-CB-CG | 6.31 | 129.82 | 115.30 |
| 1 | P | 495 | LEU | CA-CB-CG | 6.31 | 129.82 | 115.30 |
| 1 | M | 495 | LEU | CA-CB-CG | 6.31 | 129.80 | 115.30 |
| 1 | K | 495 | LEU | CA-CB-CG | 6.30 | 129.80 | 115.30 |
| 1 | N | 495 | LEU | CA-CB-CG | 6.30 | 129.80 | 115.30 |
| 1 | T | 495 | LEU | CA-CB-CG | 6.30 | 129.79 | 115.30 |
| 1 | D | 495 | LEU | CA-CB-CG | 6.30 | 129.78 | 115.30 |
| 1 | F | 495 | LEU | CA-CB-CG | 6.30 | 129.78 | 115.30 |
| 1 | G | 495 | LEU | CA-CB-CG | 6.29 | 129.77 | 115.30 |
| 1 | B | 495 | LEU | CA-CB-CG | 6.29 | 129.77 | 115.30 |
| 1 | C | 495 | LEU | CA-CB-CG | 6.29 | 129.76 | 115.30 |
| 1 | H | 495 | LEU | CA-CB-CG | 6.29 | 129.76 | 115.30 |
| 1 | U | 495 | LEU | CA-CB-CG | 6.29 | 129.76 | 115.30 |
| 1 | S | 495 | LEU | CA-CB-CG | 6.28 | 129.75 | 115.30 |
| 1 | A | 495 | LEU | CA-CB-CG | 6.28 | 129.74 | 115.30 |
| 1 | Q | 495 | LEU | CA-CB-CG | 6.28 | 129.75 | 115.30 |
| 1 | J | 495 | LEU | CA-CB-CG | 6.28 | 129.74 | 115.30 |
| 1 | C | 185 | ASP | CB-CG-OD2 | 6.20 | 123.88 | 118.30 |
| 1 | W | 185 | ASP | CB-CG-OD2 | 6.18 | 123.86 | 118.30 |
| 1 | I | 185 | ASP | CB-CG-OD2 | 6.17 | 123.85 | 118.30 |
| 1 | S | 185 | ASP | CB-CG-OD2 | 6.17 | 123.85 | 118.30 |
| 1 | G | 185 | ASP | CB-CG-OD2 | 6.16 | 123.84 | 118.30 |
| 1 | X | 185 | ASP | CB-CG-OD2 | 6.16 | 123.84 | 118.30 |
| 1 | B | 185 | ASP | CB-CG-OD2 | 6.15 | 123.84 | 118.30 |
| 1 | A | 185 | ASP | CB-CG-OD2 | 6.15 | 123.83 | 118.30 |
| 1 | T | 185 | ASP | CB-CG-OD2 | 6.14 | 123.83 | 118.30 |
| 1 | U | 185 | ASP | CB-CG-OD2 | 6.14 | 123.83 | 118.30 |
| 1 | L | 185 | ASP | CB-CG-OD2 | 6.13 | 123.82 | 118.30 |
| 1 | D | 185 | ASP | CB-CG-OD2 | 6.12 | 123.81 | 118.30 |
| 1 | E | 185 | ASP | CB-CG-OD2 | 6.12 | 123.81 | 118.30 |
| 1 | N | 185 | ASP | CB-CG-OD2 | 6.12 | 123.81 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | Q | 185 | ASP | CB-CG-OD2 | 6.12 | 123.81 | 118.30 |
| 1 | M | 185 | ASP | CB-CG-OD2 | 6.12 | 123.81 | 118.30 |
| 1 | P | 185 | ASP | CB-CG-OD2 | 6.12 | 123.81 | 118.30 |
| 1 | V | 185 | ASP | CB-CG-OD2 | 6.11 | 123.80 | 118.30 |
| 1 | O | 185 | ASP | CB-CG-OD2 | 6.11 | 123.80 | 118.30 |
| 1 | F | 185 | ASP | CB-CG-OD2 | 6.10 | 123.79 | 118.30 |
| 1 | J | 185 | ASP | CB-CG-OD2 | 6.09 | 123.78 | 118.30 |
| 1 | K | 185 | ASP | CB-CG-OD2 | 6.09 | 123.78 | 118.30 |
| 1 | H | 185 | ASP | CB-CG-OD2 | 6.08 | 123.77 | 118.30 |
| 1 | R | 185 | ASP | CB-CG-OD2 | 6.08 | 123.77 | 118.30 |
| 1 | M | 269 | ILE | N-CA-C | -5.52 | 96.11 | 111.00 |
| 1 | P | 269 | ILE | N-CA-C | -5.51 | 96.13 | 111.00 |
| 1 | B | 269 | ILE | N-CA-C | -5.50 | 96.16 | 111.00 |
| 1 | E | 269 | ILE | N-CA-C | -5.50 | 96.16 | 111.00 |
| 1 | N | 269 | ILE | N-CA-C | -5.50 | 96.16 | 111.00 |
| 1 | S | 269 | ILE | N-CA-C | -5.50 | 96.16 | 111.00 |
| 1 | F | 269 | ILE | N-CA-C | -5.49 | 96.17 | 111.00 |
| 1 | V | 269 | ILE | N-CA-C | -5.49 | 96.18 | 111.00 |
| 1 | A | 269 | ILE | N-CA-C | -5.49 | 96.19 | 111.00 |
| 1 | Q | 269 | ILE | N-CA-C | -5.49 | 96.19 | 111.00 |
| 1 | U | 269 | ILE | N-CA-C | -5.49 | 96.19 | 111.00 |
| 1 | R | 269 | ILE | N-CA-C | -5.48 | 96.20 | 111.00 |
| 1 | L | 269 | ILE | N-CA-C | -5.48 | 96.21 | 111.00 |
| 1 | H | 269 | ILE | N-CA-C | -5.48 | 96.21 | 111.00 |
| 1 | I | 269 | ILE | N-CA-C | -5.47 | 96.22 | 111.00 |
| 1 | O | 269 | ILE | N-CA-C | -5.47 | 96.22 | 111.00 |
| 1 | T | 269 | ILE | N-CA-C | -5.47 | 96.22 | 111.00 |
| 1 | K | 269 | ILE | N-CA-C | -5.47 | 96.23 | 111.00 |
| 1 | D | 269 | ILE | N-CA-C | -5.47 | 96.24 | 111.00 |
| 1 | C | 269 | ILE | N-CA-C | -5.47 | 96.24 | 111.00 |
| 1 | W | 269 | ILE | N-CA-C | -5.47 | 96.24 | 111.00 |
| 1 | X | 269 | ILE | N-CA-C | -5.47 | 96.24 | 111.00 |
| 1 | G | 269 | ILE | N-CA-C | -5.46 | 96.25 | 111.00 |
| 1 | M | 265 | LEU | CB-CG-CD2 | 5.46 | 120.29 | 111.00 |
| 1 | J | 269 | ILE | N-CA-C | -5.46 | 96.26 | 111.00 |
| 1 | O | 265 | LEU | CB-CG-CD2 | 5.45 | 120.26 | 111.00 |
| 1 | C | 265 | LEU | CB-CG-CD2 | 5.44 | 120.25 | 111.00 |
| 1 | R | 265 | LEU | CB-CG-CD2 | 5.44 | 120.26 | 111.00 |
| 1 | L | 265 | LEU | CB-CG-CD2 | 5.44 | 120.25 | 111.00 |
| 1 | T | 265 | LEU | CB-CG-CD2 | 5.44 | 120.25 | 111.00 |
| 1 | H | 265 | LEU | CB-CG-CD2 | 5.44 | 120.25 | 111.00 |
| 1 | A | 265 | LEU | CB-CG-CD2 | 5.44 | 120.24 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | K | 265 | LEU | CB-CG-CD2 | 5.43 | 120.24 | 111.00 |
| 1 | B | 265 | LEU | CB-CG-CD2 | 5.43 | 120.23 | 111.00 |
| 1 | W | 265 | LEU | CB-CG-CD2 | 5.43 | 120.23 | 111.00 |
| 1 | S | 265 | LEU | CB-CG-CD2 | 5.42 | 120.22 | 111.00 |
| 1 | J | 265 | LEU | CB-CG-CD2 | 5.41 | 120.20 | 111.00 |
| 1 | F | 265 | LEU | CB-CG-CD2 | 5.41 | 120.19 | 111.00 |
| 1 | E | 265 | LEU | CB-CG-CD2 | 5.40 | 120.18 | 111.00 |
| 1 | G | 265 | LEU | CB-CG-CD2 | 5.40 | 120.18 | 111.00 |
| 1 | D | 265 | LEU | CB-CG-CD2 | 5.40 | 120.17 | 111.00 |
| 1 | Q | 265 | LEU | CB-CG-CD2 | 5.40 | 120.17 | 111.00 |
| 1 | P | 265 | LEU | CB-CG-CD2 | 5.39 | 120.17 | 111.00 |
| 1 | V | 265 | LEU | CB-CG-CD2 | 5.39 | 120.17 | 111.00 |
| 1 | N | 265 | LEU | CB-CG-CD2 | 5.38 | 120.15 | 111.00 |
| 1 | U | 265 | LEU | CB-CG-CD2 | 5.38 | 120.15 | 111.00 |
| 1 | X | 265 | LEU | CB-CG-CD2 | 5.38 | 120.15 | 111.00 |
| 1 | I | 265 | LEU | CB-CG-CD2 | 5.38 | 120.14 | 111.00 |
| 1 | N | 82 | LEU | O-C-N | 5.05 | 130.78 | 122.70 |
| 1 | B | 82 | LEU | O-C-N | 5.04 | 130.76 | 122.70 |
| 1 | Q | 82 | LEU | O-C-N | 5.04 | 130.76 | 122.70 |
| 1 | P | 82 | LEU | O-C-N | 5.03 | 130.75 | 122.70 |
| 1 | X | 82 | LEU | O-C-N | 5.03 | 130.75 | 122.70 |
| 1 | E | 82 | LEU | O-C-N | 5.02 | 130.73 | 122.70 |
| 1 | G | 82 | LEU | O-C-N | 5.02 | 130.73 | 122.70 |
| 1 | O | 82 | LEU | O-C-N | 5.02 | 130.73 | 122.70 |
| 1 | I | 82 | LEU | O-C-N | 5.01 | 130.72 | 122.70 |
| 1 | V | 82 | LEU | O-C-N | 5.01 | 130.72 | 122.70 |
| 1 | M | 82 | LEU | O-C-N | 5.01 | 130.71 | 122.70 |
| 1 | K | 82 | LEU | O-C-N | 5.00 | 130.70 | 122.70 |
| 1 | S | 82 | LEU | O-C-N | 5.00 | 130.70 | 122.70 |

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 | 3799 | 0 | 3802 | 142 | 0 |
| 1 | B | 3799 | 0 | 3802 | 165 | 0 |
| 1 | C | 3799 | 0 | 3802 | 208 | 0 |
| 1 | D | 3799 | 0 | 3802 | 134 | 0 |
| 1 | E | 3799 | 0 | 3802 | 154 | 0 |
| 1 | F | 3799 | 0 | 3802 | 144 | 3 |
| 1 | G | 3799 | 0 | 3802 | 154 | 0 |
| 1 | H | 3799 | 0 | 3802 | 238 | 0 |
| 1 | I | 3799 | 0 | 3802 | 178 | 0 |
| 1 | J | 3799 | 0 | 3802 | 197 | 1 |
| 1 | K | 3799 | 0 | 3802 | 172 | 0 |
| 1 | L | 3799 | 0 | 3802 | 229 | 0 |
| 1 | M | 3799 | 0 | 3802 | 194 | 0 |
| 1 | N | 3799 | 0 | 3802 | 235 | 0 |
| 1 | O | 3799 | 0 | 3802 | 167 | 0 |
| 1 | P | 3799 | 0 | 3802 | 197 | 0 |
| 1 | Q | 3799 | 0 | 3802 | 191 | 0 |
| 1 | R | 3799 | 0 | 3802 | 200 | 0 |
| 1 | S | 3799 | 0 | 3802 | 230 | 0 |
| 1 | T | 3799 | 0 | 3802 | 213 | 1 |
| 1 | U | 3799 | 0 | 3802 | 218 | 0 |
| 1 | V | 3799 | 0 | 3802 | 257 | 0 |
| 1 | W | 3799 | 0 | 3802 | 188 | 3 |
| 1 | X | 3799 | 0 | 3802 | 186 | 0 |
| 2 | A | 20 | 0 | 10 | 4 | 0 |
| 2 | B | 20 | 0 | 10 | 4 | 0 |
| 2 | C | 20 | 0 | 10 | 4 | 0 |
| 2 | D | 20 | 0 | 10 | 4 | 0 |
| 2 | E | 20 | 0 | 10 | 4 | 0 |
| 2 | F | 20 | 0 | 10 | 4 | 0 |
| 2 | G | 20 | 0 | 10 | 4 | 0 |
| 2 | H | 20 | 0 | 10 | 5 | 0 |
| 2 | I | 20 | 0 | 10 | 4 | 0 |
| 2 | J | 20 | 0 | 10 | 4 | 0 |
| 2 | K | 20 | 0 | 10 | 5 | 0 |
| 2 | L | 20 | 0 | 10 | 5 | 0 |
| 2 | M | 20 | 0 | 10 | 4 | 0 |
| 2 | N | 20 | 0 | 10 | 4 | 0 |
| 2 | O | 20 | 0 | 10 | 5 | 0 |
| 2 | P | 20 | 0 | 10 | 5 | 0 |
| 2 | Q | 20 | 0 | 10 | 4 | 0 |
| 2 | R | 20 | 0 | 10 | 5 | 0 |
| 2 | S | 20 | 0 | 10 | 4 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | T | 20 | 0 | 10 | 5 | 0 |
| 2 | U | 20 | 0 | 10 | 4 | 0 |
| 2 | V | 20 | 0 | 10 | 5 | 0 |
| 2 | W | 20 | 0 | 10 | 5 | 0 |
| 2 | X | 20 | 0 | 10 | 5 | 0 |
| All | All | 91656 | 0 | 91488 | 3536 | 4 |

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 19.

All (3536) 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:C:216:ALA:CB | 1:N:446:LYS:HD3 | 1.49 | 1.42 |
| 1:C:250:SER:CB | 1:N:446:LYS:HG2 | 1.49 | 1.41 |
| 1:U:242:HIS:HE1 | 1:W:12:PHE:CZ | 1.42 | 1.38 |
| 1:H:12:PHE:CZ | 1:J:242:HIS:HE1 | 1.41 | 1.37 |
| 1:P:487:GLY:HA2 | 1:V:229:LYS:CE | 1.56 | 1.33 |
| 1:F:188:ALA:CB | 1:F:218:GLN:HG3 | 1.62 | 1.30 |
| 1:M:188:ALA:CB | 1:M:218:GLN:HG3 | 1.62 | 1.30 |
| 1:B:188:ALA:CB | 1:B:218:GLN:HG3 | 1.62 | 1.30 |
| 1:J:188:ALA:CB | 1:J:218:GLN:HG3 | 1.62 | 1.30 |
| 1:D:188:ALA:CB | 1:D:218:GLN:HG3 | 1.62 | 1.29 |
| 1:K:12:PHE:CZ | 1:M:242:HIS:HE1 | 1.49 | 1.29 |
| 1:G:188:ALA:CB | 1:G:218:GLN:HG3 | 1.62 | 1.29 |
| 1:U:188:ALA:CB | 1:U:218:GLN:HG3 | 1.62 | 1.29 |
| 1:O:188:ALA:CB | 1:O:218:GLN:HG3 | 1.62 | 1.28 |
| 1:R:188:ALA:CB | 1:R:218:GLN:HG3 | 1.62 | 1.28 |
| 1:C:250:SER:HB2 | 1:N:446:LYS:CG | 1.61 | 1.28 |
| 1:K:188:ALA:CB | 1:K:218:GLN:HG3 | 1.62 | 1.28 |
| 1:V:284:LYS:HG3 | 1:X:7:LEU:CD2 | 1.60 | 1.28 |
| 1:L:188:ALA:CB | 1:L:218:GLN:HG3 | 1.62 | 1.28 |
| 1:N:188:ALA:CB | 1:N:218:GLN:HG3 | 1.62 | 1.28 |
| 1:T:188:ALA:CB | 1:T:218:GLN:HG3 | 1.62 | 1.28 |
| 1:E:188:ALA:CB | 1:E:218:GLN:HG3 | 1.62 | 1.28 |
| 1:U:242:HIS:CE1 | 1:W:12:PHE:CZ | 2.20 | 1.28 |
| 1:C:188:ALA:CB | 1:C:218:GLN:HG3 | 1.62 | 1.28 |
| 1:V:188:ALA:CB | 1:V:218:GLN:HG3 | 1.62 | 1.28 |
| 1:W:188:ALA:CB | 1:W:218:GLN:HG3 | 1.62 | 1.28 |
| 1:S:188:ALA:CB | 1:S:218:GLN:HG3 | 1.62 | 1.28 |
| 1:A:188:ALA:CB | 1:A:218:GLN:HG3 | 1.62 | 1.27 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:188:ALA:CB | 1:I:218:GLN:HG3 | 1.62 | 1.27 |
| 1:P:188:ALA:CB | 1:P:218:GLN:HG3 | 1.62 | 1.27 |
| 1:X:188:ALA:CB | 1:X:218:GLN:HG3 | 1.62 | 1.27 |
| 1:Q:188:ALA:CB | 1:Q:218:GLN:HG3 | 1.62 | 1.27 |
| 1:H:188:ALA:CB | 1:H:218:GLN:HG3 | 1.62 | 1.27 |
| 1:L:242:HIS:HE1 | 1:N:12:PHE:CE2 | 1.51 | 1.27 |
| 1:I:229:LYS:CE | 1:M:487:GLY:HA2 | 1.64 | 1.26 |
| 1:R:280:ILE:HG12 | 1:T:6:ASN:O | 1.35 | 1.23 |
| 1:L:242:HIS:CE1 | 1:N:12:PHE:CE2 | 2.28 | 1.21 |
| 1:R:284:LYS:HG3 | 1:T:7:LEU:CD2 | 1.69 | 1.21 |
| 1:K:12:PHE:CE2 | 1:M:242:HIS:CE1 | 2.28 | 1.20 |
| 1:U:372:ILE:HG13 | 1:V:390:GLU:HA | 1.22 | 1.19 |
| 1:E:297:GLN:OE1 | 1:G:310:ARG:HG2 | 1.44 | 1.18 |
| 1:D:472:THR:HG22 | 1:D:498:GLU:HA | 1.25 | 1.17 |
| 1:Q:472:THR:HG22 | 1:Q:498:GLU:HA | 1.25 | 1.17 |
| 1:S:373:PRO:HB3 | 1:T:391:THR:HA | 1.25 | 1.17 |
| 1:H:310:ARG:HG2 | 1:J:297:GLN:CG | 1.75 | 1.17 |
| 1:C:390:GLU:HA | 1:P:372:ILE:HG13 | 1.23 | 1.17 |
| 1:H:310:ARG:HG2 | 1:J:297:GLN:CB | 1.73 | 1.17 |
| 1:I:487:GLY:CA | 1:M:229:LYS:HG3 | 1.73 | 1.17 |
| 1:M:472:THR:HG22 | 1:M:498:GLU:HA | 1.25 | 1.16 |
| 1:L:283:SER:HB3 | 1:N:3:LEU:CD2 | 1.75 | 1.16 |
| 1:H:12:PHE:CZ | 1:J:242:HIS:CE1 | 2.31 | 1.16 |
| 1:H:371:HIS:O | 1:H:374:MET:HG2 | 1.44 | 1.16 |
| 1:R:472:THR:HG22 | 1:R:498:GLU:HA | 1.25 | 1.16 |
| 1:K:472:THR:HG22 | 1:K:498:GLU:HA | 1.25 | 1.16 |
| 1:F:373:PRO:HA | 1:G:390:GLU:O | 1.40 | 1.15 |
| 1:I:487:GLY:HA2 | 1:M:229:LYS:CG | 1.76 | 1.15 |
| 1:A:472:THR:HG22 | 1:A:498:GLU:HA | 1.25 | 1.15 |
| 1:U:12:PHE:CE2 | 1:W:242:HIS:HE1 | 1.64 | 1.15 |
| 1:L:472:THR:HG22 | 1:L:498:GLU:HA | 1.25 | 1.14 |
| 1:S:472:THR:HG22 | 1:S:498:GLU:HA | 1.25 | 1.14 |
| 1:V:472:THR:HG22 | 1:V:498:GLU:HA | 1.25 | 1.14 |
| 1:H:310:ARG:CG | 1:J:297:GLN:HB2 | 1.76 | 1.14 |
| 1:S:372:ILE:HD11 | 1:T:390:GLU:HG2 | 1.29 | 1.13 |
| 1:P:487:GLY:HA2 | 1:V:229:LYS:CD | 1.77 | 1.13 |
| 1:B:12:PHE:CE2 | 1:C:242:HIS:HE1 | 1.65 | 1.13 |
| 1:B:472:THR:HG22 | 1:B:498:GLU:HA | 1.25 | 1.13 |
| 1:H:297:GLN:HB2 | 1:J:310:ARG:HG2 | 1.26 | 1.13 |
| 1:S:372:ILE:CG1 | 1:T:390:GLU:HA | 1.77 | 1.13 |
| 1:U:242:HIS:CE1 | 1:W:12:PHE:CE2 | 2.37 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:Q:297:GLN:OE1 | 1:S:310:ARG:HG2 | 1.43 | 1.13 |
| 1:U:11:ILE:HB | 1:W:273:LYS:CG | 1.77 | 1.12 |
| 1:H:312:GLU:HA | 1:J:311:ALA:CB | 1.78 | 1.12 |
| 1:K:12:PHE:CZ | 1:M:242:HIS:CE1 | 2.36 | 1.12 |
| 1:U:297:GLN:HB2 | 1:W:310:ARG:HG2 | 1.32 | 1.12 |
| 1:W:472:THR:HG22 | 1:W:498:GLU:HA | 1.25 | 1.12 |
| 1:K:12:PHE:CE2 | 1:M:242:HIS:HE1 | 1.65 | 1.12 |
| 1:U:472:THR:HG22 | 1:U:498:GLU:HA | 1.25 | 1.12 |
| 1:B:188:ALA:CB | 1:B:218:GLN:CG | 2.28 | 1.12 |
| 1:L:188:ALA:CB | 1:L:218:GLN:CG | 2.28 | 1.12 |
| 1:T:3:LEU:HD23 | 1:T:3:LEU:C | 1.70 | 1.12 |
| 1:F:188:ALA:CB | 1:F:218:GLN:CG | 2.28 | 1.11 |
| 1:O:472:THR:HG22 | 1:O:498:GLU:HA | 1.25 | 1.11 |
| 1:T:188:ALA:CB | 1:T:218:GLN:CG | 2.28 | 1.11 |
| 1:S:373:PRO:HA | 1:T:390:GLU:O | 1.49 | 1.11 |
| 1:M:188:ALA:CB | 1:M:218:GLN:CG | 2.28 | 1.11 |
| 1:C:472:THR:HG22 | 1:C:498:GLU:HA | 1.25 | 1.11 |
| 1:H:188:ALA:CB | 1:H:218:GLN:CG | 2.28 | 1.11 |
| 1:U:188:ALA:CB | 1:U:218:GLN:CG | 2.28 | 1.11 |
| 1:O:188:ALA:CB | 1:O:218:GLN:CG | 2.28 | 1.11 |
| 1:S:188:ALA:CB | 1:S:218:GLN:CG | 2.28 | 1.11 |
| 1:U:11:ILE:HB | 1:W:273:LYS:HG2 | 1.13 | 1.11 |
| 1:F:472:THR:HG22 | 1:F:498:GLU:HA | 1.25 | 1.11 |
| 1:Q:188:ALA:CB | 1:Q:218:GLN:CG | 2.28 | 1.11 |
| 1:I:188:ALA:CB | 1:I:218:GLN:CG | 2.28 | 1.11 |
| 1:C:188:ALA:CB | 1:C:218:GLN:CG | 2.28 | 1.11 |
| 1:H:242:HIS:CE1 | 1:J:12:PHE:CE2 | 2.39 | 1.11 |
| 1:I:229:LYS:HE3 | 1:M:487:GLY:HA2 | 1.15 | 1.11 |
| 1:V:242:HIS:CE1 | 1:X:12:PHE:CE2 | 2.39 | 1.11 |
| 1:X:472:THR:HG22 | 1:X:498:GLU:HA | 1.25 | 1.11 |
| 1:O:11:ILE:HB | 1:P:273:LYS:HG2 | 1.27 | 1.10 |
| 1:R:371:HIS:O | 1:R:374:MET:HG2 | 1.48 | 1.10 |
| 1:V:188:ALA:CB | 1:V:218:GLN:CG | 2.29 | 1.10 |
| 1:V:280:ILE:HG12 | 1:X:6:ASN:O | 1.51 | 1.10 |
| 1:X:188:ALA:CB | 1:X:218:GLN:CG | 2.28 | 1.10 |
| 1:U:11:ILE:CB | 1:W:273:LYS:HG2 | 1.81 | 1.10 |
| 1:W:188:ALA:CB | 1:W:218:GLN:CG | 2.28 | 1.10 |
| 1:A:188:ALA:CB | 1:A:218:GLN:CG | 2.28 | 1.10 |
| 1:J:188:ALA:CB | 1:J:218:GLN:CG | 2.28 | 1.10 |
| 1:P:487:GLY:CA | 1:V:229:LYS:HE3 | 1.82 | 1.10 |
| 1:A:392:LYS:HD2 | 1:J:373:PRO:HD3 | 1.34 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:P:188:ALA:CB | 1:P:218:GLN:CG | 2.28 | 1.10 |
| 1:E:188:ALA:CB | 1:E:218:GLN:CG | 2.28 | 1.10 |
| 1:G:472:THR:HG22 | 1:G:498:GLU:HA | 1.25 | 1.10 |
| 1:K:188:ALA:CB | 1:K:218:GLN:CG | 2.28 | 1.10 |
| 1:E:472:THR:HG22 | 1:E:498:GLU:HA | 1.25 | 1.09 |
| 1:I:188:ALA:HB2 | 1:I:218:GLN:CG | 1.82 | 1.09 |
| 1:N:188:ALA:CB | 1:N:218:GLN:CG | 2.28 | 1.09 |
| 1:R:188:ALA:CB | 1:R:218:GLN:CG | 2.28 | 1.09 |
| 1:S:188:ALA:HB2 | 1:S:218:GLN:CG | 1.82 | 1.09 |
| 1:D:188:ALA:CB | 1:D:218:GLN:CG | 2.28 | 1.09 |
| 1:I:472:THR:HG22 | 1:I:498:GLU:HA | 1.25 | 1.09 |
| 1:O:12:PHE:CE2 | 1:P:242:HIS:HE1 | 1.69 | 1.09 |
| 1:P:188:ALA:HB2 | 1:P:218:GLN:CG | 1.82 | 1.09 |
| 1:U:312:GLU:HA | 1:W:311:ALA:HB1 | 1.32 | 1.09 |
| 1:A:188:ALA:HB2 | 1:A:218:GLN:CG | 1.83 | 1.09 |
| 1:G:188:ALA:CB | 1:G:218:GLN:CG | 2.28 | 1.09 |
| 1:G:188:ALA:HB2 | 1:G:218:GLN:CG | 1.82 | 1.09 |
| 1:M:188:ALA:HB2 | 1:M:218:GLN:CG | 1.82 | 1.09 |
| 1:L:188:ALA:HB2 | 1:L:218:GLN:CG | 1.83 | 1.09 |
| 1:Q:188:ALA:HB2 | 1:Q:218:GLN:CG | 1.82 | 1.09 |
| 1:S:372:ILE:HG12 | 1:T:390:GLU:HA | 1.30 | 1.09 |
| 1:C:188:ALA:HB2 | 1:C:218:GLN:CG | 1.83 | 1.09 |
| 1:N:472:THR:HG22 | 1:N:498:GLU:HA | 1.25 | 1.09 |
| 1:F:390:GLU:O | 1:G:373:PRO:HA | 1.52 | 1.09 |
| 1:R:272:GLU:CG | 1:T:352:GLU:HG2 | 1.80 | 1.09 |
| 1:D:188:ALA:HB2 | 1:D:218:GLN:CG | 1.83 | 1.08 |
| 1:K:188:ALA:HB2 | 1:K:218:GLN:CG | 1.83 | 1.08 |
| 1:P:472:THR:HG22 | 1:P:498:GLU:HA | 1.25 | 1.08 |
| 1:R:269:ILE:HG12 | 1:T:11:ILE:HD12 | 1.29 | 1.08 |
| 1:R:270:PRO:HG2 | 1:R:273:LYS:HE2 | 1.36 | 1.08 |
| 1:V:188:ALA:HB2 | 1:V:218:GLN:CG | 1.83 | 1.08 |
| 1:X:188:ALA:HB2 | 1:X:218:GLN:CG | 1.83 | 1.08 |
| 1:E:270:PRO:HG2 | 1:E:273:LYS:HE2 | 1.35 | 1.08 |
| 1:P:371:HIS:O | 1:P:374:MET:HG2 | 1.51 | 1.08 |
| 1:V:270:PRO:HG2 | 1:V:273:LYS:HE2 | 1.35 | 1.08 |
| 1:L:424:ARG:HG2 | 1:L:424:ARG:NH1 | 1.55 | 1.08 |
| 1:B:188:ALA:HB2 | 1:B:218:GLN:CG | 1.83 | 1.08 |
| 1:H:188:ALA:HB2 | 1:H:218:GLN:CG | 1.83 | 1.08 |
| 1:O:188:ALA:HB2 | 1:O:218:GLN:CG | 1.82 | 1.08 |
| 1:T:472:THR:HG22 | 1:T:498:GLU:HA | 1.25 | 1.08 |
| 1:U:371:HIS:O | 1:U:374:MET:HG2 | 1.54 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:188:ALA:HB2 | 1:F:218:GLN:CG | 1.83 | 1.08 |
| 1:C:216:ALA:HB3 | 1:N:446:LYS:HD3 | 1.28 | 1.08 |
| 1:T:188:ALA:HB2 | 1:T:218:GLN:CG | 1.83 | 1.07 |
| 1:C:424:ARG:HG2 | 1:C:424:ARG:NH1 | 1.55 | 1.07 |
| 1:H:472:THR:HG22 | 1:H:498:GLU:HA | 1.25 | 1.07 |
| 1:B:424:ARG:HG2 | 1:B:424:ARG:NH1 | 1.56 | 1.07 |
| 1:N:188:ALA:HB2 | 1:N:218:GLN:CG | 1.83 | 1.07 |
| 1:L:270:PRO:HG2 | 1:L:273:LYS:HE2 | 1.35 | 1.07 |
| 1:U:188:ALA:HB2 | 1:U:218:GLN:CG | 1.83 | 1.07 |
| 1:I:424:ARG:NH1 | 1:I:424:ARG:HG2 | 1.55 | 1.07 |
| 1:H:242:HIS:HE1 | 1:J:12:PHE:CE2 | 1.69 | 1.07 |
| 1:L:297:GLN:OE1 | 1:N:310:ARG:HG2 | 1.50 | 1.07 |
| 1:U:11:ILE:O | 1:W:273:LYS:HE3 | 1.54 | 1.07 |
| 1:E:188:ALA:HB2 | 1:E:218:GLN:CG | 1.83 | 1.07 |
| 1:H:496:LEU:HG | 1:M:195:VAL:CG2 | 1.85 | 1.07 |
| 1:H:242:HIS:HE1 | 1:J:12:PHE:CZ | 1.72 | 1.07 |
| 1:J:472:THR:HG22 | 1:J:498:GLU:HA | 1.25 | 1.06 |
| 1:T:424:ARG:HH11 | 1:T:424:ARG:CG | 1.68 | 1.06 |
| 1:J:188:ALA:HB2 | 1:J:218:GLN:CG | 1.82 | 1.06 |
| 1:P:229:LYS:HG3 | 1:V:487:GLY:CA | 1.84 | 1.06 |
| 1:V:284:LYS:HG3 | 1:X:7:LEU:HD21 | 1.35 | 1.06 |
| 1:I:270:PRO:HG2 | 1:I:273:LYS:HE2 | 1.36 | 1.06 |
| 1:R:188:ALA:HB2 | 1:R:218:GLN:CG | 1.83 | 1.06 |
| 1:J:296:THR:HG22 | 1:J:297:GLN:HG2 | 1.37 | 1.06 |
| 1:H:496:LEU:CD2 | 1:M:195:VAL:HG22 | 1.83 | 1.06 |
| 1:C:216:ALA:HB3 | 1:N:446:LYS:O | 1.55 | 1.06 |
| 1:S:424:ARG:CG | 1:S:424:ARG:HH11 | 1.68 | 1.06 |
| 1:W:188:ALA:HB2 | 1:W:218:GLN:CG | 1.83 | 1.06 |
| 1:B:424:ARG:CG | 1:B:424:ARG:HH11 | 1.68 | 1.06 |
| 1:B:297:GLN:OE1 | 1:C:310:ARG:HG2 | 1.55 | 1.06 |
| 1:I:424:ARG:HH11 | 1:I:424:ARG:CG | 1.68 | 1.06 |
| 1:H:311:ALA:CB | 1:J:312:GLU:HA | 1.85 | 1.06 |
| 1:I:229:LYS:HE3 | 1:M:487:GLY:CA | 1.86 | 1.06 |
| 1:I:229:LYS:CD | 1:M:487:GLY:HA2 | 1.86 | 1.06 |
| 1:U:311:ALA:HB1 | 1:W:312:GLU:HA | 1.32 | 1.06 |
| 1:C:216:ALA:CB | 1:N:446:LYS:CD | 2.34 | 1.06 |
| 1:D:424:ARG:CG | 1:D:424:ARG:HH11 | 1.68 | 1.06 |
| 1:I:371:HIS:O | 1:I:374:MET:HG2 | 1.55 | 1.06 |
| 1:O:12:PHE:CZ | 1:P:242:HIS:HE1 | 1.73 | 1.05 |
| 1:W:424:ARG:NH1 | 1:W:424:ARG:HG2 | 1.55 | 1.05 |
| 1:U:372:ILE:HG13 | 1:V:390:GLU:CA | 1.87 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:424:ARG:HH11 | 1:N:424:ARG:CG | 1.69 | 1.05 |
| 1:A:424:ARG:CG | 1:A:424:ARG:HH11 | 1.68 | 1.05 |
| 1:C:424:ARG:HH11 | 1:C:424:ARG:CG | 1.68 | 1.05 |
| 1:F:424:ARG:NH1 | 1:F:424:ARG:HG2 | 1.55 | 1.05 |
| 1:R:424:ARG:NH1 | 1:R:424:ARG:HG2 | 1.55 | 1.05 |
| 1:P:229:LYS:HG3 | 1:V:487:GLY:HA2 | 1.36 | 1.05 |
| 1:H:496:LEU:CG | 1:M:195:VAL:HG22 | 1.85 | 1.04 |
| 1:H:312:GLU:HA | 1:J:311:ALA:HB1 | 1.06 | 1.04 |
| 1:G:424:ARG:CG | 1:G:424:ARG:HH11 | 1.68 | 1.04 |
| 1:O:12:PHE:CE2 | 1:P:242:HIS:CE1 | 2.45 | 1.04 |
| 1:U:12:PHE:HE2 | 1:W:242:HIS:CE1 | 1.75 | 1.04 |
| 1:L:371:HIS:O | 1:L:374:MET:HG2 | 1.58 | 1.04 |
| 1:K:424:ARG:HH11 | 1:K:424:ARG:CG | 1.68 | 1.04 |
| 1:V:424:ARG:HH11 | 1:V:424:ARG:CG | 1.68 | 1.04 |
| 1:M:373:PRO:HA | 1:N:390:GLU:O | 1.58 | 1.04 |
| 1:H:372:ILE:HG23 | 1:I:390:GLU:O | 1.57 | 1.04 |
| 1:R:284:LYS:HG3 | 1:T:7:LEU:HD22 | 1.36 | 1.04 |
| 1:M:424:ARG:HH11 | 1:M:424:ARG:CG | 1.68 | 1.04 |
| 1:L:424:ARG:CG | 1:L:424:ARG:HH11 | 1.68 | 1.04 |
| 1:X:424:ARG:CG | 1:X:424:ARG:HH11 | 1.68 | 1.03 |
| 1:V:242:HIS:HE1 | 1:X:12:PHE:CE2 | 1.74 | 1.03 |
| 1:O:424:ARG:HH11 | 1:O:424:ARG:CG | 1.68 | 1.03 |
| 1:P:424:ARG:CG | 1:P:424:ARG:HH11 | 1.68 | 1.03 |
| 1:Q:424:ARG:CG | 1:Q:424:ARG:HH11 | 1.68 | 1.03 |
| 1:M:372:ILE:HG13 | 1:N:390:GLU:HA | 1.36 | 1.03 |
| 1:W:424:ARG:HH11 | 1:W:424:ARG:CG | 1.68 | 1.03 |
| 1:H:424:ARG:CG | 1:H:424:ARG:HH11 | 1.68 | 1.03 |
| 1:J:424:ARG:CG | 1:J:424:ARG:HH11 | 1.68 | 1.03 |
| 1:Q:242:HIS:CE1 | 1:S:12:PHE:CE2 | 2.47 | 1.03 |
| 1:S:371:HIS:O | 1:S:374:MET:HG2 | 1.58 | 1.03 |
| 1:U:424:ARG:CG | 1:U:424:ARG:HH11 | 1.68 | 1.02 |
| 1:F:424:ARG:HH11 | 1:F:424:ARG:CG | 1.69 | 1.02 |
| 1:U:373:PRO:HA | 1:V:390:GLU:O | 1.59 | 1.02 |
| 1:V:276:VAL:HG12 | 1:V:280:ILE:HD11 | 1.36 | 1.02 |
| 1:R:269:ILE:HG12 | 1:T:11:ILE:CD1 | 1.89 | 1.02 |
| 1:S:372:ILE:HG13 | 1:T:390:GLU:CA | 1.89 | 1.02 |
| 1:R:297:GLN:HG3 | 1:T:310:ARG:HG3 | 1.40 | 1.02 |
| 1:H:372:ILE:HG13 | 1:I:390:GLU:HA | 1.40 | 1.02 |
| 1:P:487:GLY:HA2 | 1:V:229:LYS:HE3 | 1.06 | 1.02 |
| 1:H:310:ARG:HG2 | 1:J:297:GLN:HB2 | 1.30 | 1.01 |
| 1:S:372:ILE:HG13 | 1:T:390:GLU:O | 1.59 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:373:PRO:HB3 | 1:X:391:THR:HA | 1.39 | 1.01 |
| 1:K:424:ARG:HG2 | 1:K:424:ARG:NH1 | 1.55 | 1.01 |
| 1:O:311:ALA:HB1 | 1:P:312:GLU:HA | 1.41 | 1.01 |
| 1:H:310:ARG:HG2 | 1:J:297:GLN:HG3 | 1.42 | 1.01 |
| 1:L:283:SER:CB | 1:N:3:LEU:CD2 | 2.38 | 1.01 |
| 1:M:371:HIS:O | 1:M:374:MET:HG2 | 1.60 | 1.01 |
| 1:E:242:HIS:HE1 | 1:G:12:PHE:CZ | 1.77 | 1.01 |
| 1:U:12:PHE:CE2 | 1:W:242:HIS:CE1 | 2.49 | 1.01 |
| 1:V:284:LYS:CG | 1:X:7:LEU:CD2 | 2.37 | 1.00 |
| 1:T:371:HIS:O | 1:T:374:MET:HG2 | 1.61 | 1.00 |
| 1:W:372:ILE:HG13 | 1:X:390:GLU:HA | 1.39 | 1.00 |
| 1:E:424:ARG:HG2 | 1:E:424:ARG:NH1 | 1.55 | 1.00 |
| 1:K:496:LEU:HG | 1:S:195:VAL:HG22 | 1.40 | 1.00 |
| 1:R:424:ARG:HH11 | 1:R:424:ARG:CG | 1.68 | 1.00 |
| 1:P:195:VAL:HG22 | 1:U:496:LEU:HG | 1.43 | 1.00 |
| 1:H:311:ALA:HB1 | 1:J:312:GLU:CA | 1.90 | 1.00 |
| 1:Q:283:SER:HB3 | 1:S:3:LEU:CD2 | 1.92 | 1.00 |
| 1:E:424:ARG:CG | 1:E:424:ARG:HH11 | 1.68 | 1.00 |
| 1:R:272:GLU:HG3 | 1:T:352:GLU:HB2 | 1.42 | 1.00 |
| 1:D:424:ARG:NH1 | 1:D:424:ARG:HG2 | 1.55 | 0.99 |
| 1:H:496:LEU:HG | 1:M:195:VAL:HG22 | 1.39 | 0.99 |
| 1:U:372:ILE:HG23 | 1:V:390:GLU:O | 1.62 | 0.99 |
| 1:H:12:PHE:CE2 | 1:J:242:HIS:HE1 | 1.80 | 0.99 |
| 1:I:229:LYS:HG3 | 1:M:487:GLY:CA | 1.91 | 0.99 |
| 1:K:12:PHE:HE2 | 1:M:242:HIS:CE1 | 1.75 | 0.99 |
| 1:P:424:ARG:HG2 | 1:P:424:ARG:NH1 | 1.55 | 0.99 |
| 1:M:424:ARG:NH1 | 1:M:424:ARG:HG2 | 1.55 | 0.99 |
| 1:J:424:ARG:HG2 | 1:J:424:ARG:NH1 | 1.55 | 0.98 |
| 1:I:229:LYS:HG3 | 1:M:487:GLY:HA3 | 1.42 | 0.98 |
| 1:O:12:PHE:HE2 | 1:P:242:HIS:CE1 | 1.81 | 0.98 |
| 1:V:297:GLN:HE21 | 1:V:300:GLU:CB | 1.76 | 0.98 |
| 1:A:424:ARG:HG2 | 1:A:424:ARG:NH1 | 1.55 | 0.98 |
| 1:B:12:PHE:HE2 | 1:C:242:HIS:CE1 | 1.80 | 0.98 |
| 1:T:424:ARG:HG2 | 1:T:424:ARG:NH1 | 1.55 | 0.98 |
| 1:U:424:ARG:NH1 | 1:U:424:ARG:HG2 | 1.55 | 0.98 |
| 1:H:310:ARG:CB | 1:J:297:GLN:HB2 | 1.93 | 0.98 |
| 1:O:312:GLU:HA | 1:P:311:ALA:HB1 | 1.45 | 0.98 |
| 1:G:424:ARG:NH1 | 1:G:424:ARG:HG2 | 1.55 | 0.97 |
| 1:H:311:ALA:HB1 | 1:J:312:GLU:HA | 0.98 | 0.97 |
| 1:K:373:PRO:HA | 1:L:390:GLU:O | 1.63 | 0.97 |
| 1:S:373:PRO:HB3 | 1:T:391:THR:CA | 1.93 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:195:VAL:HG22 | 1:U:496:LEU:CD2 | 1.95 | 0.97 |
| 1:T:3:LEU:HD23 | 1:T:3:LEU:O | 1.63 | 0.97 |
| 1:X:424:ARG:NH1 | 1:X:424:ARG:HG2 | 1.55 | 0.97 |
| 1:H:297:GLN:CB | 1:J:310:ARG:HG2 | 1.94 | 0.97 |
| 1:K:242:HIS:CE1 | 1:M:12:PHE:CE2 | 2.53 | 0.97 |
| 1:S:424:ARG:NH1 | 1:S:424:ARG:HG2 | 1.55 | 0.97 |
| 1:C:473:GLY:HA3 | 1:V:191:ALA:HB1 | 1.46 | 0.97 |
| 1:L:283:SER:CB | 1:N:3:LEU:HD23 | 1.95 | 0.96 |
| 1:H:424:ARG:NH1 | 1:H:424:ARG:HG2 | 1.55 | 0.96 |
| 1:A:3:LEU:CD2 | 1:I:283:SER:HB3 | 1.95 | 0.96 |
| 1:S:373:PRO:CB | 1:T:391:THR:HA | 1.95 | 0.96 |
| 1:H:472:THR:HG22 | 1:H:498:GLU:CA | 1.96 | 0.96 |
| 1:F:472:THR:HG22 | 1:F:498:GLU:CA | 1.96 | 0.96 |
| 1:H:297:GLN:HB2 | 1:J:310:ARG:CG | 1.94 | 0.96 |
| 1:C:496:LEU:HG | 1:V:195:VAL:HG22 | 1.48 | 0.96 |
| 1:V:424:ARG:NH1 | 1:V:424:ARG:HG2 | 1.56 | 0.96 |
| 1:B:472:THR:HG22 | 1:B:498:GLU:CA | 1.96 | 0.96 |
| 1:L:472:THR:HG22 | 1:L:498:GLU:CA | 1.96 | 0.96 |
| 1:Q:472:THR:HG22 | 1:Q:498:GLU:CA | 1.96 | 0.96 |
| 1:V:297:GLN:NE2 | 1:V:300:GLU:CG | 2.29 | 0.96 |
| 1:D:472:THR:HG22 | 1:D:498:GLU:CA | 1.96 | 0.96 |
| 1:Q:424:ARG:HG2 | 1:Q:424:ARG:NH1 | 1.55 | 0.96 |
| 1:A:472:THR:HG22 | 1:A:498:GLU:CA | 1.96 | 0.96 |
| 1:C:390:GLU:O | 1:P:373:PRO:HA | 1.66 | 0.95 |
| 1:R:472:THR:HG22 | 1:R:498:GLU:CA | 1.96 | 0.95 |
| 1:B:373:PRO:HD3 | 1:O:392:LYS:HD2 | 1.45 | 0.95 |
| 1:F:372:ILE:HG13 | 1:G:390:GLU:HA | 1.48 | 0.95 |
| 1:K:472:THR:HG22 | 1:K:498:GLU:CA | 1.96 | 0.95 |
| 1:S:472:THR:HG22 | 1:S:498:GLU:CA | 1.96 | 0.95 |
| 1:R:269:ILE:CG1 | 1:T:11:ILE:HD12 | 1.96 | 0.95 |
| 1:P:195:VAL:HG22 | 1:U:496:LEU:CG | 1.95 | 0.95 |
| 1:U:472:THR:HG22 | 1:U:498:GLU:CA | 1.96 | 0.95 |
| 1:V:472:THR:HG22 | 1:V:498:GLU:CA | 1.96 | 0.95 |
| 1:C:472:THR:HG22 | 1:C:498:GLU:CA | 1.96 | 0.95 |
| 1:V:297:GLN:NE2 | 1:V:300:GLU:CB | 2.30 | 0.95 |
| 1:O:472:THR:HG22 | 1:O:498:GLU:CA | 1.96 | 0.95 |
| 1:X:472:THR:HG22 | 1:X:498:GLU:CA | 1.96 | 0.95 |
| 1:G:472:THR:HG22 | 1:G:498:GLU:CA | 1.96 | 0.94 |
| 1:C:373:PRO:HA | 1:P:390:GLU:O | 1.66 | 0.94 |
| 1:P:472:THR:HG22 | 1:P:498:GLU:CA | 1.96 | 0.94 |
| 1:W:472:THR:HG22 | 1:W:498:GLU:CA | 1.96 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:472:THR:HG22 | 1:E:498:GLU:CA | 1.96 | 0.94 |
| 1:D:12:PHE:CZ | 1:F:242:HIS:HE1 | 1.84 | 0.94 |
| 1:N:472:THR:HG22 | 1:N:498:GLU:CA | 1.96 | 0.94 |
| 1:I:472:THR:HG22 | 1:I:498:GLU:CA | 1.96 | 0.94 |
| 1:M:472:THR:HG22 | 1:M:498:GLU:CA | 1.96 | 0.94 |
| 1:T:472:THR:HG22 | 1:T:498:GLU:CA | 1.96 | 0.94 |
| 1:F:188:ALA:HB1 | 1:F:218:GLN:CG | 1.98 | 0.94 |
| 1:H:6:ASN:OD1 | 1:J:279:LYS:HE3 | 1.64 | 0.94 |
| 1:S:372:ILE:CG1 | 1:T:390:GLU:CA | 2.44 | 0.94 |
| 1:D:12:PHE:CE2 | 1:F:242:HIS:CE1 | 2.55 | 0.94 |
| 1:U:188:ALA:HB1 | 1:U:218:GLN:CG | 1.98 | 0.94 |
| 1:D:188:ALA:HB1 | 1:D:218:GLN:CG | 1.98 | 0.93 |
| 1:Q:390:GLU:HA | 1:R:372:ILE:HG13 | 1.45 | 0.93 |
| 1:W:372:ILE:HG13 | 1:X:390:GLU:CA | 1.98 | 0.93 |
| 1:N:188:ALA:HB1 | 1:N:218:GLN:CG | 1.98 | 0.93 |
| 1:E:242:HIS:CE1 | 1:G:12:PHE:CE2 | 2.56 | 0.93 |
| 1:N:424:ARG:HG2 | 1:N:424:ARG:NH1 | 1.55 | 0.93 |
| 1:P:487:GLY:HA3 | 1:V:229:LYS:HG3 | 1.51 | 0.93 |
| 1:R:276:VAL:HG12 | 1:R:280:ILE:HD11 | 1.50 | 0.93 |
| 1:U:373:PRO:HB3 | 1:V:391:THR:HA | 1.51 | 0.93 |
| 1:B:12:PHE:CE2 | 1:C:242:HIS:CE1 | 2.56 | 0.93 |
| 1:D:392:LYS:HD2 | 1:E:373:PRO:HD3 | 1.51 | 0.93 |
| 1:J:472:THR:HG22 | 1:J:498:GLU:CA | 1.96 | 0.93 |
| 1:R:370:GLN:HB3 | 1:R:374:MET:SD | 2.08 | 0.93 |
| 1:E:242:HIS:HE1 | 1:G:12:PHE:CE2 | 1.86 | 0.93 |
| 1:I:487:GLY:HA2 | 1:M:229:LYS:HG3 | 0.93 | 0.93 |
| 1:W:188:ALA:HB1 | 1:W:218:GLN:CG | 1.98 | 0.93 |
| 1:I:188:ALA:HB1 | 1:I:218:GLN:CG | 1.98 | 0.93 |
| 1:O:11:ILE:HB | 1:P:273:LYS:CG | 1.99 | 0.93 |
| 1:O:6:ASN:OD1 | 1:P:279:LYS:HE3 | 1.68 | 0.93 |
| 1:G:188:ALA:HB1 | 1:G:218:GLN:CG | 1.98 | 0.93 |
| 1:M:188:ALA:HB1 | 1:M:218:GLN:CG | 1.98 | 0.93 |
| 1:L:283:SER:OG | 1:N:3:LEU:HD23 | 1.67 | 0.93 |
| 1:R:272:GLU:HG3 | 1:T:352:GLU:CB | 1.98 | 0.93 |
| 1:B:188:ALA:HB1 | 1:B:218:GLN:CG | 1.98 | 0.93 |
| 1:H:473:GLY:HA3 | 1:M:191:ALA:HB1 | 1.51 | 0.93 |
| 1:K:373:PRO:HB3 | 1:L:391:THR:HA | 1.50 | 0.93 |
| 1:Q:269:ILE:HG12 | 1:S:11:ILE:HD12 | 1.51 | 0.93 |
| 1:R:188:ALA:HB1 | 1:R:218:GLN:CG | 1.98 | 0.93 |
| 1:K:188:ALA:HB1 | 1:K:218:GLN:CG | 1.98 | 0.92 |
| 1:V:276:VAL:HG12 | 1:V:280:ILE:CD1 | 1.99 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:188:ALA:HB1 | 1:A:218:GLN:CG | 1.98 | 0.92 |
| 1:O:188:ALA:HB1 | 1:O:218:GLN:CG | 1.98 | 0.92 |
| 1:P:188:ALA:HB1 | 1:P:218:GLN:CG | 1.98 | 0.92 |
| 1:D:12:PHE:CE2 | 1:F:242:HIS:HE1 | 1.88 | 0.92 |
| 1:H:242:HIS:CE1 | 1:J:12:PHE:CZ | 2.55 | 0.92 |
| 1:J:188:ALA:HB1 | 1:J:218:GLN:CG | 1.98 | 0.92 |
| 1:R:272:GLU:CG | 1:T:352:GLU:CG | 2.46 | 0.92 |
| 1:L:280:ILE:HG12 | 1:N:6:ASN:O | 1.69 | 0.92 |
| 1:L:487:GLY:CA | 1:S:229:LYS:HG3 | 1.99 | 0.92 |
| 1:H:188:ALA:HB1 | 1:H:218:GLN:CG | 1.98 | 0.92 |
| 1:Q:188:ALA:HB1 | 1:Q:218:GLN:CG | 1.98 | 0.91 |
| 1:F:373:PRO:HB3 | 1:G:391:THR:HA | 1.52 | 0.91 |
| 1:V:283:SER:CB | 1:X:3:LEU:HG | 2.00 | 0.91 |
| 1:K:188:ALA:HB2 | 1:K:218:GLN:HG3 | 0.91 | 0.91 |
| 1:L:188:ALA:HB2 | 1:L:218:GLN:HG3 | 0.91 | 0.91 |
| 1:M:188:ALA:HB2 | 1:M:218:GLN:HG3 | 0.91 | 0.91 |
| 1:L:242:HIS:CE1 | 1:N:12:PHE:HE2 | 1.81 | 0.91 |
| 1:X:188:ALA:HB2 | 1:X:218:GLN:HG3 | 0.91 | 0.91 |
| 1:C:188:ALA:HB1 | 1:C:218:GLN:CG | 1.98 | 0.91 |
| 1:I:188:ALA:HB2 | 1:I:218:GLN:HG3 | 0.91 | 0.91 |
| 1:L:188:ALA:HB1 | 1:L:218:GLN:CG | 1.98 | 0.91 |
| 1:U:6:ASN:OD1 | 1:W:279:LYS:HE3 | 1.69 | 0.91 |
| 1:D:188:ALA:HB2 | 1:D:218:GLN:HG3 | 0.91 | 0.91 |
| 1:A:242:HIS:CE1 | 1:I:12:PHE:CE2 | 2.59 | 0.91 |
| 1:K:312:GLU:HA | 1:M:311:ALA:HB1 | 1.53 | 0.91 |
| 1:N:371:HIS:O | 1:N:374:MET:HG2 | 1.71 | 0.91 |
| 1:O:424:ARG:HG2 | 1:O:424:ARG:NH1 | 1.55 | 0.91 |
| 1:S:372:ILE:CD1 | 1:T:390:GLU:HG2 | 2.00 | 0.91 |
| 1:M:390:GLU:O | 1:N:373:PRO:HA | 1.69 | 0.91 |
| 1:C:216:ALA:HB2 | 1:N:446:LYS:HD3 | 1.52 | 0.91 |
| 1:E:188:ALA:HB1 | 1:E:218:GLN:CG | 1.98 | 0.91 |
| 1:O:371:HIS:O | 1:O:374:MET:HG2 | 1.71 | 0.91 |
| 1:P:487:GLY:CA | 1:V:229:LYS:HG3 | 2.00 | 0.91 |
| 1:S:188:ALA:HB1 | 1:S:218:GLN:CG | 1.98 | 0.91 |
| 1:X:188:ALA:HB1 | 1:X:218:GLN:CG | 1.98 | 0.91 |
| 1:K:242:HIS:HE1 | 1:M:12:PHE:CE2 | 1.89 | 0.90 |
| 1:T:188:ALA:HB1 | 1:T:218:GLN:CG | 1.98 | 0.90 |
| 1:S:372:ILE:HG13 | 1:T:390:GLU:C | 1.91 | 0.90 |
| 1:G:371:HIS:O | 1:G:374:MET:HG2 | 1.71 | 0.90 |
| 1:A:188:ALA:HB2 | 1:A:218:GLN:HG3 | 0.91 | 0.90 |
| 1:A:371:HIS:O | 1:A:374:MET:HG2 | 1.71 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:188:ALA:HB2 | 1:G:218:GLN:HG3 | 0.91 | 0.90 |
| 1:H:188:ALA:HB2 | 1:H:218:GLN:HG3 | 0.91 | 0.90 |
| 1:R:272:GLU:HG2 | 1:T:352:GLU:HG2 | 1.53 | 0.90 |
| 1:R:273:LYS:HD3 | 1:T:11:ILE:O | 1.69 | 0.90 |
| 1:P:195:VAL:CG2 | 1:U:496:LEU:HG | 2.01 | 0.90 |
| 1:I:370:GLN:HB3 | 1:I:374:MET:SD | 2.11 | 0.90 |
| 1:V:297:GLN:HE21 | 1:V:300:GLU:HB2 | 1.34 | 0.90 |
| 1:R:296:THR:HG22 | 1:R:297:GLN:HG2 | 1.54 | 0.90 |
| 1:S:372:ILE:HG23 | 1:T:390:GLU:O | 1.70 | 0.90 |
| 1:U:188:ALA:HB2 | 1:U:218:GLN:HG3 | 0.91 | 0.90 |
| 1:V:188:ALA:HB1 | 1:V:218:GLN:CG | 1.98 | 0.90 |
| 1:P:487:GLY:CA | 1:V:229:LYS:CD | 2.50 | 0.90 |
| 1:I:229:LYS:CG | 1:M:487:GLY:HA2 | 2.02 | 0.90 |
| 1:E:371:HIS:O | 1:E:374:MET:HG2 | 1.71 | 0.90 |
| 1:K:371:HIS:O | 1:K:374:MET:HG2 | 1.71 | 0.90 |
| 1:Q:188:ALA:HB2 | 1:Q:218:GLN:HG3 | 0.91 | 0.90 |
| 1:R:297:GLN:HG3 | 1:T:310:ARG:CG | 2.02 | 0.90 |
| 1:V:188:ALA:HB2 | 1:V:218:GLN:HG3 | 0.91 | 0.90 |
| 1:B:371:HIS:O | 1:B:374:MET:HG2 | 1.71 | 0.90 |
| 1:C:371:HIS:O | 1:C:374:MET:HG2 | 1.71 | 0.90 |
| 1:H:312:GLU:CA | 1:J:311:ALA:HB1 | 2.00 | 0.90 |
| 1:U:263:GLY:HA2 | 1:W:310:ARG:HH11 | 1.34 | 0.90 |
| 1:R:276:VAL:CG1 | 1:T:9:LEU:HB3 | 2.02 | 0.89 |
| 1:T:188:ALA:HB2 | 1:T:218:GLN:HG3 | 0.91 | 0.89 |
| 1:F:188:ALA:HB2 | 1:F:218:GLN:HG3 | 0.91 | 0.89 |
| 1:D:11:ILE:HB | 1:F:273:LYS:HG2 | 1.52 | 0.89 |
| 1:W:373:PRO:HA | 1:X:390:GLU:O | 1.72 | 0.89 |
| 1:K:12:PHE:HZ | 1:M:242:HIS:HE1 | 1.20 | 0.89 |
| 1:P:144:ASP:O | 1:P:145:ASP:HB2 | 1.73 | 0.89 |
| 1:O:11:ILE:CB | 1:P:273:LYS:HG2 | 2.03 | 0.89 |
| 1:S:144:ASP:O | 1:S:145:ASP:HB2 | 1.73 | 0.89 |
| 1:R:284:LYS:CG | 1:T:7:LEU:HD22 | 2.01 | 0.89 |
| 1:U:312:GLU:HA | 1:W:311:ALA:CB | 2.01 | 0.89 |
| 1:E:144:ASP:O | 1:E:145:ASP:HB2 | 1.72 | 0.89 |
| 1:F:144:ASP:O | 1:F:145:ASP:HB2 | 1.72 | 0.89 |
| 1:G:144:ASP:O | 1:G:145:ASP:HB2 | 1.72 | 0.89 |
| 1:N:144:ASP:O | 1:N:145:ASP:HB2 | 1.72 | 0.89 |
| 1:C:216:ALA:HB1 | 1:N:446:LYS:HE2 | 1.54 | 0.89 |
| 1:L:487:GLY:HA2 | 1:S:229:LYS:HE3 | 1.53 | 0.89 |
| 1:S:188:ALA:HB2 | 1:S:218:GLN:HG3 | 0.91 | 0.89 |
| 1:W:144:ASP:O | 1:W:145:ASP:HB2 | 1.72 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:188:ALA:HB2 | 1:B:218:GLN:HG3 | 0.91 | 0.89 |
| 1:V:371:HIS:O | 1:V:374:MET:HG2 | 1.71 | 0.89 |
| 1:J:188:ALA:HB2 | 1:J:218:GLN:HG3 | 0.91 | 0.89 |
| 1:P:188:ALA:HB2 | 1:P:218:GLN:HG3 | 0.91 | 0.89 |
| 1:Q:144:ASP:O | 1:Q:145:ASP:HB2 | 1.72 | 0.89 |
| 1:W:188:ALA:HB2 | 1:W:218:GLN:HG3 | 0.91 | 0.89 |
| 1:X:371:HIS:O | 1:X:374:MET:HG2 | 1.71 | 0.89 |
| 1:K:144:ASP:O | 1:K:145:ASP:HB2 | 1.72 | 0.89 |
| 1:L:242:HIS:HE1 | 1:N:12:PHE:CZ | 1.90 | 0.89 |
| 1:O:144:ASP:O | 1:O:145:ASP:HB2 | 1.72 | 0.89 |
| 1:Q:371:HIS:O | 1:Q:374:MET:HG2 | 1.71 | 0.89 |
| 1:V:284:LYS:CG | 1:X:7:LEU:HD22 | 2.01 | 0.89 |
| 1:D:144:ASP:O | 1:D:145:ASP:HB2 | 1.72 | 0.88 |
| 1:W:371:HIS:O | 1:W:374:MET:HG2 | 1.71 | 0.88 |
| 1:E:188:ALA:HB2 | 1:E:218:GLN:HG3 | 0.91 | 0.88 |
| 1:R:188:ALA:HB2 | 1:R:218:GLN:HG3 | 0.91 | 0.88 |
| 1:Q:280:ILE:HG12 | 1:S:6:ASN:O | 1.71 | 0.88 |
| 1:U:272:GLU:O | 1:W:352:GLU:HG2 | 1.72 | 0.88 |
| 1:J:371:HIS:O | 1:J:374:MET:HG2 | 1.71 | 0.88 |
| 1:R:297:GLN:HB2 | 1:T:310:ARG:HB2 | 1.53 | 0.88 |
| 1:N:188:ALA:HB2 | 1:N:218:GLN:HG3 | 0.91 | 0.88 |
| 1:T:144:ASP:O | 1:T:145:ASP:HB2 | 1.72 | 0.88 |
| 1:P:229:LYS:CG | 1:V:487:GLY:HA2 | 2.03 | 0.88 |
| 1:B:144:ASP:O | 1:B:145:ASP:HB2 | 1.72 | 0.88 |
| 1:H:383:SER:HB2 | 1:I:383:SER:HB2 | 1.54 | 0.88 |
| 1:H:11:ILE:HB | 1:J:273:LYS:HG2 | 1.53 | 0.88 |
| 1:X:144:ASP:O | 1:X:145:ASP:HB2 | 1.73 | 0.88 |
| 1:F:371:HIS:O | 1:F:374:MET:HG2 | 1.71 | 0.88 |
| 1:F:373:PRO:CA | 1:G:390:GLU:O | 2.20 | 0.88 |
| 1:U:144:ASP:O | 1:U:145:ASP:HB2 | 1.72 | 0.88 |
| 1:C:144:ASP:O | 1:C:145:ASP:HB2 | 1.72 | 0.88 |
| 1:D:371:HIS:O | 1:D:374:MET:HG2 | 1.71 | 0.88 |
| 1:J:144:ASP:O | 1:J:145:ASP:HB2 | 1.72 | 0.88 |
| 1:C:390:GLU:CA | 1:P:372:ILE:HG13 | 2.04 | 0.87 |
| 1:D:297:GLN:OE1 | 1:F:310:ARG:HG2 | 1.75 | 0.87 |
| 1:V:297:GLN:HE21 | 1:V:300:GLU:CG | 1.87 | 0.87 |
| 1:B:272:GLU:HG3 | 1:C:352:GLU:HB2 | 1.55 | 0.87 |
| 1:H:144:ASP:O | 1:H:145:ASP:HB2 | 1.72 | 0.87 |
| 1:L:144:ASP:O | 1:L:145:ASP:HB2 | 1.72 | 0.87 |
| 1:Q:242:HIS:HE1 | 1:S:12:PHE:CE2 | 1.87 | 0.87 |
| 1:H:188:ALA:HB1 | 1:H:218:GLN:HG2 | 1.56 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:C:496:LEU:HG | 1:V:195:VAL:CG2 | 2.05 | 0.87 |
| 1:I:404:ARG:NH2 | 1:M:228:PRO:HG2 | 1.89 | 0.87 |
| 1:L:229:LYS:HG3 | 1:S:487:GLY:CA | 2.05 | 0.87 |
| 1:V:144:ASP:O | 1:V:145:ASP:HB2 | 1.72 | 0.87 |
| 1:B:312:GLU:HA | 1:C:311:ALA:HB1 | 1.56 | 0.87 |
| 1:C:188:ALA:HB2 | 1:C:218:GLN:HG3 | 0.91 | 0.87 |
| 1:G:188:ALA:HB1 | 1:G:218:GLN:HG2 | 1.56 | 0.87 |
| 1:O:188:ALA:HB2 | 1:O:218:GLN:HG3 | 0.91 | 0.87 |
| 1:R:188:ALA:HB1 | 1:R:218:GLN:HG2 | 1.56 | 0.87 |
| 1:R:272:GLU:HG3 | 1:T:352:GLU:CG | 2.05 | 0.87 |
| 1:T:3:LEU:CD2 | 1:T:3:LEU:C | 2.42 | 0.87 |
| 1:W:372:ILE:HG23 | 1:X:390:GLU:O | 1.75 | 0.87 |
| 1:L:269:ILE:HG12 | 1:N:11:ILE:HD12 | 1.57 | 0.87 |
| 1:M:144:ASP:O | 1:M:145:ASP:HB2 | 1.72 | 0.87 |
| 1:J:188:ALA:HB1 | 1:J:218:GLN:HG2 | 1.56 | 0.86 |
| 1:R:144:ASP:O | 1:R:145:ASP:HB2 | 1.72 | 0.86 |
| 1:F:188:ALA:HB1 | 1:F:218:GLN:HG2 | 1.56 | 0.86 |
| 1:I:144:ASP:O | 1:I:145:ASP:HB2 | 1.72 | 0.86 |
| 1:M:188:ALA:HB1 | 1:M:218:GLN:HG2 | 1.56 | 0.86 |
| 1:T:188:ALA:HB1 | 1:T:218:GLN:HG2 | 1.57 | 0.86 |
| 1:U:390:GLU:O | 1:V:373:PRO:CB | 2.22 | 0.86 |
| 1:K:311:ALA:HB1 | 1:M:312:GLU:HA | 1.57 | 0.86 |
| 1:A:144:ASP:O | 1:A:145:ASP:HB2 | 1.72 | 0.86 |
| 1:S:390:GLU:OE1 | 1:T:379:ALA:CB | 2.23 | 0.86 |
| 1:U:11:ILE:CA | 1:W:273:LYS:HG2 | 2.05 | 0.86 |
| 1:U:188:ALA:HB1 | 1:U:218:GLN:HG2 | 1.56 | 0.86 |
| 1:D:188:ALA:HB1 | 1:D:218:GLN:HG2 | 1.57 | 0.86 |
| 1:H:310:ARG:HB2 | 1:J:297:GLN:HB2 | 1.58 | 0.86 |
| 1:K:188:ALA:HB1 | 1:K:218:GLN:HG2 | 1.56 | 0.86 |
| 1:Q:188:ALA:HB1 | 1:Q:218:GLN:HG2 | 1.56 | 0.86 |
| 1:U:12:PHE:CZ | 1:W:242:HIS:HE1 | 1.93 | 0.86 |
| 1:L:188:ALA:HB1 | 1:L:218:GLN:HG2 | 1.56 | 0.86 |
| 1:O:310:ARG:HG2 | 1:P:297:GLN:OE1 | 1.75 | 0.86 |
| 1:P:188:ALA:HB1 | 1:P:218:GLN:HG2 | 1.56 | 0.86 |
| 1:R:279:LYS:HB3 | 1:T:6:ASN:CG | 1.96 | 0.86 |
| 1:E:11:ILE:CG1 | 1:E:12:PHE:CE2 | 2.60 | 0.85 |
| 1:H:11:ILE:O | 1:J:273:LYS:CD | 2.24 | 0.85 |
| 1:N:188:ALA:HB1 | 1:N:218:GLN:HG2 | 1.56 | 0.85 |
| 1:H:12:PHE:CE2 | 1:J:242:HIS:CE1 | 2.59 | 0.85 |
| 1:H:370:GLN:HB3 | 1:H:374:MET:SD | 2.16 | 0.85 |
| 1:V:424:ARG:HH11 | 1:V:424:ARG:HG2 | 0.74 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:188:ALA:HB1 | 1:A:218:GLN:HG2 | 1.56 | 0.85 |
| 1:E:242:HIS:CE1 | 1:G:12:PHE:CZ | 2.64 | 0.85 |
| 1:H:272:GLU:O | 1:J:352:GLU:HG2 | 1.76 | 0.85 |
| 1:U:310:ARG:HG2 | 1:W:297:GLN:OE1 | 1.77 | 0.85 |
| 1:C:188:ALA:HB1 | 1:C:218:GLN:HG2 | 1.56 | 0.85 |
| 1:M:383:SER:HB2 | 1:N:383:SER:HB2 | 1.59 | 0.85 |
| 1:M:424:ARG:HH11 | 1:M:424:ARG:HG2 | 0.74 | 0.85 |
| 1:O:242:HIS:HE1 | 1:P:12:PHE:CZ | 1.94 | 0.85 |
| 1:O:188:ALA:HB1 | 1:O:218:GLN:HG2 | 1.56 | 0.85 |
| 1:K:496:LEU:CG | 1:S:195:VAL:HG22 | 2.06 | 0.85 |
| 1:X:188:ALA:HB1 | 1:X:218:GLN:HG2 | 1.56 | 0.85 |
| 1:H:352:GLU:HG2 | 1:J:272:GLU:O | 1.77 | 0.85 |
| 1:I:11:ILE:CG1 | 1:I:12:PHE:CE2 | 2.60 | 0.85 |
| 1:I:188:ALA:HB1 | 1:I:218:GLN:HG2 | 1.56 | 0.85 |
| 1:I:11:ILE:HD11 | 1:I:12:PHE:CE2 | 2.12 | 0.85 |
| 1:L:11:ILE:CG1 | 1:L:12:PHE:CE2 | 2.59 | 0.85 |
| 1:U:372:ILE:CG1 | 1:V:390:GLU:HA | 2.04 | 0.85 |
| 1:U:11:ILE:O | 1:W:273:LYS:CE | 2.25 | 0.85 |
| 1:B:188:ALA:HB1 | 1:B:218:GLN:HG2 | 1.56 | 0.84 |
| 1:E:188:ALA:HB1 | 1:E:218:GLN:HG2 | 1.56 | 0.84 |
| 1:R:11:ILE:CG1 | 1:R:12:PHE:CE2 | 2.59 | 0.84 |
| 1:Q:272:GLU:HG3 | 1:S:352:GLU:HB2 | 1.59 | 0.84 |
| 1:V:11:ILE:HD11 | 1:V:12:PHE:CE2 | 2.12 | 0.84 |
| 1:L:11:ILE:HG13 | 1:L:12:PHE:CD2 | 2.12 | 0.84 |
| 1:V:188:ALA:HB1 | 1:V:218:GLN:HG2 | 1.56 | 0.84 |
| 1:S:483:HIS:CD2 | 1:T:483:HIS:NE2 | 2.44 | 0.84 |
| 1:I:11:ILE:HG13 | 1:I:12:PHE:CD2 | 2.13 | 0.84 |
| 1:K:390:GLU:HA | 1:L:372:ILE:HG13 | 1.60 | 0.84 |
| 1:O:12:PHE:CZ | 1:P:242:HIS:CE1 | 2.64 | 0.84 |
| 1:S:483:HIS:NE2 | 1:T:483:HIS:CD2 | 2.44 | 0.84 |
| 1:R:11:ILE:HD11 | 1:R:12:PHE:CE2 | 2.12 | 0.84 |
| 1:S:483:HIS:NE2 | 1:T:483:HIS:HD2 | 1.75 | 0.84 |
| 1:L:11:ILE:HD11 | 1:L:12:PHE:CE2 | 2.12 | 0.84 |
| 1:L:297:GLN:HB2 | 1:N:310:ARG:HG3 | 1.59 | 0.84 |
| 1:S:188:ALA:HB1 | 1:S:218:GLN:HG2 | 1.57 | 0.84 |
| 1:V:11:ILE:CG1 | 1:V:12:PHE:CE2 | 2.60 | 0.84 |
| 1:E:11:ILE:HD11 | 1:E:12:PHE:CE2 | 2.12 | 0.84 |
| 1:R:11:ILE:HG13 | 1:R:12:PHE:CD2 | 2.12 | 0.84 |
| 1:E:424:ARG:HG2 | 1:E:424:ARG:HH11 | 0.74 | 0.84 |
| 1:K:297:GLN:OE1 | 1:M:310:ARG:HG2 | 1.77 | 0.84 |
| 1:W:188:ALA:HB1 | 1:W:218:GLN:HG2 | 1.56 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:U:310:ARG:HG2 | 1:W:297:GLN:HB2 | 1.59 | 0.84 |
| 1:W:373:PRO:HB3 | 1:X:391:THR:CA | 2.07 | 0.84 |
| 1:R:272:GLU:CB | 1:T:352:GLU:HG2 | 2.08 | 0.83 |
| 1:U:297:GLN:HB2 | 1:W:310:ARG:CG | 2.08 | 0.83 |
| 1:E:11:ILE:HG13 | 1:E:12:PHE:CD2 | 2.12 | 0.83 |
| 1:H:10:SER:HB3 | 1:H:13:ASP:OD1 | 1.78 | 0.83 |
| 1:S:10:SER:HB3 | 1:S:13:ASP:OD1 | 1.79 | 0.83 |
| 1:I:229:LYS:CG | 1:M:487:GLY:CA | 2.56 | 0.83 |
| 1:L:11:ILE:HD11 | 1:L:12:PHE:HE2 | 1.44 | 0.83 |
| 1:R:10:SER:HB3 | 1:R:13:ASP:OD1 | 1.79 | 0.83 |
| 1:T:10:SER:HB3 | 1:T:13:ASP:OD1 | 1.78 | 0.83 |
| 1:V:11:ILE:HG13 | 1:V:12:PHE:CD2 | 2.12 | 0.83 |
| 1:B:279:LYS:HE3 | 1:C:6:ASN:OD1 | 1.78 | 0.83 |
| 1:L:10:SER:HB3 | 1:L:13:ASP:OD1 | 1.78 | 0.83 |
| 1:H:496:LEU:CD2 | 1:M:195:VAL:CG2 | 2.56 | 0.83 |
| 1:G:10:SER:HB3 | 1:G:13:ASP:OD1 | 1.79 | 0.83 |
| 1:M:10:SER:HB3 | 1:M:13:ASP:OD1 | 1.79 | 0.83 |
| 1:C:254:GLU:HG2 | 1:N:446:LYS:HE2 | 1.60 | 0.83 |
| 1:O:10:SER:HB3 | 1:O:13:ASP:OD1 | 1.78 | 0.83 |
| 1:R:11:ILE:HD11 | 1:R:12:PHE:HE2 | 1.43 | 0.83 |
| 1:V:272:GLU:CG | 1:X:352:GLU:HG2 | 2.09 | 0.83 |
| 1:E:279:LYS:HE3 | 1:G:6:ASN:OD1 | 1.76 | 0.83 |
| 1:I:11:ILE:HD11 | 1:I:12:PHE:HE2 | 1.44 | 0.83 |
| 1:A:242:HIS:NE2 | 1:I:12:PHE:CZ | 2.47 | 0.83 |
| 1:H:315:ASP:HB2 | 1:J:311:ALA:HA | 1.61 | 0.83 |
| 1:M:390:GLU:O | 1:N:373:PRO:CB | 2.27 | 0.83 |
| 1:A:10:SER:HB3 | 1:A:13:ASP:OD1 | 1.78 | 0.83 |
| 1:V:10:SER:HB3 | 1:V:13:ASP:OD1 | 1.79 | 0.83 |
| 1:F:10:SER:HB3 | 1:F:13:ASP:OD1 | 1.79 | 0.83 |
| 1:N:10:SER:HB3 | 1:N:13:ASP:OD1 | 1.79 | 0.83 |
| 1:M:390:GLU:O | 1:N:373:PRO:CA | 2.26 | 0.83 |
| 1:U:10:SER:HB3 | 1:U:13:ASP:OD1 | 1.78 | 0.83 |
| 1:V:3:LEU:HD23 | 1:X:283:SER:HB3 | 1.61 | 0.83 |
| 1:I:10:SER:HB3 | 1:I:13:ASP:OD1 | 1.79 | 0.83 |
| 1:J:10:SER:HB3 | 1:J:13:ASP:OD1 | 1.79 | 0.83 |
| 1:K:424:ARG:HH11 | 1:K:424:ARG:HG2 | 0.74 | 0.83 |
| 1:L:280:ILE:CG1 | 1:N:6:ASN:O | 2.26 | 0.83 |
| 1:R:280:ILE:HD11 | 1:T:9:LEU:HB2 | 1.59 | 0.82 |
| 1:V:7:LEU:CD2 | 1:X:284:LYS:HG3 | 2.08 | 0.82 |
| 1:E:10:SER:HB3 | 1:E:13:ASP:OD1 | 1.79 | 0.82 |
| 1:H:310:ARG:CG | 1:J:297:GLN:CG | 2.57 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:3:LEU:HD21 | 1:I:283:SER:HB3 | 1.61 | 0.82 |
| 1:K:12:PHE:HZ | 1:M:242:HIS:CE1 | 1.91 | 0.82 |
| 1:I:229:LYS:CD | 1:M:487:GLY:CA | 2.57 | 0.82 |
| 1:C:10:SER:HB3 | 1:C:13:ASP:OD1 | 1.78 | 0.82 |
| 1:F:390:GLU:O | 1:G:373:PRO:CA | 2.26 | 0.82 |
| 1:V:284:LYS:CG | 1:X:7:LEU:HD21 | 2.07 | 0.82 |
| 1:B:10:SER:HB3 | 1:B:13:ASP:OD1 | 1.79 | 0.82 |
| 1:F:373:PRO:CB | 1:G:391:THR:HA | 2.09 | 0.82 |
| 1:A:453:LYS:NZ | 2:A:700:FDP:O1P | 2.12 | 0.82 |
| 1:C:453:LYS:NZ | 2:C:700:FDP:O1P | 2.12 | 0.82 |
| 1:O:424:ARG:HG2 | 1:O:424:ARG:HH11 | 0.74 | 0.82 |
| 1:D:10:SER:HB3 | 1:D:13:ASP:OD1 | 1.79 | 0.82 |
| 1:H:11:ILE:CA | 1:J:273:LYS:HG2 | 2.08 | 0.82 |
| 1:Q:310:ARG:HG2 | 1:S:297:GLN:OE1 | 1.80 | 0.82 |
| 1:C:496:LEU:CG | 1:V:195:VAL:HG22 | 2.10 | 0.82 |
| 1:F:453:LYS:NZ | 2:F:700:FDP:O1P | 2.13 | 0.82 |
| 1:I:424:ARG:HH11 | 1:I:424:ARG:HG2 | 0.74 | 0.82 |
| 1:V:11:ILE:HD11 | 1:V:12:PHE:HE2 | 1.44 | 0.82 |
| 1:W:10:SER:HB3 | 1:W:13:ASP:OD1 | 1.79 | 0.82 |
| 1:A:424:ARG:HG2 | 1:A:424:ARG:HH11 | 0.74 | 0.82 |
| 1:Q:283:SER:CB | 1:S:3:LEU:CD2 | 2.57 | 0.82 |
| 1:Q:283:SER:CB | 1:S:3:LEU:HD23 | 2.09 | 0.82 |
| 1:X:10:SER:HB3 | 1:X:13:ASP:OD1 | 1.78 | 0.82 |
| 1:B:453:LYS:NZ | 2:B:700:FDP:O1P | 2.13 | 0.81 |
| 1:E:453:LYS:NZ | 2:E:700:FDP:O1P | 2.13 | 0.81 |
| 1:K:10:SER:HB3 | 1:K:13:ASP:OD1 | 1.79 | 0.81 |
| 1:L:11:ILE:O | 1:N:273:LYS:HE3 | 1.79 | 0.81 |
| 1:P:487:GLY:HA2 | 1:V:229:LYS:CG | 2.09 | 0.81 |
| 1:R:424:ARG:HH11 | 1:R:424:ARG:HG2 | 0.74 | 0.81 |
| 1:D:453:LYS:NZ | 2:D:700:FDP:O1P | 2.13 | 0.81 |
| 1:J:453:LYS:NZ | 2:J:700:FDP:O1P | 2.13 | 0.81 |
| 1:H:496:LEU:CG | 1:M:195:VAL:CG2 | 2.52 | 0.81 |
| 1:N:453:LYS:NZ | 2:N:700:FDP:O1P | 2.13 | 0.81 |
| 1:Q:10:SER:HB3 | 1:Q:13:ASP:OD1 | 1.78 | 0.81 |
| 1:L:487:GLY:HA2 | 1:S:229:LYS:HG3 | 1.59 | 0.81 |
| 1:Q:453:LYS:NZ | 2:Q:700:FDP:O1P | 2.13 | 0.81 |
| 1:C:424:ARG:HH11 | 1:C:424:ARG:HG2 | 0.74 | 0.81 |
| 1:D:12:PHE:HE2 | 1:F:242:HIS:CE1 | 1.95 | 0.81 |
| 1:E:11:ILE:HD11 | 1:E:12:PHE:HE2 | 1.44 | 0.81 |
| 1:N:446:LYS:O | 1:N:446:LYS:HD2 | 1.81 | 0.81 |
| 1:S:453:LYS:NZ | 2:S:700:FDP:O1P | 2.13 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:10:SER:HB3 | 1:P:13:ASP:OD1 | 1.79 | 0.81 |
| 1:F:373:PRO:HB3 | 1:G:391:THR:CA | 2.11 | 0.81 |
| 1:V:280:ILE:CG1 | 1:X:6:ASN:O | 2.29 | 0.81 |
| 1:L:311:ALA:HB1 | 1:N:312:GLU:HA | 1.63 | 0.81 |
| 1:V:12:PHE:CE2 | 1:X:242:HIS:CE1 | 2.69 | 0.81 |
| 1:D:12:PHE:CZ | 1:F:242:HIS:CE1 | 2.69 | 0.81 |
| 1:L:229:LYS:HE3 | 1:S:487:GLY:HA2 | 1.61 | 0.81 |
| 1:L:487:GLY:HA2 | 1:S:229:LYS:CE | 2.09 | 0.81 |
| 1:M:370:GLN:HB3 | 1:M:374:MET:SD | 2.20 | 0.81 |
| 1:K:496:LEU:HG | 1:S:195:VAL:CG2 | 2.10 | 0.81 |
| 1:S:483:HIS:CD2 | 1:T:483:HIS:CD2 | 2.69 | 0.81 |
| 1:T:424:ARG:HG2 | 1:T:424:ARG:HH11 | 0.74 | 0.81 |
| 1:W:390:GLU:OE1 | 1:X:379:ALA:CB | 2.29 | 0.81 |
| 1:I:453:LYS:NZ | 2:I:700:FDP:O1P | 2.13 | 0.81 |
| 1:S:424:ARG:HG2 | 1:S:424:ARG:HH11 | 0.74 | 0.81 |
| 1:U:390:GLU:OE1 | 1:V:379:ALA:CB | 2.29 | 0.81 |
| 1:K:372:ILE:HG13 | 1:L:390:GLU:HA | 1.61 | 0.81 |
| 1:H:11:ILE:HB | 1:J:273:LYS:CG | 2.10 | 0.80 |
| 1:R:453:LYS:NZ | 2:R:700:FDP:O1P | 2.13 | 0.80 |
| 1:I:270:PRO:HG2 | 1:I:273:LYS:CE | 2.11 | 0.80 |
| 1:D:424:ARG:HG2 | 1:D:424:ARG:HH11 | 0.74 | 0.80 |
| 1:G:424:ARG:HG2 | 1:G:424:ARG:HH11 | 0.74 | 0.80 |
| 1:V:283:SER:OG | 1:X:3:LEU:HG | 1.82 | 0.80 |
| 1:E:270:PRO:HG2 | 1:E:273:LYS:CE | 2.11 | 0.80 |
| 1:H:315:ASP:CB | 1:J:311:ALA:HA | 2.12 | 0.80 |
| 1:R:280:ILE:CG1 | 1:T:6:ASN:O | 2.26 | 0.80 |
| 1:U:310:ARG:CG | 1:W:297:GLN:HB2 | 2.11 | 0.80 |
| 1:V:453:LYS:NZ | 2:V:700:FDP:O1P | 2.15 | 0.80 |
| 1:W:453:LYS:NZ | 2:W:700:FDP:O1P | 2.15 | 0.80 |
| 1:B:269:ILE:HG12 | 1:C:11:ILE:HD12 | 1.64 | 0.80 |
| 1:H:390:GLU:O | 1:I:373:PRO:HA | 1.79 | 0.80 |
| 1:R:270:PRO:HG2 | 1:R:273:LYS:CE | 2.11 | 0.80 |
| 1:V:270:PRO:HG2 | 1:V:273:LYS:CE | 2.11 | 0.80 |
| 1:X:424:ARG:HH11 | 1:X:424:ARG:HG2 | 0.74 | 0.80 |
| 1:U:453:LYS:NZ | 2:U:700:FDP:O1P | 2.13 | 0.80 |
| 1:X:453:LYS:NZ | 2:X:700:FDP:O1P | 2.15 | 0.80 |
| 1:H:453:LYS:NZ | 2:H:700:FDP:O1P | 2.15 | 0.79 |
| 1:K:453:LYS:NZ | 2:K:700:FDP:O1P | 2.15 | 0.79 |
| 1:O:453:LYS:NZ | 2:O:700:FDP:O1P | 2.14 | 0.79 |
| 1:N:142:TYR:HB3 | 1:N:146:GLY:HA2 | 1.65 | 0.79 |
| 1:U:242:HIS:NE2 | 1:W:12:PHE:CE2 | 2.49 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:372:ILE:HG13 | 1:O:390:GLU:HA | 1.64 | 0.79 |
| 1:H:11:ILE:O | 1:J:273:LYS:CG | 2.30 | 0.79 |
| 1:L:142:TYR:HB3 | 1:L:146:GLY:HA2 | 1.65 | 0.79 |
| 1:H:496:LEU:HD23 | 1:M:195:VAL:HG22 | 1.64 | 0.79 |
| 1:L:487:GLY:HA2 | 1:S:229:LYS:CG | 2.11 | 0.79 |
| 1:V:276:VAL:CG1 | 1:V:280:ILE:HD11 | 2.11 | 0.79 |
| 1:W:390:GLU:OE1 | 1:X:379:ALA:HB1 | 1.82 | 0.79 |
| 1:H:424:ARG:HH11 | 1:H:424:ARG:HG2 | 0.74 | 0.79 |
| 1:N:446:LYS:O | 1:N:446:LYS:CD | 2.30 | 0.79 |
| 1:O:312:GLU:HA | 1:P:311:ALA:CB | 2.13 | 0.79 |
| 1:P:370:GLN:HB3 | 1:P:374:MET:SD | 2.22 | 0.79 |
| 1:P:453:LYS:NZ | 2:P:700:FDP:O1P | 2.15 | 0.79 |
| 1:G:142:TYR:HB3 | 1:G:146:GLY:HA2 | 1.65 | 0.79 |
| 1:L:312:GLU:HA | 1:N:311:ALA:HB1 | 1.64 | 0.79 |
| 1:T:142:TYR:HB3 | 1:T:146:GLY:HA2 | 1.65 | 0.79 |
| 1:T:453:LYS:NZ | 2:T:700:FDP:O1P | 2.15 | 0.79 |
| 1:V:242:HIS:HE1 | 1:X:12:PHE:CZ | 2.00 | 0.79 |
| 1:P:487:GLY:CA | 1:V:229:LYS:CG | 2.61 | 0.79 |
| 1:Q:280:ILE:HD11 | 1:S:9:LEU:HB2 | 1.65 | 0.79 |
| 1:K:142:TYR:HB3 | 1:K:146:GLY:HA2 | 1.65 | 0.79 |
| 1:Q:142:TYR:HB3 | 1:Q:146:GLY:HA2 | 1.65 | 0.79 |
| 1:H:11:ILE:O | 1:J:273:LYS:HE3 | 1.83 | 0.79 |
| 1:L:12:PHE:CZ | 1:N:242:HIS:CE1 | 2.70 | 0.79 |
| 1:M:453:LYS:NZ | 2:M:700:FDP:O1P | 2.15 | 0.79 |
| 1:R:3:LEU:HD13 | 1:T:369:LEU:HD12 | 1.65 | 0.79 |
| 1:W:142:TYR:HB3 | 1:W:146:GLY:HA2 | 1.65 | 0.79 |
| 1:B:424:ARG:HG2 | 1:B:424:ARG:HH11 | 0.74 | 0.79 |
| 1:L:453:LYS:NZ | 2:L:700:FDP:O1P | 2.15 | 0.79 |
| 1:R:371:HIS:O | 1:R:374:MET:CG | 2.30 | 0.79 |
| 1:V:269:ILE:HG12 | 1:X:11:ILE:HD12 | 1.64 | 0.79 |
| 1:A:142:TYR:HB3 | 1:A:146:GLY:HA2 | 1.65 | 0.78 |
| 1:B:142:TYR:HB3 | 1:B:146:GLY:HA2 | 1.65 | 0.78 |
| 1:H:11:ILE:CB | 1:J:273:LYS:HG2 | 2.13 | 0.78 |
| 1:B:4:ALA:O | 1:B:7:LEU:HB2 | 1.84 | 0.78 |
| 1:H:142:TYR:HB3 | 1:H:146:GLY:HA2 | 1.64 | 0.78 |
| 1:L:270:PRO:HG2 | 1:L:273:LYS:CE | 2.11 | 0.78 |
| 1:C:216:ALA:HB1 | 1:N:446:LYS:CE | 2.13 | 0.78 |
| 1:L:284:LYS:HG3 | 1:N:7:LEU:CD2 | 2.13 | 0.78 |
| 1:S:4:ALA:O | 1:S:7:LEU:HB2 | 1.83 | 0.78 |
| 1:N:424:ARG:HG2 | 1:N:424:ARG:HH11 | 0.74 | 0.78 |
| 1:T:4:ALA:O | 1:T:7:LEU:HB2 | 1.84 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:284:LYS:HG3 | 1:T:7:LEU:HD21 | 1.59 | 0.78 |
| 1:W:373:PRO:CB | 1:X:391:THR:HA | 2.12 | 0.78 |
| 1:D:142:TYR:HB3 | 1:D:146:GLY:HA2 | 1.65 | 0.78 |
| 1:L:370:GLN:HB3 | 1:L:374:MET:SD | 2.22 | 0.78 |
| 1:K:242:HIS:HE1 | 1:M:12:PHE:CZ | 2.01 | 0.78 |
| 1:P:4:ALA:O | 1:P:7:LEU:HB2 | 1.84 | 0.78 |
| 1:W:4:ALA:O | 1:W:7:LEU:HB2 | 1.84 | 0.78 |
| 1:G:453:LYS:NZ | 2:G:700:FDP:O1P | 2.15 | 0.78 |
| 1:I:4:ALA:O | 1:I:7:LEU:HB2 | 1.84 | 0.78 |
| 1:J:142:TYR:HB3 | 1:J:146:GLY:HA2 | 1.65 | 0.78 |
| 1:N:4:ALA:O | 1:N:7:LEU:HB2 | 1.84 | 0.78 |
| 1:R:142:TYR:HB3 | 1:R:146:GLY:HA2 | 1.65 | 0.78 |
| 1:U:142:TYR:HB3 | 1:U:146:GLY:HA2 | 1.65 | 0.78 |
| 1:H:373:PRO:HA | 1:I:390:GLU:O | 1.84 | 0.78 |
| 1:K:4:ALA:O | 1:K:7:LEU:HB2 | 1.84 | 0.78 |
| 1:R:284:LYS:CG | 1:T:7:LEU:CD2 | 2.56 | 0.78 |
| 1:C:223:ARG:HH11 | 1:C:223:ARG:HG2 | 1.49 | 0.78 |
| 1:F:424:ARG:HG2 | 1:F:424:ARG:HH11 | 0.74 | 0.78 |
| 1:L:272:GLU:CG | 1:N:352:GLU:HG2 | 2.13 | 0.78 |
| 1:P:223:ARG:HG2 | 1:P:223:ARG:HH11 | 1.49 | 0.78 |
| 1:Q:283:SER:HB3 | 1:S:3:LEU:HD23 | 1.65 | 0.78 |
| 1:D:4:ALA:O | 1:D:7:LEU:HB2 | 1.83 | 0.78 |
| 1:E:4:ALA:O | 1:E:7:LEU:HB2 | 1.84 | 0.78 |
| 1:H:372:ILE:HG13 | 1:I:390:GLU:CA | 2.14 | 0.78 |
| 1:K:390:GLU:O | 1:L:373:PRO:HA | 1.83 | 0.78 |
| 1:V:7:LEU:CD2 | 1:X:284:LYS:CG | 2.62 | 0.78 |
| 1:B:223:ARG:HH11 | 1:B:223:ARG:HG2 | 1.49 | 0.78 |
| 1:C:4:ALA:O | 1:C:7:LEU:HB2 | 1.84 | 0.78 |
| 1:R:4:ALA:O | 1:R:7:LEU:HB2 | 1.84 | 0.78 |
| 1:W:223:ARG:HG2 | 1:W:223:ARG:HH11 | 1.49 | 0.78 |
| 1:D:223:ARG:HG2 | 1:D:223:ARG:HH11 | 1.49 | 0.78 |
| 1:L:223:ARG:HG2 | 1:L:223:ARG:HH11 | 1.49 | 0.78 |
| 1:L:4:ALA:O | 1:L:7:LEU:HB2 | 1.83 | 0.78 |
| 1:P:142:TYR:HB3 | 1:P:146:GLY:HA2 | 1.65 | 0.78 |
| 1:C:142:TYR:HB3 | 1:C:146:GLY:HA2 | 1.65 | 0.77 |
| 1:F:223:ARG:HH11 | 1:F:223:ARG:HG2 | 1.49 | 0.77 |
| 1:X:4:ALA:O | 1:X:7:LEU:HB2 | 1.84 | 0.77 |
| 1:P:424:ARG:HG2 | 1:P:424:ARG:HH11 | 0.74 | 0.77 |
| 1:A:4:ALA:O | 1:A:7:LEU:HB2 | 1.84 | 0.77 |
| 1:G:4:ALA:O | 1:G:7:LEU:HB2 | 1.83 | 0.77 |
| 1:I:142:TYR:HB3 | 1:I:146:GLY:HA2 | 1.65 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:223:ARG:HG2 | 1:J:223:ARG:HH11 | 1.49 | 0.77 |
| 1:L:487:GLY:HA3 | 1:S:229:LYS:HG3 | 1.64 | 0.77 |
| 1:X:142:TYR:HB3 | 1:X:146:GLY:HA2 | 1.64 | 0.77 |
| 1:J:4:ALA:O | 1:J:7:LEU:HB2 | 1.84 | 0.77 |
| 1:O:4:ALA:O | 1:O:7:LEU:HB2 | 1.84 | 0.77 |
| 1:Q:424:ARG:HG2 | 1:Q:424:ARG:HH11 | 0.74 | 0.77 |
| 1:R:279:LYS:HE3 | 1:T:6:ASN:OD1 | 1.85 | 0.77 |
| 1:V:276:VAL:O | 1:V:280:ILE:HD12 | 1.85 | 0.77 |
| 1:A:223:ARG:HG2 | 1:A:223:ARG:HH11 | 1.49 | 0.77 |
| 1:H:297:GLN:CG | 1:J:310:ARG:HG2 | 2.15 | 0.77 |
| 1:V:142:TYR:HB3 | 1:V:146:GLY:HA2 | 1.65 | 0.77 |
| 1:B:311:ALA:HB1 | 1:C:312:GLU:HA | 1.65 | 0.77 |
| 1:E:142:TYR:HB3 | 1:E:146:GLY:HA2 | 1.65 | 0.77 |
| 1:F:4:ALA:O | 1:F:7:LEU:HB2 | 1.83 | 0.77 |
| 1:Q:223:ARG:HH11 | 1:Q:223:ARG:HG2 | 1.49 | 0.77 |
| 1:S:223:ARG:HG2 | 1:S:223:ARG:HH11 | 1.49 | 0.77 |
| 1:S:370:GLN:HB3 | 1:S:374:MET:SD | 2.25 | 0.77 |
| 1:W:424:ARG:HG2 | 1:W:424:ARG:HH11 | 0.74 | 0.77 |
| 1:D:372:ILE:HG13 | 1:E:390:GLU:HA | 1.67 | 0.77 |
| 1:F:142:TYR:HB3 | 1:F:146:GLY:HA2 | 1.65 | 0.77 |
| 1:H:4:ALA:O | 1:H:7:LEU:HB2 | 1.84 | 0.77 |
| 1:M:4:ALA:O | 1:M:7:LEU:HB2 | 1.84 | 0.77 |
| 1:M:142:TYR:HB3 | 1:M:146:GLY:HA2 | 1.65 | 0.77 |
| 1:O:142:TYR:HB3 | 1:O:146:GLY:HA2 | 1.65 | 0.77 |
| 1:Q:283:SER:OG | 1:S:3:LEU:HD23 | 1.83 | 0.77 |
| 1:Q:284:LYS:HG3 | 1:S:7:LEU:CD2 | 2.15 | 0.77 |
| 1:T:223:ARG:HH11 | 1:T:223:ARG:HG2 | 1.49 | 0.77 |
| 1:U:223:ARG:HG2 | 1:U:223:ARG:HH11 | 1.49 | 0.77 |
| 1:U:4:ALA:O | 1:U:7:LEU:HB2 | 1.84 | 0.77 |
| 1:V:283:SER:HB3 | 1:X:3:LEU:HG | 1.66 | 0.77 |
| 1:G:223:ARG:HG2 | 1:G:223:ARG:HH11 | 1.49 | 0.76 |
| 1:H:223:ARG:HG2 | 1:H:223:ARG:HH11 | 1.49 | 0.76 |
| 1:M:214:ARG:H | 1:M:218:GLN:HE22 | 1.33 | 0.76 |
| 1:Q:4:ALA:O | 1:Q:7:LEU:HB2 | 1.84 | 0.76 |
| 1:S:142:TYR:HB3 | 1:S:146:GLY:HA2 | 1.64 | 0.76 |
| 1:V:12:PHE:CZ | 1:X:242:HIS:CE1 | 2.72 | 0.76 |
| 1:V:283:SER:HB3 | 1:X:3:LEU:CD2 | 2.15 | 0.76 |
| 1:Q:390:GLU:O | 1:R:372:ILE:HG23 | 1.86 | 0.76 |
| 1:V:214:ARG:H | 1:V:218:GLN:HE22 | 1.33 | 0.76 |
| 1:A:392:LYS:CD | 1:J:373:PRO:HD3 | 2.13 | 0.76 |
| 1:K:223:ARG:HH11 | 1:K:223:ARG:HG2 | 1.49 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:269:ILE:HG12 | 1:N:11:ILE:CD1 | 2.15 | 0.76 |
| 1:X:223:ARG:HH11 | 1:X:223:ARG:HG2 | 1.49 | 0.76 |
| 1:K:214:ARG:H | 1:K:218:GLN:HE22 | 1.34 | 0.76 |
| 1:N:223:ARG:HH11 | 1:N:223:ARG:HG2 | 1.49 | 0.76 |
| 1:B:373:PRO:HB3 | 1:O:391:THR:C | 2.06 | 0.76 |
| 1:B:214:ARG:H | 1:B:218:GLN:HE22 | 1.33 | 0.76 |
| 1:I:214:ARG:H | 1:I:218:GLN:HE22 | 1.33 | 0.76 |
| 1:O:223:ARG:HH11 | 1:O:223:ARG:HG2 | 1.49 | 0.76 |
| 1:L:229:LYS:HG3 | 1:S:487:GLY:HA3 | 1.67 | 0.76 |
| 1:I:223:ARG:HG2 | 1:I:223:ARG:HH11 | 1.49 | 0.76 |
| 1:R:223:ARG:HH11 | 1:R:223:ARG:HG2 | 1.49 | 0.76 |
| 1:L:229:LYS:HG3 | 1:S:487:GLY:HA2 | 1.66 | 0.76 |
| 1:M:223:ARG:HG2 | 1:M:223:ARG:HH11 | 1.49 | 0.76 |
| 1:C:373:PRO:CA | 1:P:390:GLU:O | 2.34 | 0.76 |
| 1:B:12:PHE:HE2 | 1:C:242:HIS:HE1 | 0.88 | 0.75 |
| 1:O:11:ILE:O | 1:P:273:LYS:HE3 | 1.85 | 0.75 |
| 1:U:390:GLU:O | 1:V:373:PRO:HB3 | 1.85 | 0.75 |
| 1:L:283:SER:HB3 | 1:N:3:LEU:HD23 | 1.57 | 0.75 |
| 1:C:214:ARG:H | 1:C:218:GLN:HE22 | 1.33 | 0.75 |
| 1:F:383:SER:HB2 | 1:G:383:SER:HB2 | 1.69 | 0.75 |
| 1:V:223:ARG:HG2 | 1:V:223:ARG:HH11 | 1.49 | 0.75 |
| 1:V:4:ALA:O | 1:V:7:LEU:HB2 | 1.84 | 0.75 |
| 1:B:297:GLN:HB2 | 1:C:310:ARG:CG | 2.15 | 0.75 |
| 1:D:373:PRO:HA | 1:E:390:GLU:O | 1.85 | 0.75 |
| 1:Q:12:PHE:HE2 | 1:S:242:HIS:CE1 | 2.05 | 0.75 |
| 1:H:310:ARG:CG | 1:J:297:GLN:CB | 2.49 | 0.75 |
| 1:P:214:ARG:H | 1:P:218:GLN:HE22 | 1.33 | 0.75 |
| 1:S:390:GLU:OE1 | 1:T:379:ALA:HB1 | 1.86 | 0.75 |
| 1:A:214:ARG:H | 1:A:218:GLN:HE22 | 1.33 | 0.75 |
| 1:E:214:ARG:H | 1:E:218:GLN:HE22 | 1.33 | 0.75 |
| 1:O:214:ARG:H | 1:O:218:GLN:HE22 | 1.34 | 0.75 |
| 1:L:214:ARG:H | 1:L:218:GLN:HE22 | 1.33 | 0.74 |
| 1:K:272:GLU:HG3 | 1:M:352:GLU:HB2 | 1.68 | 0.74 |
| 1:R:276:VAL:CG1 | 1:T:9:LEU:CB | 2.64 | 0.74 |
| 1:E:223:ARG:HG2 | 1:E:223:ARG:HH11 | 1.49 | 0.74 |
| 1:H:297:GLN:HG3 | 1:J:310:ARG:HG2 | 1.69 | 0.74 |
| 1:S:491:GLN:HG3 | 1:T:491:GLN:HG3 | 1.68 | 0.74 |
| 1:U:242:HIS:CE1 | 1:W:12:PHE:HZ | 2.00 | 0.74 |
| 1:V:280:ILE:HD11 | 1:X:9:LEU:HB2 | 1.68 | 0.74 |
| 1:I:195:VAL:HG22 | 1:N:496:LEU:HG | 1.69 | 0.74 |
| 1:X:214:ARG:H | 1:X:218:GLN:HE22 | 1.33 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:390:GLU:HA | 1:G:372:ILE:HG13 | 1.69 | 0.74 |
| 1:K:11:ILE:HB | 1:M:273:LYS:HG2 | 1.68 | 0.74 |
| 1:P:229:LYS:HG3 | 1:V:487:GLY:HA3 | 1.69 | 0.74 |
| 1:L:191:ALA:HB1 | 1:T:473:GLY:HA3 | 1.69 | 0.74 |
| 1:U:214:ARG:H | 1:U:218:GLN:HE22 | 1.33 | 0.74 |
| 1:Q:280:ILE:CG1 | 1:S:6:ASN:O | 2.34 | 0.74 |
| 1:D:214:ARG:H | 1:D:218:GLN:HE22 | 1.33 | 0.74 |
| 1:G:214:ARG:H | 1:G:218:GLN:HE22 | 1.33 | 0.74 |
| 1:C:373:PRO:HB3 | 1:P:391:THR:HA | 1.69 | 0.74 |
| 1:T:214:ARG:H | 1:T:218:GLN:HE22 | 1.33 | 0.74 |
| 1:V:297:GLN:NE2 | 1:V:300:GLU:HG2 | 2.02 | 0.74 |
| 1:I:193:ASP:HA | 1:I:196:ASP:HB2 | 1.70 | 0.74 |
| 1:F:391:THR:HA | 1:G:373:PRO:HB3 | 1.70 | 0.74 |
| 1:J:214:ARG:H | 1:J:218:GLN:HE22 | 1.33 | 0.74 |
| 1:K:193:ASP:HA | 1:K:196:ASP:HB2 | 1.70 | 0.74 |
| 1:M:193:ASP:HA | 1:M:196:ASP:HB2 | 1.70 | 0.74 |
| 1:Q:214:ARG:H | 1:Q:218:GLN:HE22 | 1.33 | 0.74 |
| 1:Q:12:PHE:CE2 | 1:S:242:HIS:HE1 | 2.06 | 0.74 |
| 1:W:193:ASP:HA | 1:W:196:ASP:HB2 | 1.70 | 0.74 |
| 1:O:193:ASP:HA | 1:O:196:ASP:HB2 | 1.70 | 0.74 |
| 1:R:276:VAL:HG13 | 1:T:9:LEU:CB | 2.18 | 0.74 |
| 1:W:392:LYS:HD2 | 1:X:373:PRO:HD3 | 1.69 | 0.74 |
| 1:V:9:LEU:HB2 | 1:X:280:ILE:HD11 | 1.68 | 0.74 |
| 1:V:297:GLN:OE1 | 1:X:309:THR:HB | 1.88 | 0.74 |
| 1:L:193:ASP:HA | 1:L:196:ASP:HB2 | 1.70 | 0.73 |
| 1:L:283:SER:CB | 1:N:3:LEU:HD21 | 2.17 | 0.73 |
| 1:S:494:ILE:HD12 | 1:T:376:ALA:HB1 | 1.68 | 0.73 |
| 1:H:214:ARG:H | 1:H:218:GLN:HE22 | 1.34 | 0.73 |
| 1:Q:390:GLU:O | 1:R:373:PRO:HA | 1.88 | 0.73 |
| 1:S:214:ARG:H | 1:S:218:GLN:HE22 | 1.33 | 0.73 |
| 1:A:179:LEU:HB3 | 1:A:182:CYS:HB2 | 1.71 | 0.73 |
| 1:E:11:ILE:CG1 | 1:E:12:PHE:CD2 | 2.71 | 0.73 |
| 1:F:193:ASP:HA | 1:F:196:ASP:HB2 | 1.70 | 0.73 |
| 1:N:179:LEU:HB3 | 1:N:182:CYS:HB2 | 1.70 | 0.73 |
| 1:P:193:ASP:HA | 1:P:196:ASP:HB2 | 1.70 | 0.73 |
| 1:C:383:SER:HB2 | 1:P:383:SER:HB2 | 1.70 | 0.73 |
| 1:V:310:ARG:HG2 | 1:X:297:GLN:OE1 | 1.88 | 0.73 |
| 1:I:11:ILE:CG1 | 1:I:12:PHE:CD2 | 2.71 | 0.73 |
| 1:R:11:ILE:CG1 | 1:R:12:PHE:CD2 | 2.71 | 0.73 |
| 1:C:216:ALA:HB3 | 1:N:446:LYS:CD | 2.12 | 0.73 |
| 1:F:214:ARG:H | 1:F:218:GLN:HE22 | 1.33 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:179:LEU:HB3 | 1:J:182:CYS:HB2 | 1.70 | 0.73 |
| 1:U:193:ASP:HA | 1:U:196:ASP:HB2 | 1.70 | 0.73 |
| 1:K:242:HIS:CE1 | 1:M:12:PHE:CZ | 2.75 | 0.73 |
| 1:L:424:ARG:HG2 | 1:L:424:ARG:HH11 | 0.74 | 0.73 |
| 1:B:373:PRO:HA | 1:O:390:GLU:O | 1.88 | 0.73 |
| 1:O:242:HIS:CE1 | 1:P:12:PHE:CZ | 2.77 | 0.73 |
| 1:Q:297:GLN:OE1 | 1:S:310:ARG:CG | 2.31 | 0.73 |
| 1:R:214:ARG:H | 1:R:218:GLN:HE22 | 1.33 | 0.73 |
| 1:S:193:ASP:HA | 1:S:196:ASP:HB2 | 1.70 | 0.73 |
| 1:C:216:ALA:HB1 | 1:N:446:LYS:CD | 2.15 | 0.73 |
| 1:D:179:LEU:HB3 | 1:D:182:CYS:HB2 | 1.70 | 0.73 |
| 1:N:214:ARG:H | 1:N:218:GLN:HE22 | 1.33 | 0.73 |
| 1:Q:312:GLU:HA | 1:S:311:ALA:HB1 | 1.70 | 0.73 |
| 1:V:11:ILE:CG1 | 1:V:12:PHE:CD2 | 2.71 | 0.73 |
| 1:W:179:LEU:HB3 | 1:W:182:CYS:HB2 | 1.70 | 0.73 |
| 1:C:179:LEU:HB3 | 1:C:182:CYS:HB2 | 1.70 | 0.73 |
| 1:D:193:ASP:HA | 1:D:196:ASP:HB2 | 1.70 | 0.73 |
| 1:I:179:LEU:HB3 | 1:I:182:CYS:HB2 | 1.70 | 0.73 |
| 1:N:193:ASP:HA | 1:N:196:ASP:HB2 | 1.70 | 0.73 |
| 1:T:179:LEU:HB3 | 1:T:182:CYS:HB2 | 1.70 | 0.73 |
| 1:U:179:LEU:HB3 | 1:U:182:CYS:HB2 | 1.70 | 0.73 |
| 1:C:496:LEU:CD2 | 1:V:195:VAL:HG22 | 2.19 | 0.73 |
| 1:W:214:ARG:H | 1:W:218:GLN:HE22 | 1.33 | 0.73 |
| 1:O:179:LEU:HB3 | 1:O:182:CYS:HB2 | 1.71 | 0.73 |
| 1:T:370:GLN:HB3 | 1:T:374:MET:SD | 2.29 | 0.73 |
| 1:A:193:ASP:HA | 1:A:196:ASP:HB2 | 1.70 | 0.72 |
| 1:L:11:ILE:CG1 | 1:L:12:PHE:CD2 | 2.71 | 0.72 |
| 1:Q:193:ASP:HA | 1:Q:196:ASP:HB2 | 1.70 | 0.72 |
| 1:U:424:ARG:HH11 | 1:U:424:ARG:HG2 | 0.74 | 0.72 |
| 1:X:179:LEU:HB3 | 1:X:182:CYS:HB2 | 1.70 | 0.72 |
| 1:M:390:GLU:O | 1:N:373:PRO:HB3 | 1.87 | 0.72 |
| 1:Q:373:PRO:HA | 1:R:390:GLU:O | 1.89 | 0.72 |
| 1:L:229:LYS:CE | 1:S:487:GLY:HA2 | 2.19 | 0.72 |
| 1:R:193:ASP:HA | 1:R:196:ASP:HB2 | 1.70 | 0.72 |
| 1:U:370:GLN:HB3 | 1:U:374:MET:SD | 2.29 | 0.72 |
| 1:P:191:ALA:HB1 | 1:U:473:GLY:HA3 | 1.69 | 0.72 |
| 1:L:487:GLY:HA2 | 1:S:229:LYS:CD | 2.20 | 0.72 |
| 1:V:179:LEU:HB3 | 1:V:182:CYS:HB2 | 1.70 | 0.72 |
| 1:Q:179:LEU:HB3 | 1:Q:182:CYS:HB2 | 1.71 | 0.72 |
| 1:V:193:ASP:HA | 1:V:196:ASP:HB2 | 1.70 | 0.72 |
| 1:C:193:ASP:HA | 1:C:196:ASP:HB2 | 1.70 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:193:ASP:HA | 1:J:196:ASP:HB2 | 1.70 | 0.72 |
| 1:S:179:LEU:HB3 | 1:S:182:CYS:HB2 | 1.70 | 0.72 |
| 1:Q:11:ILE:HB | 1:S:273:LYS:HG2 | 1.72 | 0.72 |
| 1:Q:3:LEU:CD2 | 1:S:283:SER:HB3 | 2.20 | 0.72 |
| 1:R:276:VAL:HG13 | 1:T:9:LEU:HD13 | 1.71 | 0.72 |
| 1:U:373:PRO:CB | 1:V:391:THR:HA | 2.19 | 0.72 |
| 1:V:242:HIS:CE1 | 1:X:12:PHE:CZ | 2.75 | 0.72 |
| 1:F:179:LEU:HB3 | 1:F:182:CYS:HB2 | 1.70 | 0.72 |
| 1:L:272:GLU:HG3 | 1:N:352:GLU:HB2 | 1.70 | 0.72 |
| 1:Q:373:PRO:HD3 | 1:R:392:LYS:HD2 | 1.72 | 0.72 |
| 1:U:373:PRO:HB3 | 1:V:391:THR:CA | 2.19 | 0.72 |
| 1:A:390:GLU:HA | 1:J:372:ILE:HG13 | 1.70 | 0.72 |
| 1:E:193:ASP:HA | 1:E:196:ASP:HB2 | 1.70 | 0.72 |
| 1:F:491:GLN:HG3 | 1:G:491:GLN:HG3 | 1.72 | 0.72 |
| 1:J:424:ARG:HH11 | 1:J:424:ARG:HG2 | 0.74 | 0.72 |
| 1:L:179:LEU:HB3 | 1:L:182:CYS:HB2 | 1.70 | 0.72 |
| 1:P:179:LEU:HB3 | 1:P:182:CYS:HB2 | 1.70 | 0.72 |
| 1:U:372:ILE:HD11 | 1:V:390:GLU:HG2 | 1.71 | 0.72 |
| 1:H:11:ILE:O | 1:J:273:LYS:HG2 | 1.90 | 0.72 |
| 1:M:179:LEU:HB3 | 1:M:182:CYS:HB2 | 1.70 | 0.72 |
| 1:R:276:VAL:HG13 | 1:T:9:LEU:HB3 | 1.71 | 0.72 |
| 1:U:315:ASP:HB2 | 1:W:311:ALA:HA | 1.71 | 0.72 |
| 1:B:193:ASP:HA | 1:B:196:ASP:HB2 | 1.70 | 0.72 |
| 1:A:242:HIS:CE1 | 1:I:12:PHE:CZ | 2.77 | 0.72 |
| 1:V:6:ASN:O | 1:X:280:ILE:HG12 | 1.90 | 0.72 |
| 1:H:193:ASP:HA | 1:H:196:ASP:HB2 | 1.70 | 0.71 |
| 1:H:179:LEU:HB3 | 1:H:182:CYS:HB2 | 1.70 | 0.71 |
| 1:K:179:LEU:HB3 | 1:K:182:CYS:HB2 | 1.70 | 0.71 |
| 1:G:179:LEU:HB3 | 1:G:182:CYS:HB2 | 1.70 | 0.71 |
| 1:H:11:ILE:O | 1:J:273:LYS:CE | 2.37 | 0.71 |
| 1:S:376:ALA:HA | 1:T:494:ILE:HD12 | 1.71 | 0.71 |
| 1:K:297:GLN:HB2 | 1:M:310:ARG:HG2 | 1.71 | 0.71 |
| 1:R:179:LEU:HB3 | 1:R:182:CYS:HB2 | 1.70 | 0.71 |
| 1:A:283:SER:HB3 | 1:I:3:LEU:CD2 | 2.21 | 0.71 |
| 1:Q:272:GLU:CG | 1:S:352:GLU:HG2 | 2.21 | 0.71 |
| 1:I:370:GLN:CB | 1:I:374:MET:SD | 2.78 | 0.71 |
| 1:K:473:GLY:HA3 | 1:S:191:ALA:HB1 | 1.73 | 0.71 |
| 1:L:273:LYS:HD3 | 1:N:11:ILE:O | 1.90 | 0.71 |
| 1:R:276:VAL:HG12 | 1:R:280:ILE:CD1 | 2.21 | 0.71 |
| 1:P:487:GLY:CA | 1:V:229:LYS:CE | 2.49 | 0.71 |
| 1:U:315:ASP:CB | 1:W:311:ALA:HA | 2.21 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:254:GLU:CG | 1:N:446:LYS:HE2 | 2.21 | 0.71 |
| 1:E:179:LEU:HB3 | 1:E:182:CYS:HB2 | 1.70 | 0.71 |
| 1:G:193:ASP:HA | 1:G:196:ASP:HB2 | 1.70 | 0.71 |
| 1:O:310:ARG:HG2 | 1:P:297:GLN:HB2 | 1.72 | 0.71 |
| 1:L:229:LYS:CG | 1:S:487:GLY:HA2 | 2.20 | 0.71 |
| 1:X:193:ASP:HA | 1:X:196:ASP:HB2 | 1.70 | 0.71 |
| 1:B:179:LEU:HB3 | 1:B:182:CYS:HB2 | 1.70 | 0.70 |
| 1:L:273:LYS:CG | 1:N:11:ILE:HB | 2.21 | 0.70 |
| 1:C:270:PRO:HG2 | 1:C:273:LYS:CD | 2.21 | 0.70 |
| 1:B:297:GLN:HB2 | 1:C:310:ARG:HG2 | 1.73 | 0.70 |
| 1:V:3:LEU:CD2 | 1:X:283:SER:HB3 | 2.20 | 0.70 |
| 1:H:311:ALA:HB3 | 1:J:312:GLU:HG3 | 1.73 | 0.70 |
| 1:K:496:LEU:CD2 | 1:S:195:VAL:HG22 | 2.21 | 0.70 |
| 1:Q:270:PRO:HG2 | 1:Q:273:LYS:CD | 2.22 | 0.70 |
| 1:Q:311:ALA:HB1 | 1:S:312:GLU:HA | 1.74 | 0.70 |
| 1:L:242:HIS:CE1 | 1:N:12:PHE:CZ | 2.71 | 0.70 |
| 1:R:276:VAL:O | 1:R:280:ILE:HG13 | 1.91 | 0.70 |
| 1:T:193:ASP:HA | 1:T:196:ASP:HB2 | 1.70 | 0.70 |
| 1:V:7:LEU:HD22 | 1:X:284:LYS:HG2 | 1.74 | 0.70 |
| 1:M:491:GLN:HG3 | 1:N:491:GLN:HG3 | 1.72 | 0.70 |
| 1:R:370:GLN:CB | 1:R:374:MET:SD | 2.78 | 0.70 |
| 1:X:456:ARG:NH2 | 2:X:700:FDP:O1P | 2.25 | 0.70 |
| 1:A:270:PRO:HG2 | 1:A:273:LYS:CD | 2.21 | 0.70 |
| 1:R:11:ILE:CD1 | 1:R:12:PHE:CE2 | 2.75 | 0.70 |
| 1:S:372:ILE:CG1 | 1:T:390:GLU:O | 2.36 | 0.70 |
| 1:U:390:GLU:OE1 | 1:V:379:ALA:HB1 | 1.91 | 0.70 |
| 1:A:135:VAL:HG11 | 1:A:152:VAL:HG21 | 1.74 | 0.70 |
| 1:I:11:ILE:CD1 | 1:I:12:PHE:CE2 | 2.75 | 0.70 |
| 1:B:373:PRO:HD3 | 1:O:392:LYS:CD | 2.22 | 0.70 |
| 1:R:280:ILE:HG23 | 1:T:7:LEU:HA | 1.74 | 0.70 |
| 1:Q:38:LYS:HE3 | 1:Q:73:GLU:OE1 | 1.92 | 0.70 |
| 1:R:38:LYS:HE3 | 1:R:73:GLU:OE1 | 1.92 | 0.70 |
| 1:B:135:VAL:HG11 | 1:B:152:VAL:HG21 | 1.74 | 0.70 |
| 1:C:38:LYS:HE3 | 1:C:73:GLU:OE1 | 1.92 | 0.70 |
| 1:E:11:ILE:CD1 | 1:E:12:PHE:CE2 | 2.75 | 0.70 |
| 1:O:38:LYS:HE3 | 1:O:73:GLU:OE1 | 1.92 | 0.70 |
| 1:T:38:LYS:HE3 | 1:T:73:GLU:OE1 | 1.92 | 0.70 |
| 1:X:135:VAL:HG11 | 1:X:152:VAL:HG21 | 1.74 | 0.70 |
| 1:I:38:LYS:HE3 | 1:I:73:GLU:OE1 | 1.92 | 0.69 |
| 1:V:11:ILE:CD1 | 1:V:12:PHE:CE2 | 2.75 | 0.69 |
| 1:B:270:PRO:HG2 | 1:B:273:LYS:CD | 2.22 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:58:GLU:CD | 1:E:103:ARG:HD2 | 2.12 | 0.69 |
| 1:E:38:LYS:HE3 | 1:E:73:GLU:OE1 | 1.92 | 0.69 |
| 1:F:38:LYS:HE3 | 1:F:73:GLU:OE1 | 1.92 | 0.69 |
| 1:L:11:ILE:CD1 | 1:L:12:PHE:CE2 | 2.75 | 0.69 |
| 1:M:135:VAL:HG11 | 1:M:152:VAL:HG21 | 1.74 | 0.69 |
| 1:A:391:THR:C | 1:J:373:PRO:HB3 | 2.13 | 0.69 |
| 1:D:310:ARG:HG2 | 1:F:297:GLN:OE1 | 1.92 | 0.69 |
| 1:D:38:LYS:HE3 | 1:D:73:GLU:OE1 | 1.92 | 0.69 |
| 1:K:270:PRO:HG2 | 1:K:273:LYS:CD | 2.22 | 0.69 |
| 1:K:383:SER:HB2 | 1:L:383:SER:HB2 | 1.74 | 0.69 |
| 1:N:38:LYS:HE3 | 1:N:73:GLU:OE1 | 1.92 | 0.69 |
| 1:R:276:VAL:HG11 | 1:T:9:LEU:HB3 | 1.74 | 0.69 |
| 1:U:38:LYS:HE3 | 1:U:73:GLU:OE1 | 1.92 | 0.69 |
| 1:V:272:GLU:HG3 | 1:X:352:GLU:HB2 | 1.73 | 0.69 |
| 1:A:38:LYS:HE3 | 1:A:73:GLU:OE1 | 1.92 | 0.69 |
| 1:F:373:PRO:HD3 | 1:G:392:LYS:HD2 | 1.75 | 0.69 |
| 1:H:270:PRO:HG2 | 1:H:273:LYS:CD | 2.22 | 0.69 |
| 1:H:456:ARG:NH2 | 2:H:700:FDP:O1P | 2.25 | 0.69 |
| 1:L:38:LYS:HE3 | 1:L:73:GLU:OE1 | 1.92 | 0.69 |
| 1:O:297:GLN:HB2 | 1:P:310:ARG:HG2 | 1.74 | 0.69 |
| 1:X:38:LYS:HE3 | 1:X:73:GLU:OE1 | 1.92 | 0.69 |
| 1:A:3:LEU:HD23 | 1:I:283:SER:HB3 | 1.74 | 0.69 |
| 1:B:272:GLU:CG | 1:C:352:GLU:HG2 | 2.23 | 0.69 |
| 1:D:270:PRO:HG2 | 1:D:273:LYS:CD | 2.22 | 0.69 |
| 1:J:38:LYS:HE3 | 1:J:73:GLU:OE1 | 1.92 | 0.69 |
| 1:U:270:PRO:HG2 | 1:U:273:LYS:CD | 2.22 | 0.69 |
| 1:V:135:VAL:HG11 | 1:V:152:VAL:HG21 | 1.74 | 0.69 |
| 1:H:12:PHE:HZ | 1:J:242:HIS:CE1 | 2.02 | 0.69 |
| 1:K:272:GLU:O | 1:M:352:GLU:HG2 | 1.92 | 0.69 |
| 1:M:456:ARG:NH2 | 2:M:700:FDP:O1P | 2.25 | 0.69 |
| 1:V:276:VAL:HG13 | 1:X:9:LEU:HD13 | 1.75 | 0.69 |
| 1:U:297:GLN:CB | 1:W:310:ARG:HG2 | 2.17 | 0.69 |
| 1:W:38:LYS:HE3 | 1:W:73:GLU:OE1 | 1.92 | 0.69 |
| 1:J:135:VAL:HG11 | 1:J:152:VAL:HG21 | 1.74 | 0.69 |
| 1:O:310:ARG:CG | 1:P:297:GLN:HB2 | 2.22 | 0.69 |
| 1:T:135:VAL:HG11 | 1:T:152:VAL:HG21 | 1.74 | 0.69 |
| 1:H:38:LYS:HE3 | 1:H:73:GLU:OE1 | 1.92 | 0.69 |
| 1:W:372:ILE:HG13 | 1:X:390:GLU:O | 1.93 | 0.69 |
| 1:G:135:VAL:HG11 | 1:G:152:VAL:HG21 | 1.74 | 0.69 |
| 1:O:135:VAL:HG11 | 1:O:152:VAL:HG21 | 1.74 | 0.69 |
| 1:O:270:PRO:HG2 | 1:O:273:LYS:CD | 2.21 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:456:ARG:NH2 | 2:P:700:FDP:O1P | 2.25 | 0.69 |
| 1:R:135:VAL:HG11 | 1:R:152:VAL:HG21 | 1.74 | 0.69 |
| 1:S:38:LYS:HE3 | 1:S:73:GLU:OE1 | 1.92 | 0.69 |
| 1:W:456:ARG:NH2 | 2:W:700:FDP:O1P | 2.25 | 0.69 |
| 1:G:38:LYS:HE3 | 1:G:73:GLU:OE1 | 1.92 | 0.69 |
| 1:H:11:ILE:HB | 1:J:273:LYS:HB3 | 1.74 | 0.69 |
| 1:H:11:ILE:HD12 | 1:J:269:ILE:HG12 | 1.74 | 0.69 |
| 1:H:311:ALA:HB3 | 1:J:312:GLU:CG | 2.23 | 0.69 |
| 1:M:38:LYS:HE3 | 1:M:73:GLU:OE1 | 1.92 | 0.69 |
| 1:P:38:LYS:HE3 | 1:P:73:GLU:OE1 | 1.92 | 0.69 |
| 1:V:272:GLU:HG2 | 1:X:352:GLU:HG2 | 1.73 | 0.69 |
| 1:G:456:ARG:NH2 | 2:G:700:FDP:O1P | 2.25 | 0.69 |
| 1:N:135:VAL:HG11 | 1:N:152:VAL:HG21 | 1.74 | 0.69 |
| 1:O:456:ARG:NH2 | 2:O:700:FDP:O1P | 2.25 | 0.69 |
| 1:V:38:LYS:HE3 | 1:V:73:GLU:OE1 | 1.92 | 0.69 |
| 1:E:135:VAL:HG11 | 1:E:152:VAL:HG21 | 1.74 | 0.68 |
| 1:L:297:GLN:HB2 | 1:N:310:ARG:CG | 2.24 | 0.68 |
| 1:S:372:ILE:CG2 | 1:T:390:GLU:O | 2.42 | 0.68 |
| 1:K:38:LYS:HE3 | 1:K:73:GLU:OE1 | 1.92 | 0.68 |
| 1:S:135:VAL:HG11 | 1:S:152:VAL:HG21 | 1.74 | 0.68 |
| 1:B:273:LYS:HB3 | 1:C:11:ILE:HB | 1.75 | 0.68 |
| 1:K:297:GLN:HB2 | 1:M:310:ARG:CG | 2.23 | 0.68 |
| 1:P:135:VAL:HG11 | 1:P:152:VAL:HG21 | 1.74 | 0.68 |
| 1:V:297:GLN:HE21 | 1:V:300:GLU:CD | 1.97 | 0.68 |
| 1:B:38:LYS:HE3 | 1:B:73:GLU:OE1 | 1.92 | 0.68 |
| 1:L:456:ARG:NH2 | 2:L:700:FDP:O1P | 2.25 | 0.68 |
| 1:Q:135:VAL:HG11 | 1:Q:152:VAL:HG21 | 1.74 | 0.68 |
| 1:F:392:LYS:HD2 | 1:G:373:PRO:HD3 | 1.74 | 0.68 |
| 1:H:135:VAL:HG11 | 1:H:152:VAL:HG21 | 1.74 | 0.68 |
| 1:V:242:HIS:CE1 | 1:X:12:PHE:HE2 | 2.06 | 0.68 |
| 1:K:456:ARG:NH2 | 2:K:700:FDP:O1P | 2.25 | 0.68 |
| 1:L:11:ILE:HG13 | 1:L:12:PHE:CE2 | 2.29 | 0.68 |
| 1:R:372:ILE:HD12 | 1:R:374:MET:HG3 | 1.75 | 0.68 |
| 1:W:135:VAL:HG11 | 1:W:152:VAL:HG21 | 1.74 | 0.68 |
| 1:F:135:VAL:HG11 | 1:F:152:VAL:HG21 | 1.74 | 0.68 |
| 1:I:135:VAL:HG11 | 1:I:152:VAL:HG21 | 1.74 | 0.68 |
| 1:C:390:GLU:O | 1:P:372:ILE:HG23 | 1.92 | 0.68 |
| 1:Q:269:ILE:HG12 | 1:S:11:ILE:CD1 | 2.22 | 0.68 |
| 1:S:483:HIS:HD2 | 1:T:483:HIS:NE2 | 1.90 | 0.68 |
| 1:K:279:LYS:HE3 | 1:M:6:ASN:OD1 | 1.94 | 0.68 |
| 1:U:135:VAL:HG11 | 1:U:152:VAL:HG21 | 1.74 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:371:HIS:CD2 | 1:U:373:PRO:O | 2.47 | 0.68 |
| 1:V:11:ILE:HG13 | 1:V:12:PHE:CE2 | 2.29 | 0.68 |
| 1:L:135:VAL:HG11 | 1:L:152:VAL:HG21 | 1.74 | 0.68 |
| 1:R:297:GLN:CG | 1:T:310:ARG:CG | 2.71 | 0.68 |
| 1:V:456:ARG:NH2 | 2:V:700:FDP:O1P | 2.25 | 0.68 |
| 1:B:297:GLN:OE1 | 1:C:310:ARG:CG | 2.39 | 0.67 |
| 1:T:456:ARG:NH2 | 2:T:700:FDP:O1P | 2.25 | 0.67 |
| 1:U:242:HIS:NE2 | 1:W:12:PHE:HE2 | 1.93 | 0.67 |
| 1:L:12:PHE:CE2 | 1:N:242:HIS:CE1 | 2.82 | 0.67 |
| 1:N:446:LYS:C | 1:N:446:LYS:HD2 | 2.14 | 0.67 |
| 1:R:296:THR:HG22 | 1:R:297:GLN:CG | 2.25 | 0.67 |
| 1:Q:12:PHE:HE2 | 1:S:242:HIS:HE1 | 1.40 | 0.67 |
| 1:C:135:VAL:HG11 | 1:C:152:VAL:HG21 | 1.74 | 0.67 |
| 1:H:370:GLN:CB | 1:H:374:MET:SD | 2.82 | 0.67 |
| 1:A:390:GLU:O | 1:J:373:PRO:HA | 1.94 | 0.67 |
| 1:C:391:THR:HA | 1:P:373:PRO:HB3 | 1.75 | 0.67 |
| 1:S:383:SER:HB2 | 1:T:383:SER:HB2 | 1.76 | 0.67 |
| 1:D:135:VAL:HG11 | 1:D:152:VAL:HG21 | 1.74 | 0.67 |
| 1:A:371:HIS:CD2 | 1:A:373:PRO:O | 2.48 | 0.67 |
| 1:D:390:GLU:O | 1:E:373:PRO:HA | 1.94 | 0.67 |
| 1:L:283:SER:HB3 | 1:N:3:LEU:HD21 | 1.71 | 0.67 |
| 1:W:371:HIS:CD2 | 1:W:373:PRO:O | 2.48 | 0.67 |
| 1:X:371:HIS:CD2 | 1:X:373:PRO:O | 2.48 | 0.67 |
| 1:B:371:HIS:CD2 | 1:B:373:PRO:O | 2.48 | 0.67 |
| 1:C:371:HIS:CD2 | 1:C:373:PRO:O | 2.48 | 0.67 |
| 1:L:273:LYS:HB3 | 1:N:11:ILE:HB | 1.77 | 0.67 |
| 1:K:392:LYS:HD2 | 1:L:373:PRO:HD3 | 1.77 | 0.67 |
| 1:H:263:GLY:HA2 | 1:J:310:ARG:HH11 | 1.60 | 0.67 |
| 1:C:254:GLU:HG2 | 1:N:446:LYS:CE | 2.24 | 0.67 |
| 1:R:11:ILE:HG13 | 1:R:12:PHE:CE2 | 2.29 | 0.67 |
| 1:V:283:SER:HB3 | 1:X:3:LEU:CG | 2.25 | 0.67 |
| 1:D:373:PRO:HD3 | 1:E:392:LYS:HD2 | 1.76 | 0.67 |
| 1:J:371:HIS:CD2 | 1:J:373:PRO:O | 2.48 | 0.67 |
| 1:K:135:VAL:HG11 | 1:K:152:VAL:HG21 | 1.74 | 0.67 |
| 1:L:280:ILE:HD11 | 1:N:9:LEU:HB2 | 1.76 | 0.67 |
| 1:N:371:HIS:CD2 | 1:N:373:PRO:O | 2.48 | 0.66 |
| 1:U:311:ALA:CB | 1:W:312:GLU:HA | 2.19 | 0.66 |
| 1:L:272:GLU:CB | 1:N:352:GLU:HG2 | 2.24 | 0.66 |
| 1:S:491:GLN:HG3 | 1:T:491:GLN:CG | 2.24 | 0.66 |
| 1:V:371:HIS:CD2 | 1:V:373:PRO:O | 2.48 | 0.66 |
| 1:H:53:SER:OG | 1:H:85:LYS:HA | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:K:371:HIS:CD2 | 1:K:373:PRO:O | 2.48 | 0.66 |
| 1:F:371:HIS:CD2 | 1:F:373:PRO:O | 2.48 | 0.66 |
| 1:F:391:THR:HA | 1:G:373:PRO:CB | 2.25 | 0.66 |
| 1:H:310:ARG:CG | 1:J:297:GLN:HG3 | 2.22 | 0.66 |
| 1:L:53:SER:OG | 1:L:85:LYS:HA | 1.96 | 0.66 |
| 1:S:373:PRO:HB3 | 1:T:391:THR:C | 2.16 | 0.66 |
| 1:U:242:HIS:HE1 | 1:W:12:PHE:CE2 | 1.85 | 0.66 |
| 1:G:53:SER:OG | 1:G:85:LYS:HA | 1.96 | 0.66 |
| 1:R:53:SER:OG | 1:R:85:LYS:HA | 1.96 | 0.66 |
| 1:R:279:LYS:HB3 | 1:T:6:ASN:OD1 | 1.95 | 0.66 |
| 1:V:12:PHE:CZ | 1:X:242:HIS:NE2 | 2.63 | 0.66 |
| 1:V:3:LEU:HD23 | 1:X:283:SER:CB | 2.26 | 0.66 |
| 1:D:53:SER:OG | 1:D:85:LYS:HA | 1.96 | 0.66 |
| 1:E:371:HIS:CD2 | 1:E:373:PRO:O | 2.48 | 0.66 |
| 1:F:53:SER:OG | 1:F:85:LYS:HA | 1.96 | 0.66 |
| 1:L:352:GLU:HG2 | 1:N:272:GLU:O | 1.96 | 0.66 |
| 1:O:12:PHE:HZ | 1:P:242:HIS:HE1 | 1.42 | 0.66 |
| 1:Q:371:HIS:CD2 | 1:Q:373:PRO:O | 2.48 | 0.66 |
| 1:X:53:SER:OG | 1:X:85:LYS:HA | 1.96 | 0.66 |
| 1:D:371:HIS:CD2 | 1:D:373:PRO:O | 2.48 | 0.66 |
| 1:O:371:HIS:CD2 | 1:O:373:PRO:O | 2.48 | 0.66 |
| 1:C:53:SER:OG | 1:C:85:LYS:HA | 1.96 | 0.66 |
| 1:F:373:PRO:HB3 | 1:G:391:THR:C | 2.16 | 0.66 |
| 1:H:352:GLU:HG2 | 1:J:272:GLU:C | 2.16 | 0.66 |
| 1:L:279:LYS:HE3 | 1:N:6:ASN:OD1 | 1.96 | 0.66 |
| 1:S:53:SER:OG | 1:S:85:LYS:HA | 1.96 | 0.66 |
| 1:R:283:SER:HB3 | 1:T:3:LEU:HG | 1.77 | 0.66 |
| 1:A:53:SER:OG | 1:A:85:LYS:HA | 1.96 | 0.66 |
| 1:C:250:SER:HB3 | 1:N:446:LYS:HG2 | 1.71 | 0.66 |
| 1:E:283:SER:OG | 1:G:3:LEU:HD23 | 1.97 | 0.65 |
| 1:M:53:SER:OG | 1:M:85:LYS:HA | 1.96 | 0.65 |
| 1:U:11:ILE:O | 1:W:273:LYS:CD | 2.45 | 0.65 |
| 1:B:144:ASP:O | 1:B:145:ASP:CB | 2.45 | 0.65 |
| 1:E:11:ILE:HG13 | 1:E:12:PHE:CE2 | 2.29 | 0.65 |
| 1:E:53:SER:OG | 1:E:85:LYS:HA | 1.96 | 0.65 |
| 1:N:53:SER:OG | 1:N:85:LYS:HA | 1.96 | 0.65 |
| 1:V:269:ILE:HG12 | 1:X:11:ILE:CD1 | 2.27 | 0.65 |
| 1:W:53:SER:OG | 1:W:85:LYS:HA | 1.96 | 0.65 |
| 1:A:242:HIS:HE1 | 1:I:12:PHE:CE2 | 2.10 | 0.65 |
| 1:B:272:GLU:O | 1:C:352:GLU:HG2 | 1.96 | 0.65 |
| 1:H:352:GLU:HB2 | 1:J:272:GLU:HG3 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:53:SER:OG | 1:I:85:LYS:HA | 1.96 | 0.65 |
| 1:T:53:SER:OG | 1:T:85:LYS:HA | 1.96 | 0.65 |
| 1:U:390:GLU:O | 1:V:373:PRO:CA | 2.44 | 0.65 |
| 1:A:3:LEU:CD2 | 1:I:283:SER:CB | 2.74 | 0.65 |
| 1:V:144:ASP:O | 1:V:145:ASP:CB | 2.45 | 0.65 |
| 1:W:144:ASP:O | 1:W:145:ASP:CB | 2.45 | 0.65 |
| 1:E:312:GLU:HA | 1:G:311:ALA:HB1 | 1.78 | 0.65 |
| 1:G:371:HIS:CD2 | 1:G:373:PRO:O | 2.48 | 0.65 |
| 1:H:144:ASP:O | 1:H:145:ASP:CB | 2.45 | 0.65 |
| 1:J:53:SER:OG | 1:J:85:LYS:HA | 1.96 | 0.65 |
| 1:O:242:HIS:CE1 | 1:P:12:PHE:CE2 | 2.84 | 0.65 |
| 1:U:315:ASP:CG | 1:W:311:ALA:HA | 2.16 | 0.65 |
| 1:A:144:ASP:O | 1:A:145:ASP:CB | 2.45 | 0.65 |
| 1:O:53:SER:OG | 1:O:85:LYS:HA | 1.96 | 0.65 |
| 1:R:269:ILE:CG1 | 1:T:11:ILE:CD1 | 2.65 | 0.65 |
| 1:K:53:SER:OG | 1:K:85:LYS:HA | 1.96 | 0.65 |
| 1:Q:144:ASP:O | 1:Q:145:ASP:CB | 2.45 | 0.65 |
| 1:Q:373:PRO:CB | 1:R:390:GLU:O | 2.45 | 0.65 |
| 1:V:297:GLN:HE22 | 1:V:300:GLU:HG2 | 1.62 | 0.65 |
| 1:D:144:ASP:O | 1:D:145:ASP:CB | 2.45 | 0.65 |
| 1:O:311:ALA:CB | 1:P:312:GLU:HA | 2.23 | 0.65 |
| 1:P:53:SER:OG | 1:P:85:LYS:HA | 1.96 | 0.65 |
| 1:Q:53:SER:OG | 1:Q:85:LYS:HA | 1.96 | 0.65 |
| 1:U:372:ILE:CG2 | 1:V:390:GLU:O | 2.43 | 0.65 |
| 1:B:53:SER:OG | 1:B:85:LYS:HA | 1.96 | 0.65 |
| 1:H:11:ILE:HB | 1:J:273:LYS:CB | 2.27 | 0.65 |
| 1:R:3:LEU:HD13 | 1:T:369:LEU:CD1 | 2.26 | 0.65 |
| 1:T:371:HIS:CD2 | 1:T:373:PRO:O | 2.49 | 0.65 |
| 1:V:370:GLN:HB3 | 1:V:374:MET:SD | 2.37 | 0.65 |
| 1:Q:390:GLU:CA | 1:R:372:ILE:HG13 | 2.24 | 0.64 |
| 1:U:53:SER:OG | 1:U:85:LYS:HA | 1.96 | 0.64 |
| 1:V:269:ILE:CG1 | 1:X:11:ILE:HD12 | 2.27 | 0.64 |
| 1:T:214:ARG:N | 1:T:218:GLN:HE22 | 1.96 | 0.64 |
| 1:Q:383:SER:HB2 | 1:R:383:SER:HB2 | 1.79 | 0.64 |
| 1:R:144:ASP:O | 1:R:145:ASP:CB | 2.45 | 0.64 |
| 1:X:370:GLN:HB3 | 1:X:374:MET:SD | 2.37 | 0.64 |
| 1:F:144:ASP:O | 1:F:145:ASP:CB | 2.45 | 0.64 |
| 1:G:370:GLN:HB3 | 1:G:374:MET:SD | 2.38 | 0.64 |
| 1:K:370:GLN:HB3 | 1:K:374:MET:SD | 2.37 | 0.64 |
| 1:L:269:ILE:CG1 | 1:N:11:ILE:HD12 | 2.27 | 0.64 |
| 1:U:245:VAL:HG11 | 1:W:11:ILE:HD13 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:272:GLU:HG3 | 1:C:352:GLU:CB | 2.26 | 0.64 |
| 1:M:214:ARG:N | 1:M:218:GLN:HE22 | 1.96 | 0.64 |
| 1:L:310:ARG:HG2 | 1:N:297:GLN:HB2 | 1.78 | 0.64 |
| 1:Q:370:GLN:HB3 | 1:Q:374:MET:SD | 2.38 | 0.64 |
| 1:X:214:ARG:N | 1:X:218:GLN:HE22 | 1.96 | 0.64 |
| 1:B:370:GLN:HB3 | 1:B:374:MET:SD | 2.38 | 0.64 |
| 1:C:214:ARG:N | 1:C:218:GLN:HE22 | 1.96 | 0.64 |
| 1:D:370:GLN:HB3 | 1:D:374:MET:SD | 2.38 | 0.64 |
| 1:N:370:GLN:HB3 | 1:N:374:MET:SD | 2.37 | 0.64 |
| 1:R:273:LYS:CD | 1:T:11:ILE:O | 2.42 | 0.64 |
| 1:Q:373:PRO:CA | 1:R:390:GLU:O | 2.46 | 0.64 |
| 1:Q:272:GLU:HG3 | 1:S:352:GLU:CB | 2.27 | 0.64 |
| 1:U:11:ILE:HB | 1:W:273:LYS:CB | 2.27 | 0.64 |
| 1:V:53:SER:OG | 1:V:85:LYS:HA | 1.96 | 0.64 |
| 1:W:370:GLN:HB3 | 1:W:374:MET:SD | 2.37 | 0.64 |
| 1:O:370:GLN:HB3 | 1:O:374:MET:SD | 2.37 | 0.64 |
| 1:S:390:GLU:OE1 | 1:T:379:ALA:HB2 | 1.98 | 0.64 |
| 1:U:310:ARG:NH2 | 1:W:297:GLN:OE1 | 2.30 | 0.64 |
| 1:E:370:GLN:HB3 | 1:E:374:MET:SD | 2.37 | 0.64 |
| 1:I:371:HIS:CD2 | 1:I:373:PRO:O | 2.50 | 0.64 |
| 1:E:144:ASP:O | 1:E:145:ASP:CB | 2.45 | 0.64 |
| 1:F:370:GLN:HB3 | 1:F:374:MET:SD | 2.38 | 0.64 |
| 1:K:373:PRO:CA | 1:L:390:GLU:O | 2.42 | 0.64 |
| 1:K:373:PRO:CB | 1:L:391:THR:HA | 2.25 | 0.64 |
| 1:W:214:ARG:N | 1:W:218:GLN:HE22 | 1.96 | 0.64 |
| 1:A:370:GLN:HB3 | 1:A:374:MET:SD | 2.38 | 0.64 |
| 1:B:214:ARG:N | 1:B:218:GLN:HE22 | 1.96 | 0.64 |
| 1:C:370:GLN:HB3 | 1:C:374:MET:SD | 2.37 | 0.64 |
| 1:H:214:ARG:N | 1:H:218:GLN:HE22 | 1.96 | 0.64 |
| 1:J:214:ARG:N | 1:J:218:GLN:HE22 | 1.96 | 0.64 |
| 1:Q:6:ASN:O | 1:S:280:ILE:HG12 | 1.98 | 0.64 |
| 1:U:214:ARG:N | 1:U:218:GLN:HE22 | 1.96 | 0.64 |
| 1:T:144:ASP:O | 1:T:145:ASP:CB | 2.45 | 0.63 |
| 1:E:297:GLN:OE1 | 1:G:310:ARG:CG | 2.35 | 0.63 |
| 1:Q:214:ARG:N | 1:Q:218:GLN:HE22 | 1.95 | 0.63 |
| 1:A:214:ARG:N | 1:A:218:GLN:HE22 | 1.96 | 0.63 |
| 1:O:11:ILE:CA | 1:P:273:LYS:HG2 | 2.28 | 0.63 |
| 1:V:214:ARG:N | 1:V:218:GLN:HE22 | 1.96 | 0.63 |
| 1:F:214:ARG:N | 1:F:218:GLN:HE22 | 1.96 | 0.63 |
| 1:F:391:THR:CA | 1:G:373:PRO:HB3 | 2.29 | 0.63 |
| 1:H:297:GLN:HB2 | 1:J:310:ARG:CB | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:492:THR:HG22 | 1:J:492:THR:HG22 | 1.79 | 0.63 |
| 1:L:311:ALA:CB | 1:N:312:GLU:HA | 2.28 | 0.63 |
| 1:G:214:ARG:N | 1:G:218:GLN:HE22 | 1.96 | 0.63 |
| 1:I:371:HIS:O | 1:I:374:MET:CG | 2.41 | 0.63 |
| 1:J:370:GLN:HB3 | 1:J:374:MET:SD | 2.37 | 0.63 |
| 1:M:370:GLN:CB | 1:M:374:MET:SD | 2.86 | 0.63 |
| 1:R:214:ARG:N | 1:R:218:GLN:HE22 | 1.96 | 0.63 |
| 1:P:195:VAL:CG2 | 1:U:496:LEU:CD2 | 2.73 | 0.63 |
| 1:L:272:GLU:CG | 1:N:352:GLU:CG | 2.76 | 0.63 |
| 1:P:214:ARG:N | 1:P:218:GLN:HE22 | 1.96 | 0.63 |
| 1:D:214:ARG:N | 1:D:218:GLN:HE22 | 1.96 | 0.63 |
| 1:K:214:ARG:N | 1:K:218:GLN:HE22 | 1.96 | 0.63 |
| 1:L:9:LEU:HB2 | 1:N:280:ILE:HD11 | 1.81 | 0.63 |
| 1:L:11:ILE:HD12 | 1:N:269:ILE:HG12 | 1.80 | 0.63 |
| 1:X:144:ASP:O | 1:X:145:ASP:CB | 2.45 | 0.63 |
| 1:H:315:ASP:CG | 1:J:311:ALA:HA | 2.19 | 0.63 |
| 1:O:144:ASP:O | 1:O:145:ASP:CB | 2.45 | 0.63 |
| 1:O:214:ARG:N | 1:O:218:GLN:HE22 | 1.96 | 0.63 |
| 1:P:487:GLY:CA | 1:V:229:LYS:HD2 | 2.27 | 0.63 |
| 1:V:7:LEU:HD23 | 1:X:284:LYS:HG3 | 1.80 | 0.63 |
| 1:B:272:GLU:C | 1:C:352:GLU:HG2 | 2.20 | 0.62 |
| 1:L:214:ARG:N | 1:L:218:GLN:HE22 | 1.96 | 0.62 |
| 1:S:214:ARG:N | 1:S:218:GLN:HE22 | 1.96 | 0.62 |
| 1:E:11:ILE:CD1 | 1:E:12:PHE:HE2 | 2.12 | 0.62 |
| 1:I:11:ILE:HG13 | 1:I:12:PHE:CE2 | 2.29 | 0.62 |
| 1:I:214:ARG:N | 1:I:218:GLN:HE22 | 1.96 | 0.62 |
| 1:K:456:ARG:NH1 | 2:K:700:FDP:O2P | 2.28 | 0.62 |
| 1:M:373:PRO:HB3 | 1:N:391:THR:HA | 1.80 | 0.62 |
| 1:P:144:ASP:O | 1:P:145:ASP:CB | 2.45 | 0.62 |
| 1:F:372:ILE:HD11 | 1:G:390:GLU:HG2 | 1.81 | 0.62 |
| 1:H:372:ILE:HD12 | 1:H:374:MET:HG3 | 1.81 | 0.62 |
| 1:G:144:ASP:O | 1:G:145:ASP:CB | 2.45 | 0.62 |
| 1:K:310:ARG:HG2 | 1:M:297:GLN:HB2 | 1.80 | 0.62 |
| 1:S:371:HIS:CD2 | 1:S:373:PRO:O | 2.53 | 0.62 |
| 1:H:372:ILE:CG2 | 1:I:390:GLU:O | 2.43 | 0.62 |
| 1:L:370:GLN:CB | 1:L:374:MET:SD | 2.87 | 0.62 |
| 1:H:273:LYS:HB3 | 1:J:11:ILE:HB | 1.82 | 0.62 |
| 1:O:315:ASP:HB2 | 1:P:311:ALA:HA | 1.82 | 0.62 |
| 1:P:371:HIS:CD2 | 1:P:373:PRO:O | 2.53 | 0.62 |
| 1:P:456:ARG:NH1 | 2:P:700:FDP:O2P | 2.28 | 0.62 |
| 1:L:310:ARG:HG2 | 1:N:297:GLN:OE1 | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:144:ASP:O | 1:L:145:ASP:CB | 2.45 | 0.62 |
| 1:N:214:ARG:N | 1:N:218:GLN:HE22 | 1.96 | 0.62 |
| 1:Q:372:ILE:HD11 | 1:Q:374:MET:HE1 | 1.81 | 0.62 |
| 1:R:276:VAL:CG1 | 1:R:280:ILE:HD11 | 2.27 | 0.62 |
| 1:L:242:HIS:NE2 | 1:N:12:PHE:HE2 | 1.98 | 0.61 |
| 1:B:283:SER:OG | 1:C:3:LEU:HD23 | 1.99 | 0.61 |
| 1:K:269:ILE:HG12 | 1:M:11:ILE:HD12 | 1.82 | 0.61 |
| 1:S:144:ASP:O | 1:S:145:ASP:CB | 2.45 | 0.61 |
| 1:L:283:SER:HB3 | 1:N:3:LEU:HD22 | 1.79 | 0.61 |
| 1:D:492:THR:HG22 | 1:E:492:THR:HG22 | 1.83 | 0.61 |
| 1:H:315:ASP:HB2 | 1:J:311:ALA:CA | 2.30 | 0.61 |
| 1:C:250:SER:HB2 | 1:N:446:LYS:HG2 | 0.69 | 0.61 |
| 1:V:456:ARG:NH1 | 2:V:700:FDP:O2P | 2.28 | 0.61 |
| 1:C:390:GLU:HA | 1:P:372:ILE:CG1 | 2.15 | 0.61 |
| 1:E:214:ARG:N | 1:E:218:GLN:HE22 | 1.96 | 0.61 |
| 1:C:391:THR:C | 1:P:373:PRO:HB3 | 2.21 | 0.61 |
| 1:Q:270:PRO:HG2 | 1:Q:273:LYS:HE2 | 1.83 | 0.61 |
| 1:V:272:GLU:HG3 | 1:X:352:GLU:CB | 2.30 | 0.61 |
| 1:V:7:LEU:CD2 | 1:X:284:LYS:HG2 | 2.30 | 0.61 |
| 1:H:352:GLU:CG | 1:J:272:GLU:O | 2.49 | 0.61 |
| 1:S:373:PRO:CA | 1:T:390:GLU:O | 2.37 | 0.61 |
| 1:S:491:GLN:HG3 | 1:T:491:GLN:CD | 2.21 | 0.61 |
| 1:V:297:GLN:NE2 | 1:V:300:GLU:CD | 2.53 | 0.61 |
| 1:B:270:PRO:HG2 | 1:B:273:LYS:HE2 | 1.83 | 0.61 |
| 1:C:250:SER:CB | 1:N:446:LYS:CG | 2.46 | 0.61 |
| 1:L:11:ILE:CD1 | 1:L:12:PHE:HE2 | 2.12 | 0.61 |
| 1:P:370:GLN:CB | 1:P:374:MET:SD | 2.88 | 0.61 |
| 1:U:270:PRO:HG2 | 1:U:273:LYS:HE2 | 1.83 | 0.61 |
| 1:U:352:GLU:HG2 | 1:W:272:GLU:CB | 2.30 | 0.61 |
| 1:U:310:ARG:CZ | 1:W:297:GLN:OE1 | 2.49 | 0.61 |
| 1:E:11:ILE:HB | 1:G:273:LYS:HG2 | 1.82 | 0.61 |
| 1:H:279:LYS:HE3 | 1:J:6:ASN:OD1 | 2.01 | 0.61 |
| 1:J:144:ASP:O | 1:J:145:ASP:CB | 2.45 | 0.61 |
| 1:K:373:PRO:HB3 | 1:L:391:THR:CA | 2.26 | 0.61 |
| 1:O:456:ARG:NH1 | 2:O:700:FDP:O2P | 2.28 | 0.61 |
| 1:R:287:VAL:HG23 | 1:T:3:LEU:HD11 | 1.83 | 0.61 |
| 1:M:456:ARG:NH1 | 2:M:700:FDP:O2P | 2.28 | 0.61 |
| 1:T:456:ARG:NH1 | 2:T:700:FDP:O2P | 2.28 | 0.61 |
| 1:B:103:ARG:HD2 | 1:G:58:GLU:OE1 | 2.01 | 0.60 |
| 1:Q:456:ARG:NH2 | 2:Q:700:FDP:O1P | 2.34 | 0.60 |
| 1:D:400:SER:HB2 | 1:D:405:SER:HB2 | 1.84 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:311:ALA:HB1 | 1:G:312:GLU:HA | 1.82 | 0.60 |
| 1:H:270:PRO:HG2 | 1:H:273:LYS:HE2 | 1.83 | 0.60 |
| 1:N:446:LYS:O | 1:N:446:LYS:HD3 | 2.00 | 0.60 |
| 1:V:7:LEU:HD22 | 1:X:284:LYS:CG | 2.28 | 0.60 |
| 1:D:270:PRO:HG2 | 1:D:273:LYS:HE2 | 1.83 | 0.60 |
| 1:N:456:ARG:NH2 | 2:N:700:FDP:O1P | 2.34 | 0.60 |
| 1:O:400:SER:HB2 | 1:O:405:SER:HB2 | 1.83 | 0.60 |
| 1:Q:400:SER:HB2 | 1:Q:405:SER:HB2 | 1.84 | 0.60 |
| 1:K:270:PRO:HG2 | 1:K:273:LYS:HE2 | 1.83 | 0.60 |
| 1:M:400:SER:HB2 | 1:M:405:SER:HB2 | 1.83 | 0.60 |
| 1:O:270:PRO:HG2 | 1:O:273:LYS:HE2 | 1.83 | 0.60 |
| 1:B:272:GLU:CB | 1:C:352:GLU:HG2 | 2.30 | 0.60 |
| 1:C:58:GLU:OE1 | 1:E:103:ARG:HD2 | 2.02 | 0.60 |
| 1:E:472:THR:CG2 | 1:E:498:GLU:C | 2.70 | 0.60 |
| 1:H:296:THR:HG22 | 1:H:297:GLN:HG2 | 1.83 | 0.60 |
| 1:N:472:THR:CG2 | 1:N:498:GLU:C | 2.70 | 0.60 |
| 1:T:472:THR:CG2 | 1:T:498:GLU:C | 2.70 | 0.60 |
| 1:U:390:GLU:O | 1:V:373:PRO:HA | 2.02 | 0.60 |
| 1:U:372:ILE:HG13 | 1:V:390:GLU:O | 2.01 | 0.60 |
| 1:V:242:HIS:NE2 | 1:X:12:PHE:HE2 | 1.99 | 0.60 |
| 1:X:472:THR:CG2 | 1:X:498:GLU:C | 2.70 | 0.60 |
| 1:F:490:ASN:H | 1:F:490:ASN:HD22 | 1.50 | 0.60 |
| 1:E:242:HIS:CE1 | 1:G:12:PHE:HE2 | 2.17 | 0.60 |
| 1:H:400:SER:HB2 | 1:H:405:SER:HB2 | 1.84 | 0.60 |
| 1:K:400:SER:HB2 | 1:K:405:SER:HB2 | 1.84 | 0.60 |
| 1:L:400:SER:HB2 | 1:L:405:SER:HB2 | 1.84 | 0.60 |
| 1:S:490:ASN:H | 1:S:490:ASN:HD22 | 1.50 | 0.60 |
| 1:T:400:SER:HB2 | 1:T:405:SER:HB2 | 1.83 | 0.60 |
| 1:A:242:HIS:NE2 | 1:I:12:PHE:HZ | 1.99 | 0.60 |
| 1:A:270:PRO:HG2 | 1:A:273:LYS:HE2 | 1.83 | 0.60 |
| 1:A:472:THR:CG2 | 1:A:498:GLU:C | 2.70 | 0.60 |
| 1:D:212:PHE:CE1 | 1:D:241:ASN:ND2 | 2.70 | 0.60 |
| 1:E:212:PHE:CE1 | 1:E:241:ASN:ND2 | 2.70 | 0.60 |
| 1:G:400:SER:HB2 | 1:G:405:SER:HB2 | 1.83 | 0.60 |
| 1:G:472:THR:CG2 | 1:G:498:GLU:C | 2.70 | 0.60 |
| 1:O:490:ASN:HD22 | 1:O:490:ASN:H | 1.50 | 0.60 |
| 1:W:212:PHE:CE1 | 1:W:241:ASN:ND2 | 2.70 | 0.60 |
| 1:W:472:THR:CG2 | 1:W:498:GLU:C | 2.70 | 0.60 |
| 1:F:472:THR:CG2 | 1:F:498:GLU:C | 2.70 | 0.60 |
| 1:J:472:THR:CG2 | 1:J:498:GLU:C | 2.70 | 0.60 |
| 1:L:276:VAL:CG1 | 1:N:9:LEU:HB3 | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:472:THR:CG2 | 1:P:498:GLU:C | 2.70 | 0.60 |
| 1:R:472:THR:CG2 | 1:R:498:GLU:C | 2.70 | 0.60 |
| 1:U:144:ASP:O | 1:U:145:ASP:CB | 2.45 | 0.60 |
| 1:U:12:PHE:CZ | 1:W:242:HIS:CE1 | 2.84 | 0.60 |
| 1:W:490:ASN:H | 1:W:490:ASN:HD22 | 1.50 | 0.60 |
| 1:B:103:ARG:HB3 | 1:G:58:GLU:OE1 | 2.02 | 0.60 |
| 1:B:472:THR:CG2 | 1:B:498:GLU:C | 2.70 | 0.60 |
| 1:D:456:ARG:NH2 | 2:D:700:FDP:O1P | 2.34 | 0.60 |
| 1:E:11:ILE:O | 1:G:273:LYS:HE3 | 2.01 | 0.60 |
| 1:H:472:THR:CG2 | 1:H:498:GLU:C | 2.70 | 0.60 |
| 1:H:390:GLU:O | 1:I:373:PRO:CA | 2.48 | 0.60 |
| 1:J:490:ASN:H | 1:J:490:ASN:HD22 | 1.50 | 0.60 |
| 1:N:472:THR:HG22 | 1:N:498:GLU:C | 2.22 | 0.60 |
| 1:P:212:PHE:CE1 | 1:P:241:ASN:ND2 | 2.70 | 0.60 |
| 1:R:400:SER:HB2 | 1:R:405:SER:HB2 | 1.84 | 0.60 |
| 1:S:372:ILE:CG1 | 1:T:390:GLU:HG2 | 2.32 | 0.60 |
| 1:U:383:SER:HB2 | 1:V:383:SER:HB2 | 1.81 | 0.60 |
| 1:V:472:THR:CG2 | 1:V:498:GLU:C | 2.70 | 0.60 |
| 1:C:270:PRO:HG2 | 1:C:273:LYS:HE2 | 1.83 | 0.60 |
| 1:C:456:ARG:NH2 | 2:C:700:FDP:O1P | 2.34 | 0.60 |
| 1:F:456:ARG:NH2 | 2:F:700:FDP:O1P | 2.35 | 0.60 |
| 1:J:456:ARG:NH2 | 2:J:700:FDP:O1P | 2.34 | 0.60 |
| 1:M:490:ASN:HD22 | 1:M:490:ASN:H | 1.50 | 0.60 |
| 1:O:472:THR:CG2 | 1:O:498:GLU:C | 2.70 | 0.60 |
| 1:P:400:SER:HB2 | 1:P:405:SER:HB2 | 1.83 | 0.60 |
| 1:R:11:ILE:CD1 | 1:R:12:PHE:HE2 | 2.12 | 0.60 |
| 1:R:297:GLN:CG | 1:T:310:ARG:HG2 | 2.32 | 0.60 |
| 1:P:195:VAL:CG2 | 1:U:496:LEU:CG | 2.68 | 0.60 |
| 1:B:147:ILE:CG2 | 1:B:169:HIS:CD2 | 2.85 | 0.59 |
| 1:C:400:SER:HB2 | 1:C:405:SER:HB2 | 1.84 | 0.59 |
| 1:C:490:ASN:H | 1:C:490:ASN:HD22 | 1.50 | 0.59 |
| 1:F:400:SER:HB2 | 1:F:405:SER:HB2 | 1.83 | 0.59 |
| 1:I:472:THR:CG2 | 1:I:498:GLU:C | 2.70 | 0.59 |
| 1:L:472:THR:CG2 | 1:L:498:GLU:C | 2.70 | 0.59 |
| 1:Q:3:LEU:HD23 | 1:S:283:SER:HB3 | 1.84 | 0.59 |
| 1:U:472:THR:CG2 | 1:U:498:GLU:C | 2.70 | 0.59 |
| 1:X:456:ARG:HH22 | 2:X:700:FDP:P1 | 2.25 | 0.59 |
| 1:A:490:ASN:HD22 | 1:A:490:ASN:H | 1.50 | 0.59 |
| 1:C:212:PHE:CE1 | 1:C:241:ASN:ND2 | 2.70 | 0.59 |
| 1:H:147:ILE:CG2 | 1:H:169:HIS:CD2 | 2.85 | 0.59 |
| 1:O:147:ILE:CG2 | 1:O:169:HIS:CD2 | 2.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:472:THR:HG22 | 1:O:498:GLU:C | 2.23 | 0.59 |
| 1:R:276:VAL:HG13 | 1:T:9:LEU:CD1 | 2.32 | 0.59 |
| 1:U:311:ALA:HB1 | 1:W:312:GLU:CA | 2.21 | 0.59 |
| 1:V:147:ILE:CG2 | 1:V:169:HIS:CD2 | 2.85 | 0.59 |
| 1:V:297:GLN:NE2 | 1:V:300:GLU:HB2 | 2.05 | 0.59 |
| 1:V:456:ARG:HH22 | 2:V:700:FDP:P1 | 2.25 | 0.59 |
| 1:V:490:ASN:H | 1:V:490:ASN:HD22 | 1.50 | 0.59 |
| 1:X:400:SER:HB2 | 1:X:405:SER:HB2 | 1.83 | 0.59 |
| 1:X:456:ARG:NH1 | 2:X:700:FDP:O2P | 2.28 | 0.59 |
| 1:B:400:SER:HB2 | 1:B:405:SER:HB2 | 1.83 | 0.59 |
| 1:C:144:ASP:O | 1:C:145:ASP:CB | 2.45 | 0.59 |
| 1:G:147:ILE:CG2 | 1:G:169:HIS:CD2 | 2.86 | 0.59 |
| 1:J:472:THR:HG22 | 1:J:498:GLU:C | 2.23 | 0.59 |
| 1:M:147:ILE:CG2 | 1:M:169:HIS:CD2 | 2.86 | 0.59 |
| 1:M:472:THR:HG22 | 1:M:498:GLU:C | 2.23 | 0.59 |
| 1:U:147:ILE:CG2 | 1:U:169:HIS:CD2 | 2.85 | 0.59 |
| 1:U:400:SER:HB2 | 1:U:405:SER:HB2 | 1.84 | 0.59 |
| 1:V:400:SER:HB2 | 1:V:405:SER:HB2 | 1.84 | 0.59 |
| 1:D:472:THR:HG22 | 1:D:498:GLU:C | 2.22 | 0.59 |
| 1:E:400:SER:HB2 | 1:E:405:SER:HB2 | 1.84 | 0.59 |
| 1:F:472:THR:HG22 | 1:F:498:GLU:C | 2.23 | 0.59 |
| 1:I:147:ILE:CG2 | 1:I:169:HIS:CD2 | 2.85 | 0.59 |
| 1:I:404:ARG:CZ | 1:M:228:PRO:HG2 | 2.31 | 0.59 |
| 1:K:490:ASN:HD22 | 1:K:490:ASN:H | 1.50 | 0.59 |
| 1:Q:297:GLN:HB2 | 1:S:310:ARG:CG | 2.32 | 0.59 |
| 1:S:456:ARG:NH2 | 2:S:700:FDP:O1P | 2.34 | 0.59 |
| 1:T:472:THR:HG22 | 1:T:498:GLU:C | 2.23 | 0.59 |
| 1:V:472:THR:HG22 | 1:V:498:GLU:C | 2.23 | 0.59 |
| 1:C:472:THR:CG2 | 1:C:498:GLU:C | 2.70 | 0.59 |
| 1:D:472:THR:CG2 | 1:D:498:GLU:C | 2.70 | 0.59 |
| 1:F:212:PHE:CE1 | 1:F:241:ASN:ND2 | 2.70 | 0.59 |
| 1:H:472:THR:HG22 | 1:H:498:GLU:C | 2.23 | 0.59 |
| 1:L:371:HIS:CD2 | 1:L:373:PRO:O | 2.55 | 0.59 |
| 1:P:490:ASN:HD22 | 1:P:490:ASN:H | 1.50 | 0.59 |
| 1:S:383:SER:HB2 | 1:T:383:SER:CB | 2.33 | 0.59 |
| 1:A:147:ILE:CG2 | 1:A:169:HIS:CD2 | 2.85 | 0.59 |
| 1:A:456:ARG:NH2 | 2:A:700:FDP:O1P | 2.34 | 0.59 |
| 1:B:272:GLU:CG | 1:C:352:GLU:CG | 2.79 | 0.59 |
| 1:G:456:ARG:NH1 | 2:G:700:FDP:O2P | 2.28 | 0.59 |
| 1:I:11:ILE:CD1 | 1:I:12:PHE:HE2 | 2.12 | 0.59 |
| 1:H:352:GLU:HG2 | 1:J:272:GLU:CB | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:352:GLU:HG2 | 1:M:272:GLU:O | 2.03 | 0.59 |
| 1:K:472:THR:CG2 | 1:K:498:GLU:C | 2.70 | 0.59 |
| 1:L:490:ASN:HD22 | 1:L:490:ASN:H | 1.50 | 0.59 |
| 1:M:472:THR:CG2 | 1:M:498:GLU:C | 2.70 | 0.59 |
| 1:Q:147:ILE:CG2 | 1:Q:169:HIS:CD2 | 2.85 | 0.59 |
| 1:Q:472:THR:CG2 | 1:Q:498:GLU:C | 2.70 | 0.59 |
| 1:Q:472:THR:HG22 | 1:Q:498:GLU:C | 2.23 | 0.59 |
| 1:S:147:ILE:CG2 | 1:S:169:HIS:CD2 | 2.85 | 0.59 |
| 1:S:370:GLN:CB | 1:S:374:MET:SD | 2.90 | 0.59 |
| 1:U:456:ARG:NH2 | 2:U:700:FDP:O1P | 2.35 | 0.59 |
| 1:A:400:SER:HB2 | 1:A:405:SER:HB2 | 1.83 | 0.59 |
| 1:B:311:ALA:CB | 1:C:312:GLU:HA | 2.32 | 0.59 |
| 1:E:456:ARG:NH2 | 2:E:700:FDP:O1P | 2.34 | 0.59 |
| 1:F:147:ILE:CG2 | 1:F:169:HIS:CD2 | 2.85 | 0.59 |
| 1:H:371:HIS:O | 1:H:374:MET:CG | 2.36 | 0.59 |
| 1:K:212:PHE:CE1 | 1:K:241:ASN:ND2 | 2.70 | 0.59 |
| 1:K:311:ALA:CB | 1:M:312:GLU:HA | 2.32 | 0.59 |
| 1:K:456:ARG:HH22 | 2:K:700:FDP:P1 | 2.26 | 0.59 |
| 1:L:147:ILE:CG2 | 1:L:169:HIS:CD2 | 2.86 | 0.59 |
| 1:L:472:THR:HG22 | 1:L:498:GLU:C | 2.22 | 0.59 |
| 1:L:272:GLU:HG3 | 1:N:352:GLU:CG | 2.33 | 0.59 |
| 1:O:456:ARG:HH22 | 2:O:700:FDP:P1 | 2.25 | 0.59 |
| 1:P:147:ILE:CG2 | 1:P:169:HIS:CD2 | 2.86 | 0.59 |
| 1:P:456:ARG:HH22 | 2:P:700:FDP:P1 | 2.26 | 0.59 |
| 1:R:147:ILE:CG2 | 1:R:169:HIS:CD2 | 2.85 | 0.59 |
| 1:W:147:ILE:CG2 | 1:W:169:HIS:CD2 | 2.85 | 0.59 |
| 1:X:472:THR:HG22 | 1:X:498:GLU:C | 2.23 | 0.59 |
| 1:C:373:PRO:CB | 1:P:390:GLU:O | 2.51 | 0.59 |
| 1:H:383:SER:HB2 | 1:I:383:SER:CB | 2.29 | 0.59 |
| 1:L:273:LYS:CB | 1:N:11:ILE:HB | 2.33 | 0.59 |
| 1:L:270:PRO:CG | 1:L:273:LYS:HE2 | 2.23 | 0.59 |
| 1:O:242:HIS:HE1 | 1:P:12:PHE:CE2 | 2.20 | 0.59 |
| 1:Q:372:ILE:HD11 | 1:Q:374:MET:CE | 2.33 | 0.59 |
| 1:S:400:SER:HB2 | 1:S:405:SER:HB2 | 1.84 | 0.59 |
| 1:T:490:ASN:H | 1:T:490:ASN:HD22 | 1.50 | 0.59 |
| 1:S:491:GLN:CD | 1:T:491:GLN:NE2 | 2.56 | 0.59 |
| 1:W:472:THR:HG22 | 1:W:498:GLU:C | 2.23 | 0.59 |
| 1:B:372:ILE:HD11 | 1:B:374:MET:CE | 2.33 | 0.59 |
| 1:B:490:ASN:H | 1:B:490:ASN:HD22 | 1.50 | 0.59 |
| 1:G:456:ARG:HH22 | 2:G:700:FDP:P1 | 2.26 | 0.59 |
| 1:J:400:SER:HB2 | 1:J:405:SER:HB2 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:212:PHE:CE1 | 1:U:241:ASN:ND2 | 2.70 | 0.59 |
| 1:U:365:SER:HB3 | 1:W:3:LEU:HD12 | 1.84 | 0.59 |
| 1:W:372:ILE:HD11 | 1:W:374:MET:CE | 2.33 | 0.59 |
| 1:W:400:SER:HB2 | 1:W:405:SER:HB2 | 1.84 | 0.59 |
| 1:I:490:ASN:H | 1:I:490:ASN:HD22 | 1.50 | 0.59 |
| 1:J:372:ILE:HD11 | 1:J:374:MET:CE | 2.33 | 0.59 |
| 1:K:147:ILE:CG2 | 1:K:169:HIS:CD2 | 2.86 | 0.59 |
| 1:K:372:ILE:HD11 | 1:K:374:MET:CE | 2.33 | 0.59 |
| 1:L:229:LYS:HE3 | 1:S:487:GLY:CA | 2.33 | 0.59 |
| 1:L:456:ARG:NH1 | 2:L:700:FDP:O2P | 2.29 | 0.59 |
| 1:M:371:HIS:CD2 | 1:M:373:PRO:O | 2.55 | 0.59 |
| 1:M:456:ARG:HH22 | 2:M:700:FDP:P1 | 2.26 | 0.59 |
| 1:R:272:GLU:HG2 | 1:T:352:GLU:CG | 2.21 | 0.59 |
| 1:S:472:THR:CG2 | 1:S:498:GLU:C | 2.70 | 0.59 |
| 1:U:352:GLU:HG2 | 1:W:272:GLU:HB2 | 1.85 | 0.59 |
| 1:E:272:GLU:CG | 1:G:352:GLU:HG2 | 2.32 | 0.58 |
| 1:N:372:ILE:HD11 | 1:N:374:MET:CE | 2.33 | 0.58 |
| 1:P:472:THR:HG22 | 1:P:498:GLU:C | 2.23 | 0.58 |
| 1:R:490:ASN:HD22 | 1:R:490:ASN:H | 1.50 | 0.58 |
| 1:E:270:PRO:CG | 1:E:273:LYS:HE2 | 2.24 | 0.58 |
| 1:H:311:ALA:CB | 1:J:312:GLU:CG | 2.81 | 0.58 |
| 1:N:147:ILE:CG2 | 1:N:169:HIS:CD2 | 2.85 | 0.58 |
| 1:U:472:THR:HG22 | 1:U:498:GLU:C | 2.23 | 0.58 |
| 1:V:372:ILE:HD11 | 1:V:374:MET:CE | 2.33 | 0.58 |
| 1:W:372:ILE:CG1 | 1:X:390:GLU:HA | 2.23 | 0.58 |
| 1:A:472:THR:HG22 | 1:A:498:GLU:C | 2.22 | 0.58 |
| 1:C:472:THR:HG22 | 1:C:498:GLU:C | 2.23 | 0.58 |
| 1:E:490:ASN:HD22 | 1:E:490:ASN:H | 1.50 | 0.58 |
| 1:G:372:ILE:HD11 | 1:G:374:MET:CE | 2.33 | 0.58 |
| 1:I:472:THR:HG22 | 1:I:498:GLU:C | 2.23 | 0.58 |
| 1:J:147:ILE:CG2 | 1:J:169:HIS:CD2 | 2.85 | 0.58 |
| 1:N:490:ASN:H | 1:N:490:ASN:HD22 | 1.50 | 0.58 |
| 1:O:212:PHE:CE1 | 1:O:241:ASN:ND2 | 2.70 | 0.58 |
| 1:O:372:ILE:HD11 | 1:O:374:MET:CE | 2.33 | 0.58 |
| 1:R:212:PHE:CE1 | 1:R:241:ASN:ND2 | 2.70 | 0.58 |
| 1:L:487:GLY:CA | 1:S:229:LYS:HE3 | 2.28 | 0.58 |
| 1:U:372:ILE:HD12 | 1:U:374:MET:CG | 2.33 | 0.58 |
| 1:V:212:PHE:CE1 | 1:V:241:ASN:ND2 | 2.70 | 0.58 |
| 1:W:456:ARG:HH22 | 2:W:700:FDP:P1 | 2.26 | 0.58 |
| 1:A:372:ILE:HD11 | 1:A:374:MET:CE | 2.33 | 0.58 |
| 1:K:57:HIS:HE1 | 1:K:195:VAL:HG12 | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:297:GLN:HB2 | 1:N:310:ARG:HB2 | 1.84 | 0.58 |
| 1:L:456:ARG:HH22 | 2:L:700:FDP:P1 | 2.26 | 0.58 |
| 1:M:212:PHE:CE1 | 1:M:241:ASN:ND2 | 2.70 | 0.58 |
| 1:N:144:ASP:O | 1:N:145:ASP:CB | 2.45 | 0.58 |
| 1:Q:242:HIS:CE1 | 1:S:12:PHE:CZ | 2.91 | 0.58 |
| 1:T:147:ILE:CG2 | 1:T:169:HIS:CD2 | 2.85 | 0.58 |
| 1:X:372:ILE:HD11 | 1:X:374:MET:CE | 2.33 | 0.58 |
| 1:V:283:SER:O | 1:X:3:LEU:HD21 | 2.03 | 0.58 |
| 1:D:490:ASN:HD22 | 1:D:490:ASN:H | 1.50 | 0.58 |
| 1:E:147:ILE:CG2 | 1:E:169:HIS:CD2 | 2.85 | 0.58 |
| 1:F:372:ILE:HD11 | 1:F:374:MET:CE | 2.33 | 0.58 |
| 1:H:456:ARG:NH1 | 2:H:700:FDP:O2P | 2.29 | 0.58 |
| 1:I:212:PHE:CE1 | 1:I:241:ASN:ND2 | 2.70 | 0.58 |
| 1:M:57:HIS:HE1 | 1:M:195:VAL:HG12 | 1.69 | 0.58 |
| 1:N:400:SER:HB2 | 1:N:405:SER:HB2 | 1.84 | 0.58 |
| 1:T:212:PHE:CE1 | 1:T:241:ASN:ND2 | 2.70 | 0.58 |
| 1:X:57:HIS:HE1 | 1:X:195:VAL:HG12 | 1.69 | 0.58 |
| 1:B:283:SER:HB3 | 1:C:3:LEU:CD2 | 2.34 | 0.58 |
| 1:H:371:HIS:CD2 | 1:H:373:PRO:O | 2.57 | 0.58 |
| 1:H:57:HIS:HE1 | 1:H:195:VAL:HG12 | 1.69 | 0.58 |
| 1:I:400:SER:HB2 | 1:I:405:SER:HB2 | 1.84 | 0.58 |
| 1:H:11:ILE:C | 1:J:273:LYS:HG2 | 2.23 | 0.58 |
| 1:K:472:THR:HG22 | 1:K:498:GLU:C | 2.23 | 0.58 |
| 1:O:57:HIS:HE1 | 1:O:195:VAL:HG12 | 1.69 | 0.58 |
| 1:Q:212:PHE:CE1 | 1:Q:241:ASN:ND2 | 2.70 | 0.58 |
| 1:Q:269:ILE:CG1 | 1:S:11:ILE:HD12 | 2.31 | 0.58 |
| 1:Q:11:ILE:HD12 | 1:S:269:ILE:HG12 | 1.85 | 0.58 |
| 1:U:490:ASN:HD22 | 1:U:490:ASN:H | 1.50 | 0.58 |
| 1:V:57:HIS:HE1 | 1:V:195:VAL:HG12 | 1.69 | 0.58 |
| 1:X:147:ILE:CG2 | 1:X:169:HIS:CD2 | 2.86 | 0.58 |
| 1:A:212:PHE:CE1 | 1:A:241:ASN:ND2 | 2.70 | 0.58 |
| 1:C:147:ILE:CG2 | 1:C:169:HIS:CD2 | 2.86 | 0.58 |
| 1:D:11:ILE:HB | 1:F:273:LYS:CG | 2.31 | 0.58 |
| 1:A:242:HIS:CE1 | 1:I:12:PHE:HE2 | 2.18 | 0.58 |
| 1:C:391:THR:HA | 1:P:373:PRO:CB | 2.32 | 0.58 |
| 1:S:472:THR:HG22 | 1:S:498:GLU:C | 2.23 | 0.58 |
| 1:B:212:PHE:CE1 | 1:B:241:ASN:ND2 | 2.70 | 0.58 |
| 1:B:472:THR:HG22 | 1:B:498:GLU:C | 2.22 | 0.58 |
| 1:B:57:HIS:HE1 | 1:B:195:VAL:HG12 | 1.69 | 0.58 |
| 1:D:147:ILE:CG2 | 1:D:169:HIS:CD2 | 2.85 | 0.58 |
| 1:D:372:ILE:HD11 | 1:D:374:MET:CE | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:483:HIS:CD2 | 1:G:483:HIS:CD2 | 2.92 | 0.58 |
| 1:H:490:ASN:H | 1:H:490:ASN:HD22 | 1.50 | 0.58 |
| 1:I:456:ARG:NH2 | 2:I:700:FDP:O1P | 2.34 | 0.58 |
| 1:H:11:ILE:HA | 1:J:273:LYS:HG2 | 1.86 | 0.58 |
| 1:L:212:PHE:CE1 | 1:L:241:ASN:ND2 | 2.70 | 0.58 |
| 1:X:490:ASN:H | 1:X:490:ASN:HD22 | 1.50 | 0.58 |
| 1:C:372:ILE:HD11 | 1:C:374:MET:CE | 2.33 | 0.58 |
| 1:E:372:ILE:HD11 | 1:E:374:MET:CE | 2.33 | 0.58 |
| 1:D:279:LYS:HE3 | 1:F:6:ASN:OD1 | 2.04 | 0.58 |
| 1:H:11:ILE:O | 1:J:273:LYS:HD3 | 2.04 | 0.58 |
| 1:M:472:THR:HA | 1:M:497:VAL:O | 2.04 | 0.58 |
| 1:N:212:PHE:CE1 | 1:N:241:ASN:ND2 | 2.70 | 0.58 |
| 1:H:456:ARG:HH22 | 2:H:700:FDP:P1 | 2.26 | 0.58 |
| 1:L:283:SER:OG | 1:N:3:LEU:CD2 | 2.42 | 0.58 |
| 1:N:472:THR:HA | 1:N:497:VAL:O | 2.04 | 0.58 |
| 1:C:391:THR:CA | 1:P:373:PRO:HB3 | 2.33 | 0.58 |
| 1:T:456:ARG:HH22 | 2:T:700:FDP:P1 | 2.26 | 0.58 |
| 1:T:472:THR:HA | 1:T:497:VAL:O | 2.04 | 0.58 |
| 1:U:372:ILE:HG13 | 1:V:390:GLU:C | 2.24 | 0.58 |
| 1:U:310:ARG:HG2 | 1:W:297:GLN:CB | 2.30 | 0.58 |
| 1:F:57:HIS:HE1 | 1:F:195:VAL:HG12 | 1.69 | 0.57 |
| 1:G:472:THR:HA | 1:G:497:VAL:O | 2.04 | 0.57 |
| 1:H:9:LEU:HB3 | 1:J:276:VAL:HG13 | 1.85 | 0.57 |
| 1:R:472:THR:HA | 1:R:497:VAL:O | 2.04 | 0.57 |
| 1:U:472:THR:HA | 1:U:497:VAL:O | 2.04 | 0.57 |
| 1:U:272:GLU:HG3 | 1:W:352:GLU:HB2 | 1.86 | 0.57 |
| 1:E:472:THR:HG22 | 1:E:498:GLU:C | 2.23 | 0.57 |
| 1:G:212:PHE:CE1 | 1:G:241:ASN:ND2 | 2.70 | 0.57 |
| 1:N:57:HIS:HE1 | 1:N:195:VAL:HG12 | 1.69 | 0.57 |
| 1:P:472:THR:HA | 1:P:497:VAL:O | 2.04 | 0.57 |
| 1:R:472:THR:HG22 | 1:R:498:GLU:C | 2.23 | 0.57 |
| 1:C:472:THR:HA | 1:C:497:VAL:O | 2.04 | 0.57 |
| 1:E:272:GLU:HG3 | 1:G:352:GLU:HB2 | 1.85 | 0.57 |
| 1:H:491:GLN:HG3 | 1:I:491:GLN:HG3 | 1.86 | 0.57 |
| 1:I:472:THR:HA | 1:I:497:VAL:O | 2.05 | 0.57 |
| 1:U:57:HIS:HE1 | 1:U:195:VAL:HG12 | 1.69 | 0.57 |
| 1:B:456:ARG:NH2 | 2:B:700:FDP:O1P | 2.34 | 0.57 |
| 1:C:57:HIS:HE1 | 1:C:195:VAL:HG12 | 1.69 | 0.57 |
| 1:L:472:THR:HA | 1:L:497:VAL:O | 2.04 | 0.57 |
| 1:L:272:GLU:HG3 | 1:N:352:GLU:CB | 2.33 | 0.57 |
| 1:Q:490:ASN:H | 1:Q:490:ASN:HD22 | 1.50 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:280:ILE:CD1 | 1:T:9:LEU:HB2 | 2.32 | 0.57 |
| 1:A:283:SER:HB3 | 1:I:3:LEU:HD23 | 1.86 | 0.57 |
| 1:A:310:ARG:HG2 | 1:I:297:GLN:OE1 | 2.04 | 0.57 |
| 1:C:372:ILE:HG13 | 1:P:390:GLU:HA | 1.85 | 0.57 |
| 1:E:57:HIS:HE1 | 1:E:195:VAL:HG12 | 1.69 | 0.57 |
| 1:H:212:PHE:CE1 | 1:H:241:ASN:ND2 | 2.70 | 0.57 |
| 1:P:57:HIS:HE1 | 1:P:195:VAL:HG12 | 1.69 | 0.57 |
| 1:Q:472:THR:HA | 1:Q:497:VAL:O | 2.05 | 0.57 |
| 1:S:372:ILE:HG13 | 1:T:390:GLU:CB | 2.33 | 0.57 |
| 1:T:472:THR:CG2 | 1:T:498:GLU:HA | 2.18 | 0.57 |
| 1:W:372:ILE:HG13 | 1:X:390:GLU:C | 2.24 | 0.57 |
| 1:G:490:ASN:H | 1:G:490:ASN:HD22 | 1.50 | 0.57 |
| 1:H:496:LEU:HD21 | 1:M:195:VAL:CG2 | 2.33 | 0.57 |
| 1:J:57:HIS:HE1 | 1:J:195:VAL:HG12 | 1.69 | 0.57 |
| 1:T:57:HIS:HE1 | 1:T:195:VAL:HG12 | 1.69 | 0.57 |
| 1:V:242:HIS:NE2 | 1:X:12:PHE:CE2 | 2.73 | 0.57 |
| 1:X:472:THR:HA | 1:X:497:VAL:O | 2.04 | 0.57 |
| 1:A:472:THR:HA | 1:A:497:VAL:O | 2.04 | 0.57 |
| 1:B:472:THR:HA | 1:B:497:VAL:O | 2.05 | 0.57 |
| 1:D:57:HIS:HE1 | 1:D:195:VAL:HG12 | 1.69 | 0.57 |
| 1:E:472:THR:HA | 1:E:497:VAL:O | 2.04 | 0.57 |
| 1:F:472:THR:HA | 1:F:497:VAL:O | 2.04 | 0.57 |
| 1:H:242:HIS:CE1 | 1:J:12:PHE:HE2 | 2.13 | 0.57 |
| 1:I:57:HIS:HE1 | 1:I:195:VAL:HG12 | 1.69 | 0.57 |
| 1:L:57:HIS:HE1 | 1:L:195:VAL:HG12 | 1.69 | 0.57 |
| 1:L:6:ASN:O | 1:N:280:ILE:HG12 | 2.04 | 0.57 |
| 1:B:373:PRO:HB3 | 1:O:391:THR:O | 2.03 | 0.57 |
| 1:Q:11:ILE:O | 1:S:273:LYS:HE3 | 2.05 | 0.57 |
| 1:Q:57:HIS:HE1 | 1:Q:195:VAL:HG12 | 1.69 | 0.57 |
| 1:W:472:THR:HA | 1:W:497:VAL:O | 2.04 | 0.57 |
| 1:G:57:HIS:HE1 | 1:G:195:VAL:HG12 | 1.69 | 0.57 |
| 1:E:283:SER:HB3 | 1:G:3:LEU:CD2 | 2.35 | 0.57 |
| 1:G:472:THR:HG22 | 1:G:498:GLU:C | 2.23 | 0.57 |
| 1:L:280:ILE:HG13 | 1:N:6:ASN:O | 2.03 | 0.57 |
| 1:C:373:PRO:CB | 1:P:391:THR:HA | 2.33 | 0.57 |
| 1:R:11:ILE:HG12 | 1:R:12:PHE:CE2 | 2.40 | 0.57 |
| 1:R:57:HIS:HE1 | 1:R:195:VAL:HG12 | 1.69 | 0.57 |
| 1:S:212:PHE:CE1 | 1:S:241:ASN:ND2 | 2.70 | 0.57 |
| 1:H:472:THR:HA | 1:H:497:VAL:O | 2.04 | 0.57 |
| 1:L:273:LYS:CD | 1:N:11:ILE:O | 2.53 | 0.57 |
| 1:Q:12:PHE:CE2 | 1:S:242:HIS:CE1 | 2.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:273:LYS:HB3 | 1:T:11:ILE:HB | 1.85 | 0.57 |
| 1:R:456:ARG:NH2 | 2:R:700:FDP:O1P | 2.34 | 0.57 |
| 1:V:472:THR:HA | 1:V:497:VAL:O | 2.04 | 0.57 |
| 1:G:372:ILE:HD11 | 1:G:374:MET:HE1 | 1.86 | 0.57 |
| 1:J:212:PHE:CE1 | 1:J:241:ASN:ND2 | 2.70 | 0.57 |
| 1:V:272:GLU:CG | 1:X:352:GLU:CG | 2.82 | 0.57 |
| 1:W:57:HIS:HE1 | 1:W:195:VAL:HG12 | 1.69 | 0.57 |
| 1:J:472:THR:HA | 1:J:497:VAL:O | 2.04 | 0.56 |
| 1:K:472:THR:HA | 1:K:497:VAL:O | 2.04 | 0.56 |
| 1:L:472:THR:CG2 | 1:L:498:GLU:HA | 2.18 | 0.56 |
| 1:S:472:THR:HA | 1:S:497:VAL:O | 2.04 | 0.56 |
| 1:A:57:HIS:HE1 | 1:A:195:VAL:HG12 | 1.69 | 0.56 |
| 1:A:3:LEU:HD23 | 1:I:283:SER:CB | 2.34 | 0.56 |
| 1:D:472:THR:HA | 1:D:497:VAL:O | 2.04 | 0.56 |
| 1:M:372:ILE:HG23 | 1:N:390:GLU:O | 2.05 | 0.56 |
| 1:C:57:HIS:CE1 | 1:C:195:VAL:HG12 | 2.41 | 0.56 |
| 1:I:229:LYS:HE3 | 1:M:487:GLY:N | 2.19 | 0.56 |
| 1:K:310:ARG:HG2 | 1:M:297:GLN:OE1 | 2.05 | 0.56 |
| 1:U:11:ILE:HA | 1:W:273:LYS:HG2 | 1.85 | 0.56 |
| 1:C:498:GLU:HG2 | 1:V:195:VAL:HG11 | 1.87 | 0.56 |
| 1:D:373:PRO:HB3 | 1:E:391:THR:C | 2.25 | 0.56 |
| 1:F:57:HIS:CE1 | 1:F:195:VAL:HG12 | 2.41 | 0.56 |
| 1:M:372:ILE:HD11 | 1:N:390:GLU:HG2 | 1.87 | 0.56 |
| 1:O:472:THR:HA | 1:O:497:VAL:O | 2.04 | 0.56 |
| 1:P:195:VAL:HG22 | 1:U:496:LEU:HD23 | 1.85 | 0.56 |
| 1:Q:272:GLU:HG2 | 1:S:352:GLU:HG2 | 1.85 | 0.56 |
| 1:S:493:ARG:NE | 1:T:482:ASP:OD2 | 2.34 | 0.56 |
| 1:U:223:ARG:CG | 1:U:223:ARG:HH11 | 2.19 | 0.56 |
| 1:U:315:ASP:HB2 | 1:W:311:ALA:CA | 2.34 | 0.56 |
| 1:X:212:PHE:CE1 | 1:X:241:ASN:ND2 | 2.70 | 0.56 |
| 1:X:57:HIS:CE1 | 1:X:195:VAL:HG12 | 2.41 | 0.56 |
| 1:G:472:THR:CG2 | 1:G:498:GLU:HA | 2.18 | 0.56 |
| 1:K:491:GLN:HG3 | 1:L:491:GLN:HG3 | 1.87 | 0.56 |
| 1:L:352:GLU:HB2 | 1:N:272:GLU:HG3 | 1.87 | 0.56 |
| 1:N:57:HIS:CE1 | 1:N:195:VAL:HG12 | 2.41 | 0.56 |
| 1:O:57:HIS:CE1 | 1:O:195:VAL:HG12 | 2.41 | 0.56 |
| 1:P:223:ARG:CG | 1:P:223:ARG:HH11 | 2.19 | 0.56 |
| 1:U:57:HIS:CE1 | 1:U:195:VAL:HG12 | 2.41 | 0.56 |
| 1:V:57:HIS:CE1 | 1:V:195:VAL:HG12 | 2.41 | 0.56 |
| 1:D:312:GLU:HA | 1:F:311:ALA:HB1 | 1.87 | 0.56 |
| 1:E:57:HIS:CE1 | 1:E:195:VAL:HG12 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:57:HIS:CE1 | 1:G:195:VAL:HG12 | 2.41 | 0.56 |
| 1:L:11:ILE:HG12 | 1:L:12:PHE:CE2 | 2.40 | 0.56 |
| 1:S:57:HIS:HE1 | 1:S:195:VAL:HG12 | 1.69 | 0.56 |
| 1:A:223:ARG:HH11 | 1:A:223:ARG:CG | 2.19 | 0.56 |
| 1:H:390:GLU:HA | 1:I:372:ILE:HG13 | 1.88 | 0.56 |
| 1:K:57:HIS:CE1 | 1:K:195:VAL:HG12 | 2.41 | 0.56 |
| 1:Q:272:GLU:CG | 1:S:352:GLU:CG | 2.83 | 0.56 |
| 1:Q:57:HIS:CE1 | 1:Q:195:VAL:HG12 | 2.41 | 0.56 |
| 1:S:57:HIS:CE1 | 1:S:195:VAL:HG12 | 2.41 | 0.56 |
| 1:B:57:HIS:CE1 | 1:B:195:VAL:HG12 | 2.41 | 0.56 |
| 1:E:273:LYS:CG | 1:G:11:ILE:HB | 2.36 | 0.56 |
| 1:L:297:GLN:OE1 | 1:N:310:ARG:CG | 2.41 | 0.56 |
| 1:V:372:ILE:HD11 | 1:V:374:MET:HE1 | 1.87 | 0.56 |
| 1:C:223:ARG:CG | 1:C:223:ARG:HH11 | 2.19 | 0.56 |
| 1:I:57:HIS:CE1 | 1:I:195:VAL:HG12 | 2.41 | 0.56 |
| 1:J:57:HIS:CE1 | 1:J:195:VAL:HG12 | 2.41 | 0.56 |
| 1:T:370:GLN:CB | 1:T:374:MET:SD | 2.94 | 0.56 |
| 1:T:57:HIS:CE1 | 1:T:195:VAL:HG12 | 2.41 | 0.56 |
| 1:C:472:THR:CG2 | 1:C:498:GLU:HA | 2.18 | 0.56 |
| 1:I:270:PRO:CG | 1:I:273:LYS:HE2 | 2.24 | 0.56 |
| 1:R:57:HIS:CE1 | 1:R:195:VAL:HG12 | 2.41 | 0.56 |
| 1:B:269:ILE:HG12 | 1:C:11:ILE:CD1 | 2.35 | 0.56 |
| 1:A:3:LEU:HD21 | 1:I:283:SER:CB | 2.34 | 0.56 |
| 1:L:297:GLN:CB | 1:N:310:ARG:HG3 | 2.33 | 0.56 |
| 1:T:223:ARG:HH11 | 1:T:223:ARG:CG | 2.19 | 0.56 |
| 1:U:392:LYS:HD2 | 1:V:373:PRO:HD3 | 1.87 | 0.56 |
| 1:X:223:ARG:CG | 1:X:223:ARG:HH11 | 2.19 | 0.56 |
| 1:D:311:ALA:HB1 | 1:F:312:GLU:HA | 1.88 | 0.55 |
| 1:K:144:ASP:O | 1:K:145:ASP:CB | 2.45 | 0.55 |
| 1:W:223:ARG:CG | 1:W:223:ARG:HH11 | 2.19 | 0.55 |
| 1:W:456:ARG:NH1 | 2:W:700:FDP:O2P | 2.28 | 0.55 |
| 1:E:223:ARG:CG | 1:E:223:ARG:HH11 | 2.19 | 0.55 |
| 1:H:472:THR:CG2 | 1:H:498:GLU:HA | 2.18 | 0.55 |
| 1:M:144:ASP:O | 1:M:145:ASP:CB | 2.45 | 0.55 |
| 1:U:370:GLN:CB | 1:U:374:MET:SD | 2.94 | 0.55 |
| 1:D:57:HIS:CE1 | 1:D:195:VAL:HG12 | 2.41 | 0.55 |
| 1:H:57:HIS:CE1 | 1:H:195:VAL:HG12 | 2.41 | 0.55 |
| 1:I:223:ARG:CG | 1:I:223:ARG:HH11 | 2.19 | 0.55 |
| 1:K:272:GLU:C | 1:M:352:GLU:HG2 | 2.26 | 0.55 |
| 1:P:57:HIS:CE1 | 1:P:195:VAL:HG12 | 2.41 | 0.55 |
| 1:Q:9:LEU:HB2 | 1:S:280:ILE:HD11 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:57:HIS:CE1 | 1:W:195:VAL:HG12 | 2.41 | 0.55 |
| 1:B:297:GLN:HB2 | 1:C:310:ARG:HB2 | 1.87 | 0.55 |
| 1:N:446:LYS:C | 1:N:446:LYS:CD | 2.72 | 0.55 |
| 1:R:283:SER:CB | 1:T:3:LEU:HG | 2.36 | 0.55 |
| 1:D:223:ARG:CG | 1:D:223:ARG:HH11 | 2.19 | 0.55 |
| 1:H:273:LYS:HG2 | 1:J:11:ILE:O | 2.07 | 0.55 |
| 1:H:318:ASN:ND2 | 1:J:318:ASN:ND2 | 2.55 | 0.55 |
| 1:L:57:HIS:CE1 | 1:L:195:VAL:HG12 | 2.41 | 0.55 |
| 1:N:372:ILE:HD11 | 1:N:374:MET:HE1 | 1.89 | 0.55 |
| 1:P:487:GLY:HA3 | 1:V:229:LYS:CG | 2.27 | 0.55 |
| 1:U:365:SER:CB | 1:W:3:LEU:HD12 | 2.37 | 0.55 |
| 1:V:11:ILE:CD1 | 1:V:12:PHE:HE2 | 2.12 | 0.55 |
| 1:A:57:HIS:CE1 | 1:A:195:VAL:HG12 | 2.41 | 0.55 |
| 1:Q:272:GLU:O | 1:S:352:GLU:HG2 | 2.07 | 0.55 |
| 1:S:372:ILE:HG12 | 1:T:390:GLU:CA | 2.16 | 0.55 |
| 1:H:147:ILE:HG22 | 1:H:169:HIS:CD2 | 2.42 | 0.55 |
| 1:H:352:GLU:OE1 | 1:J:272:GLU:CG | 2.54 | 0.55 |
| 1:M:57:HIS:CE1 | 1:M:195:VAL:HG12 | 2.41 | 0.55 |
| 1:Q:372:ILE:HD12 | 1:Q:374:MET:HG2 | 1.89 | 0.55 |
| 1:R:272:GLU:C | 1:T:352:GLU:HG2 | 2.27 | 0.55 |
| 1:U:147:ILE:HG22 | 1:U:169:HIS:CD2 | 2.42 | 0.55 |
| 1:D:372:ILE:HD12 | 1:D:374:MET:HG2 | 1.89 | 0.55 |
| 1:D:53:SER:HA | 1:D:85:LYS:HG3 | 1.89 | 0.55 |
| 1:I:147:ILE:HG22 | 1:I:169:HIS:CD2 | 2.42 | 0.55 |
| 1:H:372:ILE:CG1 | 1:I:390:GLU:HA | 2.26 | 0.55 |
| 1:S:390:GLU:O | 1:T:373:PRO:CB | 2.55 | 0.55 |
| 1:W:147:ILE:HG22 | 1:W:169:HIS:CD2 | 2.42 | 0.55 |
| 1:X:147:ILE:HG22 | 1:X:169:HIS:CD2 | 2.42 | 0.55 |
| 1:I:11:ILE:HG12 | 1:I:12:PHE:CE2 | 2.40 | 0.55 |
| 1:J:193:ASP:O | 1:J:197:LEU:N | 2.38 | 0.55 |
| 1:N:147:ILE:HG22 | 1:N:169:HIS:CD2 | 2.42 | 0.55 |
| 1:N:223:ARG:HH11 | 1:N:223:ARG:CG | 2.19 | 0.55 |
| 1:N:372:ILE:HD12 | 1:N:374:MET:HG2 | 1.89 | 0.55 |
| 1:P:147:ILE:HG22 | 1:P:169:HIS:CD2 | 2.42 | 0.55 |
| 1:Q:242:HIS:HE1 | 1:S:12:PHE:CZ | 2.25 | 0.55 |
| 1:R:147:ILE:HG22 | 1:R:169:HIS:CD2 | 2.42 | 0.55 |
| 1:V:372:ILE:HD12 | 1:V:374:MET:HG2 | 1.89 | 0.55 |
| 1:W:372:ILE:CG2 | 1:X:390:GLU:O | 2.53 | 0.55 |
| 1:B:53:SER:HA | 1:B:85:LYS:HG3 | 1.89 | 0.54 |
| 1:C:372:ILE:HD12 | 1:C:374:MET:HG2 | 1.89 | 0.54 |
| 1:D:147:ILE:HG22 | 1:D:169:HIS:CD2 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:390:GLU:HA | 1:E:372:ILE:HG13 | 1.89 | 0.54 |
| 1:H:352:GLU:OE1 | 1:J:272:GLU:HG3 | 2.07 | 0.54 |
| 1:L:147:ILE:HG22 | 1:L:169:HIS:CD2 | 2.42 | 0.54 |
| 1:L:53:SER:HA | 1:L:85:LYS:HG3 | 1.89 | 0.54 |
| 1:W:372:ILE:HD12 | 1:W:374:MET:HG2 | 1.89 | 0.54 |
| 1:Q:147:ILE:HG22 | 1:Q:169:HIS:CD2 | 2.42 | 0.54 |
| 1:Q:223:ARG:CG | 1:Q:223:ARG:HH11 | 2.19 | 0.54 |
| 1:V:147:ILE:HG22 | 1:V:169:HIS:CD2 | 2.42 | 0.54 |
| 1:X:49:ARG:NE | 1:X:83:ASP:OD2 | 2.33 | 0.54 |
| 1:A:147:ILE:HG22 | 1:A:169:HIS:CD2 | 2.42 | 0.54 |
| 1:A:53:SER:HA | 1:A:85:LYS:HG3 | 1.89 | 0.54 |
| 1:G:372:ILE:HD12 | 1:G:374:MET:HG2 | 1.89 | 0.54 |
| 1:O:147:ILE:HG22 | 1:O:169:HIS:CD2 | 2.42 | 0.54 |
| 1:O:372:ILE:HD12 | 1:O:374:MET:HG2 | 1.89 | 0.54 |
| 1:C:147:ILE:HG22 | 1:C:169:HIS:CD2 | 2.42 | 0.54 |
| 1:J:372:ILE:HD12 | 1:J:374:MET:HG2 | 1.89 | 0.54 |
| 1:J:53:SER:HA | 1:J:85:LYS:HG3 | 1.89 | 0.54 |
| 1:K:372:ILE:HD12 | 1:K:374:MET:HG2 | 1.89 | 0.54 |
| 1:K:53:SER:HA | 1:K:85:LYS:HG3 | 1.89 | 0.54 |
| 1:L:284:LYS:HG3 | 1:N:7:LEU:HD21 | 1.89 | 0.54 |
| 1:R:270:PRO:CG | 1:R:273:LYS:HE2 | 2.23 | 0.54 |
| 1:T:147:ILE:HG22 | 1:T:169:HIS:CD2 | 2.42 | 0.54 |
| 1:V:272:GLU:HG3 | 1:X:352:GLU:CG | 2.37 | 0.54 |
| 1:B:147:ILE:HG22 | 1:B:169:HIS:CD2 | 2.42 | 0.54 |
| 1:E:11:ILE:HG12 | 1:E:12:PHE:CE2 | 2.40 | 0.54 |
| 1:M:147:ILE:HG22 | 1:M:169:HIS:CD2 | 2.42 | 0.54 |
| 1:Q:11:ILE:HB | 1:S:273:LYS:CG | 2.37 | 0.54 |
| 1:R:456:ARG:NH1 | 2:R:700:FDP:O2P | 2.34 | 0.54 |
| 1:V:276:VAL:O | 1:V:280:ILE:CD1 | 2.54 | 0.54 |
| 1:H:9:LEU:O | 1:J:280:ILE:HD11 | 2.07 | 0.54 |
| 1:K:223:ARG:CG | 1:K:223:ARG:HH11 | 2.19 | 0.54 |
| 1:K:390:GLU:HG2 | 1:L:374:MET:HE2 | 1.89 | 0.54 |
| 1:O:223:ARG:CG | 1:O:223:ARG:HH11 | 2.19 | 0.54 |
| 1:O:53:SER:HA | 1:O:85:LYS:HG3 | 1.89 | 0.54 |
| 1:S:147:ILE:HG22 | 1:S:169:HIS:CD2 | 2.42 | 0.54 |
| 1:T:53:SER:HA | 1:T:85:LYS:HG3 | 1.89 | 0.54 |
| 1:U:53:SER:HA | 1:U:85:LYS:HG3 | 1.89 | 0.54 |
| 1:V:273:LYS:HD3 | 1:X:11:ILE:O | 2.08 | 0.54 |
| 1:C:373:PRO:HB3 | 1:P:391:THR:CA | 2.38 | 0.54 |
| 1:F:193:ASP:O | 1:F:197:LEU:N | 2.38 | 0.54 |
| 1:H:223:ARG:CG | 1:H:223:ARG:HH11 | 2.19 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:144:ASP:O | 1:I:145:ASP:CB | 2.45 | 0.54 |
| 1:J:147:ILE:HG22 | 1:J:169:HIS:CD2 | 2.42 | 0.54 |
| 1:V:279:LYS:HB3 | 1:X:6:ASN:CG | 2.28 | 0.54 |
| 1:E:472:THR:CG2 | 1:E:498:GLU:HA | 2.18 | 0.54 |
| 1:F:147:ILE:HG22 | 1:F:169:HIS:CD2 | 2.42 | 0.54 |
| 1:F:223:ARG:CG | 1:F:223:ARG:HH11 | 2.19 | 0.54 |
| 1:F:53:SER:HA | 1:F:85:LYS:HG3 | 1.89 | 0.54 |
| 1:G:147:ILE:HG22 | 1:G:169:HIS:CD2 | 2.42 | 0.54 |
| 1:J:456:ARG:NH1 | 2:J:700:FDP:O2P | 2.34 | 0.54 |
| 1:N:53:SER:HA | 1:N:85:LYS:HG3 | 1.89 | 0.54 |
| 1:Q:53:SER:HA | 1:Q:85:LYS:HG3 | 1.89 | 0.54 |
| 1:R:49:ARG:NE | 1:R:83:ASP:OD2 | 2.33 | 0.54 |
| 1:S:53:SER:HA | 1:S:85:LYS:HG3 | 1.89 | 0.54 |
| 1:V:270:PRO:CG | 1:V:273:LYS:HE2 | 2.24 | 0.54 |
| 1:E:372:ILE:HD12 | 1:E:374:MET:HG2 | 1.89 | 0.54 |
| 1:H:270:PRO:HB2 | 1:H:273:LYS:HD2 | 1.90 | 0.54 |
| 1:P:53:SER:HA | 1:P:85:LYS:HG3 | 1.89 | 0.54 |
| 1:Q:273:LYS:HB3 | 1:S:11:ILE:HB | 1.88 | 0.54 |
| 1:Q:283:SER:CB | 1:S:3:LEU:HD21 | 2.38 | 0.54 |
| 1:V:276:VAL:CG1 | 1:X:9:LEU:HB3 | 2.37 | 0.54 |
| 1:W:53:SER:HA | 1:W:85:LYS:HG3 | 1.89 | 0.54 |
| 1:X:472:THR:CG2 | 1:X:498:GLU:HA | 2.18 | 0.54 |
| 1:B:273:LYS:HG2 | 1:C:11:ILE:O | 2.07 | 0.54 |
| 1:C:373:PRO:HB3 | 1:P:390:GLU:O | 2.08 | 0.54 |
| 1:D:12:PHE:HZ | 1:F:242:HIS:CE1 | 2.24 | 0.54 |
| 1:K:270:PRO:HB2 | 1:K:273:LYS:HD2 | 1.90 | 0.54 |
| 1:U:270:PRO:HB2 | 1:U:273:LYS:HD2 | 1.90 | 0.54 |
| 1:V:11:ILE:HG12 | 1:V:12:PHE:CE2 | 2.40 | 0.54 |
| 1:A:270:PRO:HG2 | 1:A:273:LYS:CE | 2.38 | 0.53 |
| 1:C:270:PRO:HB2 | 1:C:273:LYS:HD2 | 1.90 | 0.53 |
| 1:E:147:ILE:HG22 | 1:E:169:HIS:CD2 | 2.42 | 0.53 |
| 1:E:53:SER:HA | 1:E:85:LYS:HG3 | 1.89 | 0.53 |
| 1:H:11:ILE:CD1 | 1:J:269:ILE:HG12 | 2.38 | 0.53 |
| 1:I:195:VAL:HG22 | 1:N:496:LEU:CG | 2.36 | 0.53 |
| 1:L:276:VAL:HG13 | 1:N:9:LEU:HB3 | 1.90 | 0.53 |
| 1:O:272:GLU:O | 1:P:352:GLU:HG2 | 2.08 | 0.53 |
| 1:S:223:ARG:CG | 1:S:223:ARG:HH11 | 2.19 | 0.53 |
| 1:R:273:LYS:CD | 1:T:11:ILE:HB | 2.39 | 0.53 |
| 1:U:297:GLN:OE1 | 1:W:310:ARG:NH2 | 2.41 | 0.53 |
| 1:K:147:ILE:HG22 | 1:K:169:HIS:CD2 | 2.42 | 0.53 |
| 1:B:270:PRO:HB2 | 1:B:273:LYS:HD2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:390:GLU:O | 1:G:373:PRO:CB | 2.56 | 0.53 |
| 1:I:53:SER:HA | 1:I:85:LYS:HG3 | 1.89 | 0.53 |
| 1:L:229:LYS:CD | 1:S:487:GLY:HA2 | 2.38 | 0.53 |
| 1:O:12:PHE:HZ | 1:P:242:HIS:CE1 | 2.21 | 0.53 |
| 1:W:373:PRO:HB3 | 1:X:391:THR:C | 2.28 | 0.53 |
| 1:A:456:ARG:NH1 | 2:A:700:FDP:O2P | 2.34 | 0.53 |
| 1:B:270:PRO:HG2 | 1:B:273:LYS:CE | 2.38 | 0.53 |
| 1:F:372:ILE:HD12 | 1:F:374:MET:HG2 | 1.89 | 0.53 |
| 1:L:297:GLN:CB | 1:N:310:ARG:HB2 | 2.38 | 0.53 |
| 1:R:472:THR:CG2 | 1:R:498:GLU:HA | 2.18 | 0.53 |
| 1:U:494:ILE:HD12 | 1:V:376:ALA:HB1 | 1.89 | 0.53 |
| 1:D:270:PRO:HG2 | 1:D:273:LYS:CE | 2.38 | 0.53 |
| 1:L:223:ARG:CG | 1:L:223:ARG:HH11 | 2.19 | 0.53 |
| 1:N:472:THR:CG2 | 1:N:498:GLU:HA | 2.18 | 0.53 |
| 1:Q:272:GLU:C | 1:S:352:GLU:HG2 | 2.28 | 0.53 |
| 1:B:297:GLN:CD | 1:C:310:ARG:HG2 | 2.26 | 0.53 |
| 1:F:483:HIS:NE2 | 1:G:483:HIS:HD2 | 2.07 | 0.53 |
| 1:G:223:ARG:CG | 1:G:223:ARG:HH11 | 2.19 | 0.53 |
| 1:Q:270:PRO:HG2 | 1:Q:273:LYS:CE | 2.38 | 0.53 |
| 1:X:372:ILE:HD12 | 1:X:374:MET:HG2 | 1.89 | 0.53 |
| 1:G:53:SER:HA | 1:G:85:LYS:HG3 | 1.89 | 0.53 |
| 1:K:270:PRO:HG2 | 1:K:273:LYS:CE | 2.38 | 0.53 |
| 1:L:310:ARG:CG | 1:N:297:GLN:HB2 | 2.37 | 0.53 |
| 1:O:270:PRO:HB2 | 1:O:273:LYS:HD2 | 1.90 | 0.53 |
| 1:O:472:THR:CG2 | 1:O:498:GLU:HA | 2.18 | 0.53 |
| 1:Q:270:PRO:HB2 | 1:Q:273:LYS:HD2 | 1.90 | 0.53 |
| 1:Q:352:GLU:HB2 | 1:S:272:GLU:HG3 | 1.89 | 0.53 |
| 1:R:193:ASP:O | 1:R:197:LEU:N | 2.38 | 0.53 |
| 1:R:273:LYS:CG | 1:T:11:ILE:HB | 2.39 | 0.53 |
| 1:B:372:ILE:HD12 | 1:B:374:MET:HG2 | 1.89 | 0.53 |
| 1:C:89:ILE:CG2 | 1:C:177:VAL:HG22 | 2.39 | 0.53 |
| 1:H:53:SER:HA | 1:H:85:LYS:HG3 | 1.89 | 0.53 |
| 1:M:392:LYS:HD2 | 1:N:373:PRO:HD3 | 1.91 | 0.53 |
| 1:P:89:ILE:CG2 | 1:P:177:VAL:HG22 | 2.39 | 0.53 |
| 1:P:472:THR:CG2 | 1:P:498:GLU:HA | 2.18 | 0.53 |
| 1:R:53:SER:HA | 1:R:85:LYS:HG3 | 1.89 | 0.53 |
| 1:X:53:SER:HA | 1:X:85:LYS:HG3 | 1.89 | 0.53 |
| 1:B:297:GLN:CB | 1:C:310:ARG:HG2 | 2.38 | 0.53 |
| 1:D:89:ILE:CG2 | 1:D:177:VAL:HG22 | 2.39 | 0.53 |
| 1:K:89:ILE:CG2 | 1:K:177:VAL:HG22 | 2.39 | 0.53 |
| 1:L:89:ILE:CG2 | 1:L:177:VAL:HG22 | 2.39 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:89:ILE:CG2 | 1:N:177:VAL:HG22 | 2.39 | 0.53 |
| 1:O:311:ALA:HB1 | 1:P:312:GLU:CA | 2.26 | 0.53 |
| 1:S:89:ILE:CG2 | 1:S:177:VAL:HG22 | 2.39 | 0.53 |
| 1:V:11:ILE:HG13 | 1:V:12:PHE:HD2 | 1.72 | 0.53 |
| 1:V:53:SER:HA | 1:V:85:LYS:HG3 | 1.89 | 0.53 |
| 1:U:352:GLU:OE1 | 1:W:272:GLU:HG3 | 2.09 | 0.53 |
| 1:A:270:PRO:HB2 | 1:A:273:LYS:HD2 | 1.90 | 0.53 |
| 1:B:89:ILE:CG2 | 1:B:177:VAL:HG22 | 2.39 | 0.53 |
| 1:C:193:ASP:O | 1:C:197:LEU:N | 2.38 | 0.53 |
| 1:B:297:GLN:HB2 | 1:C:310:ARG:CB | 2.39 | 0.53 |
| 1:B:3:LEU:HD13 | 1:C:369:LEU:HD12 | 1.90 | 0.53 |
| 1:F:89:ILE:CG2 | 1:F:177:VAL:HG22 | 2.39 | 0.53 |
| 1:H:296:THR:HG22 | 1:H:297:GLN:CG | 2.39 | 0.53 |
| 1:J:240:GLU:HB3 | 1:J:264:ASP:HB2 | 1.91 | 0.53 |
| 1:M:240:GLU:HB3 | 1:M:264:ASP:HB2 | 1.91 | 0.53 |
| 1:R:270:PRO:O | 1:R:273:LYS:HB2 | 2.09 | 0.53 |
| 1:T:89:ILE:CG2 | 1:T:177:VAL:HG22 | 2.39 | 0.53 |
| 1:U:89:ILE:CG2 | 1:U:177:VAL:HG22 | 2.39 | 0.53 |
| 1:U:270:PRO:HG2 | 1:U:273:LYS:CE | 2.38 | 0.53 |
| 1:W:89:ILE:CG2 | 1:W:177:VAL:HG22 | 2.39 | 0.53 |
| 1:A:240:GLU:HB3 | 1:A:264:ASP:HB2 | 1.91 | 0.52 |
| 1:A:372:ILE:HD12 | 1:A:374:MET:HG2 | 1.89 | 0.52 |
| 1:E:270:PRO:O | 1:E:273:LYS:HB2 | 2.09 | 0.52 |
| 1:I:270:PRO:O | 1:I:273:LYS:HB2 | 2.09 | 0.52 |
| 1:M:383:SER:HB2 | 1:N:383:SER:CB | 2.33 | 0.52 |
| 1:L:272:GLU:HG2 | 1:N:352:GLU:HG2 | 1.91 | 0.52 |
| 1:L:276:VAL:HG13 | 1:N:9:LEU:CB | 2.39 | 0.52 |
| 1:C:270:PRO:HG2 | 1:C:273:LYS:CE | 2.38 | 0.52 |
| 1:C:390:GLU:HG2 | 1:P:372:ILE:HD11 | 1.91 | 0.52 |
| 1:C:53:SER:HA | 1:C:85:LYS:HG3 | 1.90 | 0.52 |
| 1:G:89:ILE:CG2 | 1:G:177:VAL:HG22 | 2.39 | 0.52 |
| 1:J:89:ILE:CG2 | 1:J:177:VAL:HG22 | 2.39 | 0.52 |
| 1:L:273:LYS:CD | 1:N:11:ILE:HB | 2.39 | 0.52 |
| 1:M:53:SER:HA | 1:M:85:LYS:HG3 | 1.89 | 0.52 |
| 1:N:193:ASP:O | 1:N:197:LEU:N | 2.38 | 0.52 |
| 1:S:240:GLU:HB3 | 1:S:264:ASP:HB2 | 1.91 | 0.52 |
| 1:H:372:ILE:HD12 | 1:H:374:MET:CG | 2.38 | 0.52 |
| 1:I:89:ILE:CG2 | 1:I:177:VAL:HG22 | 2.39 | 0.52 |
| 1:R:273:LYS:HG2 | 1:T:11:ILE:HA | 1.91 | 0.52 |
| 1:T:193:ASP:O | 1:T:197:LEU:N | 2.38 | 0.52 |
| 1:S:372:ILE:CG1 | 1:T:390:GLU:CB | 2.87 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:49:ARG:NE | 1:U:83:ASP:OD2 | 2.33 | 0.52 |
| 1:W:240:GLU:HB3 | 1:W:264:ASP:HB2 | 1.91 | 0.52 |
| 1:X:89:ILE:CG2 | 1:X:177:VAL:HG22 | 2.39 | 0.52 |
| 1:H:352:GLU:HG2 | 1:J:272:GLU:HB2 | 1.92 | 0.52 |
| 1:K:273:LYS:HB3 | 1:M:11:ILE:HB | 1.91 | 0.52 |
| 1:M:89:ILE:CG2 | 1:M:177:VAL:HG22 | 2.39 | 0.52 |
| 1:M:193:ASP:O | 1:M:197:LEU:N | 2.38 | 0.52 |
| 1:M:223:ARG:HH11 | 1:M:223:ARG:CG | 2.19 | 0.52 |
| 1:V:240:GLU:HB3 | 1:V:264:ASP:HB2 | 1.91 | 0.52 |
| 1:V:270:PRO:O | 1:V:273:LYS:HB2 | 2.09 | 0.52 |
| 1:X:193:ASP:O | 1:X:197:LEU:N | 2.38 | 0.52 |
| 1:B:240:GLU:HB3 | 1:B:264:ASP:HB2 | 1.91 | 0.52 |
| 1:E:240:GLU:HB3 | 1:E:264:ASP:HB2 | 1.91 | 0.52 |
| 1:H:270:PRO:HG2 | 1:H:273:LYS:CE | 2.38 | 0.52 |
| 1:O:270:PRO:HG2 | 1:O:273:LYS:CE | 2.38 | 0.52 |
| 1:O:89:ILE:CG2 | 1:O:177:VAL:HG22 | 2.39 | 0.52 |
| 1:R:89:ILE:CG2 | 1:R:177:VAL:HG22 | 2.39 | 0.52 |
| 1:V:287:VAL:HG23 | 1:X:3:LEU:CD2 | 2.40 | 0.52 |
| 1:D:270:PRO:HB2 | 1:D:273:LYS:HD2 | 1.90 | 0.52 |
| 1:D:12:PHE:HZ | 1:F:242:HIS:HE1 | 1.51 | 0.52 |
| 1:H:391:THR:HA | 1:I:373:PRO:HB3 | 1.91 | 0.52 |
| 1:J:223:ARG:CG | 1:J:223:ARG:HH11 | 2.19 | 0.52 |
| 1:J:372:ILE:HD11 | 1:J:374:MET:HE1 | 1.92 | 0.52 |
| 1:M:373:PRO:CB | 1:N:391:THR:HA | 2.39 | 0.52 |
| 1:O:193:ASP:O | 1:O:197:LEU:N | 2.38 | 0.52 |
| 1:O:270:PRO:HG2 | 1:O:273:LYS:HD2 | 1.92 | 0.52 |
| 1:P:193:ASP:O | 1:P:197:LEU:N | 2.38 | 0.52 |
| 1:Q:471:GLN:O | 1:Q:497:VAL:CG2 | 2.58 | 0.52 |
| 1:S:390:GLU:O | 1:T:373:PRO:HB3 | 2.09 | 0.52 |
| 1:U:240:GLU:HB3 | 1:U:264:ASP:HB2 | 1.91 | 0.52 |
| 1:U:471:GLN:O | 1:U:497:VAL:CG2 | 2.58 | 0.52 |
| 1:X:240:GLU:HB3 | 1:X:264:ASP:HB2 | 1.91 | 0.52 |
| 1:V:280:ILE:HA | 1:X:6:ASN:HB3 | 1.90 | 0.52 |
| 1:A:89:ILE:CG2 | 1:A:177:VAL:HG22 | 2.39 | 0.52 |
| 1:B:193:ASP:O | 1:B:197:LEU:N | 2.38 | 0.52 |
| 1:H:89:ILE:CG2 | 1:H:177:VAL:HG22 | 2.39 | 0.52 |
| 1:H:193:ASP:O | 1:H:197:LEU:N | 2.38 | 0.52 |
| 1:H:240:GLU:HB3 | 1:H:264:ASP:HB2 | 1.91 | 0.52 |
| 1:N:240:GLU:HB3 | 1:N:264:ASP:HB2 | 1.91 | 0.52 |
| 1:Q:89:ILE:CG2 | 1:Q:177:VAL:HG22 | 2.39 | 0.52 |
| 1:V:89:ILE:CG2 | 1:V:177:VAL:HG22 | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:471:GLN:O | 1:C:497:VAL:CG2 | 2.58 | 0.52 |
| 1:M:471:GLN:O | 1:M:497:VAL:CG2 | 2.58 | 0.52 |
| 1:O:310:ARG:CZ | 1:P:297:GLN:OE1 | 2.58 | 0.52 |
| 1:Q:270:PRO:HG2 | 1:Q:273:LYS:HD2 | 1.92 | 0.52 |
| 1:U:390:GLU:OE1 | 1:V:379:ALA:HB2 | 2.10 | 0.52 |
| 1:X:471:GLN:O | 1:X:497:VAL:CG2 | 2.58 | 0.52 |
| 1:A:270:PRO:HG2 | 1:A:273:LYS:HD2 | 1.92 | 0.52 |
| 1:K:270:PRO:HG2 | 1:K:273:LYS:HD2 | 1.92 | 0.52 |
| 1:O:471:GLN:O | 1:O:497:VAL:CG2 | 2.58 | 0.52 |
| 1:Q:373:PRO:HB3 | 1:R:390:GLU:O | 2.09 | 0.52 |
| 1:S:193:ASP:O | 1:S:197:LEU:N | 2.38 | 0.52 |
| 1:U:272:GLU:C | 1:W:352:GLU:HG2 | 2.29 | 0.52 |
| 1:W:471:GLN:O | 1:W:497:VAL:CG2 | 2.58 | 0.52 |
| 1:D:471:GLN:O | 1:D:497:VAL:CG2 | 2.58 | 0.51 |
| 1:E:456:ARG:HH22 | 2:E:700:FDP:P1 | 2.33 | 0.51 |
| 1:G:240:GLU:HB3 | 1:G:264:ASP:HB2 | 1.91 | 0.51 |
| 1:L:193:ASP:O | 1:L:197:LEU:N | 2.38 | 0.51 |
| 1:N:471:GLN:O | 1:N:497:VAL:CG2 | 2.58 | 0.51 |
| 1:B:223:ARG:CG | 1:B:223:ARG:HH11 | 2.19 | 0.51 |
| 1:C:240:GLU:HB3 | 1:C:264:ASP:HB2 | 1.91 | 0.51 |
| 1:B:280:ILE:HG12 | 1:C:6:ASN:O | 2.10 | 0.51 |
| 1:D:270:PRO:HG2 | 1:D:273:LYS:HD2 | 1.92 | 0.51 |
| 1:F:188:ALA:HA | 1:F:218:GLN:OE1 | 2.11 | 0.51 |
| 1:L:188:ALA:HA | 1:L:218:GLN:OE1 | 2.11 | 0.51 |
| 1:L:270:PRO:O | 1:L:273:LYS:HB2 | 2.09 | 0.51 |
| 1:L:471:GLN:O | 1:L:497:VAL:CG2 | 2.58 | 0.51 |
| 1:R:223:ARG:CG | 1:R:223:ARG:HH11 | 2.19 | 0.51 |
| 1:R:240:GLU:HB3 | 1:R:264:ASP:HB2 | 1.91 | 0.51 |
| 1:R:471:GLN:O | 1:R:497:VAL:CG2 | 2.58 | 0.51 |
| 1:B:297:GLN:OE1 | 1:C:310:ARG:CZ | 2.58 | 0.51 |
| 1:E:89:ILE:CG2 | 1:E:177:VAL:HG22 | 2.39 | 0.51 |
| 1:F:471:GLN:O | 1:F:497:VAL:CG2 | 2.58 | 0.51 |
| 1:G:471:GLN:O | 1:G:497:VAL:CG2 | 2.58 | 0.51 |
| 1:H:270:PRO:HG2 | 1:H:273:LYS:HD2 | 1.92 | 0.51 |
| 1:H:471:GLN:O | 1:H:497:VAL:CG2 | 2.58 | 0.51 |
| 1:P:240:GLU:HB3 | 1:P:264:ASP:HB2 | 1.92 | 0.51 |
| 1:S:372:ILE:HD11 | 1:T:390:GLU:CG | 2.21 | 0.51 |
| 1:S:372:ILE:CB | 1:T:390:GLU:O | 2.58 | 0.51 |
| 1:T:471:GLN:O | 1:T:497:VAL:CG2 | 2.58 | 0.51 |
| 1:V:471:GLN:O | 1:V:497:VAL:CG2 | 2.58 | 0.51 |
| 1:W:188:ALA:HA | 1:W:218:GLN:OE1 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:471:GLN:O | 1:B:497:VAL:CG2 | 2.58 | 0.51 |
| 1:I:193:ASP:O | 1:I:197:LEU:N | 2.38 | 0.51 |
| 1:L:372:ILE:HD12 | 1:L:374:MET:CG | 2.41 | 0.51 |
| 1:N:456:ARG:HH22 | 2:N:700:FDP:P1 | 2.34 | 0.51 |
| 1:P:471:GLN:O | 1:P:497:VAL:CG2 | 2.58 | 0.51 |
| 1:Q:279:LYS:HE3 | 1:S:6:ASN:OD1 | 2.10 | 0.51 |
| 1:V:223:ARG:CG | 1:V:223:ARG:HH11 | 2.19 | 0.51 |
| 1:V:352:GLU:OE1 | 1:X:273:LYS:NZ | 2.43 | 0.51 |
| 1:A:188:ALA:HA | 1:A:218:GLN:OE1 | 2.11 | 0.51 |
| 1:A:471:GLN:O | 1:A:497:VAL:CG2 | 2.58 | 0.51 |
| 1:M:188:ALA:HA | 1:M:218:GLN:OE1 | 2.11 | 0.51 |
| 1:N:456:ARG:NH1 | 2:N:700:FDP:O2P | 2.34 | 0.51 |
| 1:C:491:GLN:HG3 | 1:P:491:GLN:HG3 | 1.93 | 0.51 |
| 1:Q:3:LEU:HD23 | 1:S:283:SER:CB | 2.41 | 0.51 |
| 1:S:471:GLN:O | 1:S:497:VAL:CG2 | 2.58 | 0.51 |
| 1:T:188:ALA:HA | 1:T:218:GLN:OE1 | 2.11 | 0.51 |
| 1:V:188:ALA:HA | 1:V:218:GLN:OE1 | 2.11 | 0.51 |
| 1:B:103:ARG:CB | 1:G:58:GLU:OE1 | 2.59 | 0.51 |
| 1:B:270:PRO:HG2 | 1:B:273:LYS:HD2 | 1.92 | 0.51 |
| 1:I:188:ALA:HA | 1:I:218:GLN:OE1 | 2.11 | 0.51 |
| 1:M:483:HIS:NE2 | 1:N:483:HIS:HD2 | 2.09 | 0.51 |
| 1:B:492:THR:HG22 | 1:O:492:THR:HG22 | 1.92 | 0.51 |
| 1:P:211:SER:HA | 1:P:238:LYS:HD3 | 1.93 | 0.51 |
| 1:T:240:GLU:HB3 | 1:T:264:ASP:HB2 | 1.91 | 0.51 |
| 1:R:297:GLN:CB | 1:T:310:ARG:HB2 | 2.34 | 0.51 |
| 1:V:11:ILE:O | 1:X:273:LYS:HE3 | 2.10 | 0.51 |
| 1:C:456:ARG:NH1 | 2:C:700:FDP:O2P | 2.34 | 0.51 |
| 1:B:276:VAL:HG13 | 1:C:9:LEU:HB3 | 1.93 | 0.51 |
| 1:F:240:GLU:HB3 | 1:F:264:ASP:HB2 | 1.91 | 0.51 |
| 1:I:471:GLN:O | 1:I:497:VAL:CG2 | 2.58 | 0.51 |
| 1:Q:240:GLU:HB3 | 1:Q:264:ASP:HB2 | 1.91 | 0.51 |
| 1:U:372:ILE:HG23 | 1:V:390:GLU:C | 2.29 | 0.51 |
| 1:W:372:ILE:CG1 | 1:X:390:GLU:O | 2.58 | 0.51 |
| 1:C:211:SER:HA | 1:C:238:LYS:HD3 | 1.93 | 0.51 |
| 1:D:188:ALA:HA | 1:D:218:GLN:OE1 | 2.11 | 0.51 |
| 1:D:193:ASP:O | 1:D:197:LEU:N | 2.38 | 0.51 |
| 1:D:211:SER:HA | 1:D:238:LYS:HD3 | 1.93 | 0.51 |
| 1:E:193:ASP:O | 1:E:196:ASP:N | 2.44 | 0.51 |
| 1:E:471:GLN:O | 1:E:497:VAL:CG2 | 2.58 | 0.51 |
| 1:H:193:ASP:O | 1:H:196:ASP:N | 2.44 | 0.51 |
| 1:I:270:PRO:HD2 | 1:I:273:LYS:HD2 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:J:193:ASP:O | 1:J:196:ASP:N | 2.44 | 0.51 |
| 1:J:471:GLN:O | 1:J:497:VAL:CG2 | 2.58 | 0.51 |
| 1:J:49:ARG:NE | 1:J:83:ASP:OD2 | 2.33 | 0.51 |
| 1:K:211:SER:HA | 1:K:238:LYS:HD3 | 1.93 | 0.51 |
| 1:K:240:GLU:HB3 | 1:K:264:ASP:HB2 | 1.91 | 0.51 |
| 1:L:49:ARG:NE | 1:L:83:ASP:OD2 | 2.33 | 0.51 |
| 1:P:372:ILE:HD12 | 1:P:374:MET:CG | 2.40 | 0.51 |
| 1:S:188:ALA:HA | 1:S:218:GLN:OE1 | 2.11 | 0.51 |
| 1:U:373:PRO:HB3 | 1:V:391:THR:C | 2.32 | 0.51 |
| 1:V:193:ASP:O | 1:V:196:ASP:N | 2.44 | 0.51 |
| 1:V:49:ARG:NE | 1:V:83:ASP:OD2 | 2.33 | 0.51 |
| 1:E:269:ILE:HG12 | 1:G:11:ILE:HD12 | 1.93 | 0.51 |
| 1:I:147:ILE:HG21 | 1:I:169:HIS:CD2 | 2.46 | 0.51 |
| 1:I:240:GLU:HB3 | 1:I:264:ASP:HB2 | 1.91 | 0.51 |
| 1:H:373:PRO:HB3 | 1:I:391:THR:HA | 1.92 | 0.51 |
| 1:K:188:ALA:HA | 1:K:218:GLN:OE1 | 2.11 | 0.51 |
| 1:M:483:HIS:CD2 | 1:N:483:HIS:CD2 | 2.98 | 0.51 |
| 1:Q:193:ASP:O | 1:Q:196:ASP:N | 2.44 | 0.51 |
| 1:R:456:ARG:HH22 | 2:R:700:FDP:P1 | 2.34 | 0.51 |
| 1:S:147:ILE:HG21 | 1:S:169:HIS:NE2 | 2.26 | 0.51 |
| 1:U:211:SER:HA | 1:U:238:LYS:HD3 | 1.93 | 0.51 |
| 1:V:270:PRO:HD2 | 1:V:273:LYS:HD2 | 1.93 | 0.51 |
| 1:U:352:GLU:HG2 | 1:W:272:GLU:CG | 2.40 | 0.51 |
| 1:V:284:LYS:HG2 | 1:X:7:LEU:HD22 | 1.86 | 0.51 |
| 1:A:193:ASP:O | 1:A:196:ASP:N | 2.44 | 0.51 |
| 1:A:193:ASP:O | 1:A:197:LEU:N | 2.38 | 0.51 |
| 1:B:270:PRO:O | 1:B:273:LYS:HB2 | 2.11 | 0.51 |
| 1:B:272:GLU:HG2 | 1:C:352:GLU:HG2 | 1.93 | 0.51 |
| 1:C:270:PRO:O | 1:C:273:LYS:HB2 | 2.11 | 0.51 |
| 1:E:456:ARG:NH1 | 2:E:700:FDP:O2P | 2.34 | 0.51 |
| 1:F:483:HIS:HD2 | 1:G:483:HIS:NE2 | 2.08 | 0.51 |
| 1:K:270:PRO:O | 1:K:273:LYS:HB2 | 2.11 | 0.51 |
| 1:L:147:ILE:HG21 | 1:L:169:HIS:CD2 | 2.46 | 0.51 |
| 1:M:193:ASP:O | 1:M:196:ASP:N | 2.44 | 0.51 |
| 1:O:11:ILE:O | 1:P:273:LYS:CE | 2.56 | 0.51 |
| 1:O:188:ALA:HA | 1:O:218:GLN:OE1 | 2.11 | 0.51 |
| 1:O:240:GLU:HB3 | 1:O:264:ASP:HB2 | 1.91 | 0.51 |
| 1:Q:270:PRO:O | 1:Q:273:LYS:HB2 | 2.11 | 0.51 |
| 1:Q:456:ARG:HH22 | 2:Q:700:FDP:P1 | 2.34 | 0.51 |
| 1:S:193:ASP:O | 1:S:196:ASP:N | 2.44 | 0.51 |
| 1:S:49:ARG:NE | 1:S:83:ASP:OD2 | 2.33 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:193:ASP:O | 1:V:197:LEU:N | 2.38 | 0.51 |
| 1:W:211:SER:HA | 1:W:238:LYS:HD3 | 1.93 | 0.51 |
| 1:X:193:ASP:O | 1:X:196:ASP:N | 2.44 | 0.51 |
| 1:X:211:SER:HA | 1:X:238:LYS:HD3 | 1.93 | 0.51 |
| 1:B:188:ALA:HA | 1:B:218:GLN:OE1 | 2.11 | 0.50 |
| 1:B:310:ARG:HG2 | 1:C:297:GLN:HB2 | 1.92 | 0.50 |
| 1:D:193:ASP:O | 1:D:196:ASP:N | 2.44 | 0.50 |
| 1:E:147:ILE:HG21 | 1:E:169:HIS:NE2 | 2.27 | 0.50 |
| 1:E:188:ALA:HA | 1:E:218:GLN:OE1 | 2.11 | 0.50 |
| 1:E:283:SER:CB | 1:G:3:LEU:CD2 | 2.89 | 0.50 |
| 1:K:193:ASP:O | 1:K:196:ASP:N | 2.44 | 0.50 |
| 1:K:471:GLN:O | 1:K:497:VAL:CG2 | 2.58 | 0.50 |
| 1:O:147:ILE:HG21 | 1:O:169:HIS:NE2 | 2.26 | 0.50 |
| 1:O:270:PRO:O | 1:O:273:LYS:HB2 | 2.11 | 0.50 |
| 1:U:193:ASP:O | 1:U:196:ASP:N | 2.44 | 0.50 |
| 1:U:188:ALA:HA | 1:U:218:GLN:OE1 | 2.11 | 0.50 |
| 1:P:195:VAL:CG2 | 1:U:496:LEU:HD21 | 2.40 | 0.50 |
| 1:V:147:ILE:HG21 | 1:V:169:HIS:NE2 | 2.26 | 0.50 |
| 1:W:193:ASP:O | 1:W:197:LEU:N | 2.38 | 0.50 |
| 1:A:270:PRO:O | 1:A:273:LYS:HB2 | 2.11 | 0.50 |
| 1:B:193:ASP:O | 1:B:196:ASP:N | 2.44 | 0.50 |
| 1:C:147:ILE:HG21 | 1:C:169:HIS:NE2 | 2.27 | 0.50 |
| 1:C:456:ARG:HH22 | 2:C:700:FDP:P1 | 2.34 | 0.50 |
| 1:E:270:PRO:HD2 | 1:E:273:LYS:HD2 | 1.93 | 0.50 |
| 1:F:147:ILE:HG21 | 1:F:169:HIS:NE2 | 2.26 | 0.50 |
| 1:F:193:ASP:O | 1:F:196:ASP:N | 2.44 | 0.50 |
| 1:H:49:ARG:NE | 1:H:83:ASP:OD2 | 2.33 | 0.50 |
| 1:I:211:SER:HA | 1:I:238:LYS:HD3 | 1.93 | 0.50 |
| 1:H:311:ALA:HA | 1:J:315:ASP:HB2 | 1.93 | 0.50 |
| 1:J:456:ARG:HH22 | 2:J:700:FDP:P1 | 2.34 | 0.50 |
| 1:J:472:THR:CG2 | 1:J:498:GLU:HA | 2.18 | 0.50 |
| 1:L:193:ASP:O | 1:L:196:ASP:N | 2.44 | 0.50 |
| 1:L:240:GLU:HB3 | 1:L:264:ASP:HB2 | 1.91 | 0.50 |
| 1:L:270:PRO:HD2 | 1:L:273:LYS:HD2 | 1.93 | 0.50 |
| 1:L:297:GLN:CB | 1:N:310:ARG:CG | 2.89 | 0.50 |
| 1:L:297:GLN:HB2 | 1:N:310:ARG:CB | 2.41 | 0.50 |
| 1:M:211:SER:HA | 1:M:238:LYS:HD3 | 1.93 | 0.50 |
| 1:N:147:ILE:HG21 | 1:N:169:HIS:NE2 | 2.27 | 0.50 |
| 1:N:193:ASP:O | 1:N:196:ASP:N | 2.44 | 0.50 |
| 1:N:211:SER:HA | 1:N:238:LYS:HD3 | 1.93 | 0.50 |
| 1:O:193:ASP:O | 1:O:196:ASP:N | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:P:147:ILE:HG21 | 1:P:169:HIS:NE2 | 2.27 | 0.50 |
| 1:P:188:ALA:HA | 1:P:218:GLN:OE1 | 2.11 | 0.50 |
| 1:R:188:ALA:HA | 1:R:218:GLN:OE1 | 2.11 | 0.50 |
| 1:R:193:ASP:O | 1:R:196:ASP:N | 2.44 | 0.50 |
| 1:T:147:ILE:HG21 | 1:T:169:HIS:NE2 | 2.27 | 0.50 |
| 1:T:193:ASP:O | 1:T:196:ASP:N | 2.44 | 0.50 |
| 1:X:147:ILE:HG21 | 1:X:169:HIS:CD2 | 2.47 | 0.50 |
| 1:A:147:ILE:HG21 | 1:A:169:HIS:NE2 | 2.27 | 0.50 |
| 1:A:211:SER:HA | 1:A:238:LYS:HD3 | 1.93 | 0.50 |
| 1:A:456:ARG:HH22 | 2:A:700:FDP:P1 | 2.33 | 0.50 |
| 1:B:147:ILE:HG21 | 1:B:169:HIS:CD2 | 2.46 | 0.50 |
| 1:C:372:ILE:HD11 | 1:C:374:MET:HE1 | 1.92 | 0.50 |
| 1:D:270:PRO:O | 1:D:273:LYS:HB2 | 2.11 | 0.50 |
| 1:F:147:ILE:HG21 | 1:F:169:HIS:CD2 | 2.46 | 0.50 |
| 1:E:273:LYS:HG2 | 1:G:11:ILE:HB | 1.92 | 0.50 |
| 1:H:211:SER:HA | 1:H:238:LYS:HD3 | 1.93 | 0.50 |
| 1:J:188:ALA:HA | 1:J:218:GLN:OE1 | 2.11 | 0.50 |
| 1:P:193:ASP:O | 1:P:196:ASP:N | 2.44 | 0.50 |
| 1:R:270:PRO:HD2 | 1:R:273:LYS:HD2 | 1.93 | 0.50 |
| 1:S:211:SER:HA | 1:S:238:LYS:HD3 | 1.93 | 0.50 |
| 1:V:211:SER:HA | 1:V:238:LYS:HD3 | 1.93 | 0.50 |
| 1:D:240:GLU:HB3 | 1:D:264:ASP:HB2 | 1.91 | 0.50 |
| 1:D:456:ARG:HH22 | 2:D:700:FDP:P1 | 2.34 | 0.50 |
| 1:I:472:THR:CG2 | 1:I:498:GLU:HA | 2.18 | 0.50 |
| 1:J:193:ASP:CA | 1:J:196:ASP:HB2 | 2.41 | 0.50 |
| 1:N:147:ILE:HG21 | 1:N:169:HIS:CD2 | 2.46 | 0.50 |
| 1:N:188:ALA:HA | 1:N:218:GLN:OE1 | 2.11 | 0.50 |
| 1:Q:147:ILE:HG21 | 1:Q:169:HIS:NE2 | 2.26 | 0.50 |
| 1:U:147:ILE:HG21 | 1:U:169:HIS:CD2 | 2.46 | 0.50 |
| 1:U:270:PRO:O | 1:U:273:LYS:HB2 | 2.11 | 0.50 |
| 1:W:147:ILE:HG21 | 1:W:169:HIS:NE2 | 2.26 | 0.50 |
| 1:W:193:ASP:O | 1:W:196:ASP:N | 2.44 | 0.50 |
| 1:V:280:ILE:CD1 | 1:X:9:LEU:HB2 | 2.40 | 0.50 |
| 1:B:147:ILE:HG21 | 1:B:169:HIS:NE2 | 2.27 | 0.50 |
| 1:B:211:SER:HA | 1:B:238:LYS:HD3 | 1.93 | 0.50 |
| 1:G:188:ALA:HA | 1:G:218:GLN:OE1 | 2.11 | 0.50 |
| 1:H:312:GLU:CA | 1:J:311:ALA:CB | 2.71 | 0.50 |
| 1:M:147:ILE:HG21 | 1:M:169:HIS:CD2 | 2.46 | 0.50 |
| 1:K:352:GLU:HB2 | 1:M:272:GLU:HG3 | 1.94 | 0.50 |
| 1:O:352:GLU:HG2 | 1:P:272:GLU:O | 2.11 | 0.50 |
| 1:R:147:ILE:HG21 | 1:R:169:HIS:NE2 | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:T:193:ASP:CA | 1:T:196:ASP:HB2 | 2.42 | 0.50 |
| 1:U:11:ILE:O | 1:W:273:LYS:CG | 2.60 | 0.50 |
| 1:U:297:GLN:OE1 | 1:W:309:THR:HA | 2.12 | 0.50 |
| 1:W:390:GLU:OE1 | 1:X:379:ALA:HA | 2.12 | 0.50 |
| 1:B:456:ARG:HH22 | 2:B:700:FDP:P1 | 2.34 | 0.50 |
| 1:C:188:ALA:HA | 1:C:218:GLN:OE1 | 2.11 | 0.50 |
| 1:D:147:ILE:HG21 | 1:D:169:HIS:NE2 | 2.26 | 0.50 |
| 1:E:211:SER:HA | 1:E:238:LYS:HD3 | 1.93 | 0.50 |
| 1:J:147:ILE:HG21 | 1:J:169:HIS:CD2 | 2.46 | 0.50 |
| 1:J:147:ILE:HG21 | 1:J:169:HIS:NE2 | 2.26 | 0.50 |
| 1:K:372:ILE:HD11 | 1:L:390:GLU:HG2 | 1.93 | 0.50 |
| 1:K:297:GLN:OE1 | 1:M:310:ARG:NH2 | 2.45 | 0.50 |
| 1:O:147:ILE:HG21 | 1:O:169:HIS:CD2 | 2.46 | 0.50 |
| 1:R:211:SER:HA | 1:R:238:LYS:HD3 | 1.93 | 0.50 |
| 1:U:263:GLY:HA2 | 1:W:310:ARG:NH1 | 2.16 | 0.50 |
| 1:X:372:ILE:HD11 | 1:X:374:MET:HE2 | 1.93 | 0.50 |
| 1:B:472:THR:CG2 | 1:B:498:GLU:HA | 2.18 | 0.50 |
| 1:C:193:ASP:O | 1:C:196:ASP:N | 2.44 | 0.50 |
| 1:E:193:ASP:O | 1:E:197:LEU:N | 2.38 | 0.50 |
| 1:H:188:ALA:HA | 1:H:218:GLN:OE1 | 2.11 | 0.50 |
| 1:H:270:PRO:O | 1:H:273:LYS:HB2 | 2.11 | 0.50 |
| 1:I:11:ILE:HG13 | 1:I:12:PHE:HD2 | 1.72 | 0.50 |
| 1:L:7:LEU:CD2 | 1:N:284:LYS:HG3 | 2.42 | 0.50 |
| 1:T:211:SER:HA | 1:T:238:LYS:HD3 | 1.93 | 0.50 |
| 1:R:311:ALA:HB1 | 1:T:315:ASP:HB2 | 1.94 | 0.50 |
| 1:V:11:ILE:HG12 | 1:V:12:PHE:CD2 | 2.47 | 0.50 |
| 1:A:49:ARG:NE | 1:A:83:ASP:OD2 | 2.33 | 0.50 |
| 1:G:147:ILE:HG21 | 1:G:169:HIS:NE2 | 2.27 | 0.50 |
| 1:G:211:SER:HA | 1:G:238:LYS:HD3 | 1.93 | 0.50 |
| 1:L:211:SER:HA | 1:L:238:LYS:HD3 | 1.93 | 0.50 |
| 1:P:372:ILE:HD12 | 1:P:374:MET:HG3 | 1.92 | 0.50 |
| 1:Q:211:SER:HA | 1:Q:238:LYS:HD3 | 1.93 | 0.50 |
| 1:Q:491:GLN:HG3 | 1:R:491:GLN:HG3 | 1.93 | 0.50 |
| 1:S:51:ASN:HA | 1:S:83:ASP:HB3 | 1.94 | 0.50 |
| 1:V:284:LYS:CE | 1:X:7:LEU:HD22 | 2.41 | 0.50 |
| 1:X:188:ALA:HA | 1:X:218:GLN:OE1 | 2.11 | 0.50 |
| 1:B:51:ASN:HA | 1:B:83:ASP:HB3 | 1.94 | 0.50 |
| 1:C:51:ASN:HA | 1:C:83:ASP:HB3 | 1.94 | 0.50 |
| 1:D:49:ARG:NE | 1:D:83:ASP:OD2 | 2.33 | 0.50 |
| 1:I:193:ASP:O | 1:I:196:ASP:N | 2.44 | 0.50 |
| 1:J:211:SER:HA | 1:J:238:LYS:HD3 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:147:ILE:HG21 | 1:K:169:HIS:NE2 | 2.27 | 0.50 |
| 1:Q:272:GLU:CB | 1:S:352:GLU:HG2 | 2.42 | 0.50 |
| 1:S:456:ARG:HH22 | 2:S:700:FDP:P1 | 2.34 | 0.50 |
| 1:V:147:ILE:HG21 | 1:V:169:HIS:CD2 | 2.46 | 0.50 |
| 1:W:472:THR:CG2 | 1:W:498:GLU:HA | 2.18 | 0.50 |
| 1:X:147:ILE:HG21 | 1:X:169:HIS:NE2 | 2.27 | 0.50 |
| 1:F:211:SER:HA | 1:F:238:LYS:HD3 | 1.93 | 0.49 |
| 1:I:12:PHE:N | 1:I:12:PHE:CD2 | 2.79 | 0.49 |
| 1:K:147:ILE:HG21 | 1:K:169:HIS:CD2 | 2.47 | 0.49 |
| 1:Q:188:ALA:HA | 1:Q:218:GLN:OE1 | 2.11 | 0.49 |
| 1:Q:193:ASP:CA | 1:Q:196:ASP:HB2 | 2.42 | 0.49 |
| 1:T:147:ILE:HG21 | 1:T:169:HIS:CD2 | 2.47 | 0.49 |
| 1:U:352:GLU:HB2 | 1:W:272:GLU:HG3 | 1.94 | 0.49 |
| 1:D:147:ILE:HG21 | 1:D:169:HIS:CD2 | 2.46 | 0.49 |
| 1:F:49:ARG:NE | 1:F:83:ASP:OD2 | 2.33 | 0.49 |
| 1:G:193:ASP:O | 1:G:196:ASP:N | 2.44 | 0.49 |
| 1:H:147:ILE:HG21 | 1:H:169:HIS:NE2 | 2.26 | 0.49 |
| 1:M:147:ILE:HG21 | 1:M:169:HIS:NE2 | 2.26 | 0.49 |
| 1:N:51:ASN:HA | 1:N:83:ASP:HB3 | 1.94 | 0.49 |
| 1:R:147:ILE:HG21 | 1:R:169:HIS:CD2 | 2.46 | 0.49 |
| 1:U:456:ARG:HH22 | 2:U:700:FDP:P1 | 2.34 | 0.49 |
| 1:U:456:ARG:NH1 | 2:U:700:FDP:O2P | 2.35 | 0.49 |
| 1:U:383:SER:HB2 | 1:V:383:SER:CB | 2.42 | 0.49 |
| 1:A:147:ILE:HG21 | 1:A:169:HIS:CD2 | 2.46 | 0.49 |
| 1:A:51:ASN:HA | 1:A:83:ASP:HB3 | 1.95 | 0.49 |
| 1:F:456:ARG:HH22 | 2:F:700:FDP:P1 | 2.34 | 0.49 |
| 1:H:51:ASN:HA | 1:H:83:ASP:HB3 | 1.94 | 0.49 |
| 1:O:211:SER:HA | 1:O:238:LYS:HD3 | 1.93 | 0.49 |
| 1:Q:51:ASN:HA | 1:Q:83:ASP:HB3 | 1.94 | 0.49 |
| 1:W:390:GLU:OE1 | 1:X:379:ALA:CA | 2.60 | 0.49 |
| 1:H:147:ILE:HG21 | 1:H:169:HIS:CD2 | 2.46 | 0.49 |
| 1:I:49:ARG:NE | 1:I:83:ASP:OD2 | 2.33 | 0.49 |
| 1:L:147:ILE:HG21 | 1:L:169:HIS:NE2 | 2.27 | 0.49 |
| 1:Q:471:GLN:O | 1:Q:497:VAL:HG22 | 2.13 | 0.49 |
| 1:R:11:ILE:HG12 | 1:R:12:PHE:CD2 | 2.47 | 0.49 |
| 1:U:270:PRO:HG2 | 1:U:273:LYS:HD2 | 1.92 | 0.49 |
| 1:V:273:LYS:CD | 1:X:11:ILE:HB | 2.43 | 0.49 |
| 1:V:283:SER:HB3 | 1:X:3:LEU:HD23 | 1.93 | 0.49 |
| 1:W:147:ILE:HG21 | 1:W:169:HIS:CD2 | 2.46 | 0.49 |
| 1:X:270:PRO:O | 1:X:273:LYS:HB2 | 2.12 | 0.49 |
| 1:B:270:PRO:HD2 | 1:B:273:LYS:HD3 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:51:ASN:HA | 1:E:83:ASP:HB3 | 1.94 | 0.49 |
| 1:A:391:THR:O | 1:J:373:PRO:HB3 | 2.11 | 0.49 |
| 1:L:51:ASN:HA | 1:L:83:ASP:HB3 | 1.94 | 0.49 |
| 1:M:19:ARG:NH1 | 1:M:21:ALA:O | 2.46 | 0.49 |
| 1:L:12:PHE:CZ | 1:N:242:HIS:NE2 | 2.80 | 0.49 |
| 1:P:147:ILE:HG21 | 1:P:169:HIS:CD2 | 2.46 | 0.49 |
| 1:Q:147:ILE:HG21 | 1:Q:169:HIS:CD2 | 2.46 | 0.49 |
| 1:Q:284:LYS:HG3 | 1:S:7:LEU:HD22 | 1.93 | 0.49 |
| 1:S:147:ILE:HG21 | 1:S:169:HIS:CD2 | 2.46 | 0.49 |
| 1:U:471:GLN:O | 1:U:497:VAL:HG22 | 2.13 | 0.49 |
| 1:A:19:ARG:NH1 | 1:A:21:ALA:O | 2.46 | 0.49 |
| 1:C:471:GLN:O | 1:C:497:VAL:HG22 | 2.13 | 0.49 |
| 1:E:147:ILE:HG21 | 1:E:169:HIS:CD2 | 2.46 | 0.49 |
| 1:E:372:ILE:HD11 | 1:E:374:MET:HE1 | 1.93 | 0.49 |
| 1:G:147:ILE:HG21 | 1:G:169:HIS:CD2 | 2.47 | 0.49 |
| 1:G:19:ARG:NH1 | 1:G:21:ALA:O | 2.46 | 0.49 |
| 1:H:272:GLU:C | 1:J:352:GLU:HG2 | 2.32 | 0.49 |
| 1:I:456:ARG:HH22 | 2:I:700:FDP:P1 | 2.34 | 0.49 |
| 1:L:284:LYS:HG3 | 1:N:7:LEU:HD22 | 1.92 | 0.49 |
| 1:L:487:GLY:CA | 1:S:229:LYS:CG | 2.76 | 0.49 |
| 1:I:229:LYS:HD2 | 1:M:487:GLY:CA | 2.41 | 0.49 |
| 1:M:391:THR:HA | 1:N:373:PRO:HB3 | 1.94 | 0.49 |
| 1:Q:193:ASP:O | 1:Q:197:LEU:N | 2.38 | 0.49 |
| 1:Q:7:LEU:CD2 | 1:S:284:LYS:HG3 | 2.43 | 0.49 |
| 1:U:147:ILE:HG21 | 1:U:169:HIS:NE2 | 2.26 | 0.49 |
| 1:V:19:ARG:NH1 | 1:V:21:ALA:O | 2.46 | 0.49 |
| 1:A:193:ASP:CA | 1:A:196:ASP:HB2 | 2.41 | 0.49 |
| 1:B:471:GLN:O | 1:B:497:VAL:HG22 | 2.13 | 0.49 |
| 1:C:147:ILE:HG21 | 1:C:169:HIS:CD2 | 2.47 | 0.49 |
| 1:F:193:ASP:CA | 1:F:196:ASP:HB2 | 2.42 | 0.49 |
| 1:H:19:ARG:NH1 | 1:H:21:ALA:O | 2.46 | 0.49 |
| 1:I:147:ILE:HG21 | 1:I:169:HIS:NE2 | 2.26 | 0.49 |
| 1:I:51:ASN:HA | 1:I:83:ASP:HB3 | 1.94 | 0.49 |
| 1:N:270:PRO:O | 1:N:273:LYS:HB2 | 2.12 | 0.49 |
| 1:L:3:LEU:CD2 | 1:N:283:SER:HB3 | 2.42 | 0.49 |
| 1:T:270:PRO:O | 1:T:273:LYS:HB2 | 2.12 | 0.49 |
| 1:T:471:GLN:O | 1:T:497:VAL:HG22 | 2.13 | 0.49 |
| 1:U:51:ASN:HA | 1:U:83:ASP:HB3 | 1.94 | 0.49 |
| 1:V:482:ASP:H | 1:V:490:ASN:HD21 | 1.61 | 0.49 |
| 1:D:51:ASN:HA | 1:D:83:ASP:HB3 | 1.94 | 0.49 |
| 1:F:372:ILE:HD11 | 1:F:374:MET:HE1 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:51:ASN:HA | 1:F:83:ASP:HB3 | 1.95 | 0.49 |
| 1:G:471:GLN:O | 1:G:497:VAL:HG22 | 2.13 | 0.49 |
| 1:G:49:ARG:NE | 1:G:83:ASP:OD2 | 2.33 | 0.49 |
| 1:H:311:ALA:HA | 1:J:315:ASP:CB | 2.43 | 0.49 |
| 1:H:352:GLU:CB | 1:J:272:GLU:HB2 | 2.42 | 0.49 |
| 1:K:51:ASN:HA | 1:K:83:ASP:HB3 | 1.94 | 0.49 |
| 1:N:49:ARG:NE | 1:N:83:ASP:OD2 | 2.33 | 0.49 |
| 1:O:471:GLN:O | 1:O:497:VAL:HG22 | 2.13 | 0.49 |
| 1:S:471:GLN:O | 1:S:497:VAL:HG22 | 2.13 | 0.49 |
| 1:U:482:ASP:H | 1:U:490:ASN:HD21 | 1.61 | 0.49 |
| 1:V:471:GLN:O | 1:V:497:VAL:HG22 | 2.13 | 0.49 |
| 1:V:51:ASN:HA | 1:V:83:ASP:HB3 | 1.94 | 0.49 |
| 1:X:51:ASN:HA | 1:X:83:ASP:HB3 | 1.94 | 0.49 |
| 1:A:270:PRO:HD2 | 1:A:273:LYS:HD3 | 1.95 | 0.49 |
| 1:F:482:ASP:H | 1:F:490:ASN:HD21 | 1.61 | 0.49 |
| 1:E:273:LYS:HB3 | 1:G:11:ILE:HB | 1.95 | 0.49 |
| 1:F:391:THR:C | 1:G:373:PRO:HB3 | 2.33 | 0.49 |
| 1:C:216:ALA:CB | 1:N:446:LYS:CE | 2.81 | 0.49 |
| 1:N:482:ASP:H | 1:N:490:ASN:HD21 | 1.61 | 0.49 |
| 1:S:482:ASP:H | 1:S:490:ASN:HD21 | 1.61 | 0.49 |
| 1:V:276:VAL:C | 1:V:280:ILE:HD12 | 2.33 | 0.49 |
| 1:W:51:ASN:HA | 1:W:83:ASP:HB3 | 1.95 | 0.49 |
| 1:B:19:ARG:NH1 | 1:B:21:ALA:O | 2.46 | 0.49 |
| 1:C:19:ARG:NH1 | 1:C:21:ALA:O | 2.46 | 0.49 |
| 1:F:471:GLN:O | 1:F:497:VAL:HG22 | 2.13 | 0.49 |
| 1:A:12:PHE:CE2 | 1:I:242:HIS:CE1 | 3.00 | 0.49 |
| 1:K:310:ARG:CG | 1:M:297:GLN:HB2 | 2.43 | 0.49 |
| 1:L:11:ILE:HG13 | 1:L:12:PHE:HD2 | 1.72 | 0.49 |
| 1:L:482:ASP:H | 1:L:490:ASN:HD21 | 1.61 | 0.49 |
| 1:M:482:ASP:H | 1:M:490:ASN:HD21 | 1.61 | 0.49 |
| 1:M:471:GLN:O | 1:M:497:VAL:HG22 | 2.13 | 0.49 |
| 1:O:270:PRO:HD2 | 1:O:273:LYS:HD3 | 1.95 | 0.49 |
| 1:U:352:GLU:HG2 | 1:W:272:GLU:O | 2.13 | 0.49 |
| 1:C:482:ASP:H | 1:C:490:ASN:HD21 | 1.61 | 0.48 |
| 1:D:193:ASP:CA | 1:D:196:ASP:HB2 | 2.41 | 0.48 |
| 1:D:482:ASP:H | 1:D:490:ASN:HD21 | 1.61 | 0.48 |
| 1:G:90:ARG:HD3 | 1:G:174:ARG:O | 2.13 | 0.48 |
| 1:G:270:PRO:O | 1:G:273:LYS:HB2 | 2.12 | 0.48 |
| 1:G:51:ASN:HA | 1:G:83:ASP:HB3 | 1.94 | 0.48 |
| 1:J:471:GLN:O | 1:J:497:VAL:HG22 | 2.13 | 0.48 |
| 1:L:11:ILE:HG12 | 1:L:12:PHE:CD2 | 2.47 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:471:GLN:O | 1:L:497:VAL:HG22 | 2.13 | 0.48 |
| 1:P:471:GLN:O | 1:P:497:VAL:HG22 | 2.13 | 0.48 |
| 1:R:90:ARG:HD3 | 1:R:174:ARG:O | 2.13 | 0.48 |
| 1:T:90:ARG:HD3 | 1:T:174:ARG:O | 2.14 | 0.48 |
| 1:U:310:ARG:CB | 1:W:297:GLN:HB2 | 2.42 | 0.48 |
| 1:W:482:ASP:H | 1:W:490:ASN:HD21 | 1.61 | 0.48 |
| 1:B:283:SER:CB | 1:C:3:LEU:CD2 | 2.91 | 0.48 |
| 1:B:297:GLN:OE1 | 1:C:310:ARG:NH2 | 2.45 | 0.48 |
| 1:C:270:PRO:HD2 | 1:C:273:LYS:HD3 | 1.95 | 0.48 |
| 1:C:270:PRO:HG2 | 1:C:273:LYS:HD2 | 1.92 | 0.48 |
| 1:H:482:ASP:H | 1:H:490:ASN:HD21 | 1.61 | 0.48 |
| 1:J:90:ARG:HD3 | 1:J:174:ARG:O | 2.13 | 0.48 |
| 1:K:472:THR:CG2 | 1:K:498:GLU:HA | 2.18 | 0.48 |
| 1:L:90:ARG:HD3 | 1:L:174:ARG:O | 2.13 | 0.48 |
| 1:L:272:GLU:HB2 | 1:N:352:GLU:HG2 | 1.94 | 0.48 |
| 1:P:90:ARG:HD3 | 1:P:174:ARG:O | 2.14 | 0.48 |
| 1:P:89:ILE:HG21 | 1:P:177:VAL:HG22 | 1.96 | 0.48 |
| 1:R:12:PHE:N | 1:R:12:PHE:CD2 | 2.79 | 0.48 |
| 1:S:90:ARG:HD3 | 1:S:174:ARG:O | 2.13 | 0.48 |
| 1:V:284:LYS:HG3 | 1:X:7:LEU:HD23 | 1.80 | 0.48 |
| 1:A:482:ASP:H | 1:A:490:ASN:HD21 | 1.61 | 0.48 |
| 1:B:272:GLU:HG3 | 1:C:352:GLU:CG | 2.43 | 0.48 |
| 1:D:391:THR:C | 1:E:373:PRO:HB3 | 2.34 | 0.48 |
| 1:E:482:ASP:H | 1:E:490:ASN:HD21 | 1.61 | 0.48 |
| 1:E:471:GLN:O | 1:E:497:VAL:HG22 | 2.13 | 0.48 |
| 1:H:471:GLN:O | 1:H:497:VAL:HG22 | 2.13 | 0.48 |
| 1:I:89:ILE:HG21 | 1:I:177:VAL:HG22 | 1.96 | 0.48 |
| 1:I:90:ARG:HD3 | 1:I:174:ARG:O | 2.13 | 0.48 |
| 1:K:89:ILE:HG21 | 1:K:177:VAL:HG22 | 1.96 | 0.48 |
| 1:M:89:ILE:HG21 | 1:M:177:VAL:HG22 | 1.96 | 0.48 |
| 1:O:90:ARG:HD3 | 1:O:174:ARG:O | 2.13 | 0.48 |
| 1:O:51:ASN:HA | 1:O:83:ASP:HB3 | 1.94 | 0.48 |
| 1:Q:3:LEU:CD2 | 1:S:283:SER:CB | 2.91 | 0.48 |
| 1:U:90:ARG:HD3 | 1:U:174:ARG:O | 2.13 | 0.48 |
| 1:D:19:ARG:NH1 | 1:D:21:ALA:O | 2.46 | 0.48 |
| 1:F:90:ARG:HD3 | 1:F:174:ARG:O | 2.13 | 0.48 |
| 1:H:90:ARG:HD3 | 1:H:174:ARG:O | 2.13 | 0.48 |
| 1:H:372:ILE:HD11 | 1:I:390:GLU:HG2 | 1.94 | 0.48 |
| 1:K:471:GLN:O | 1:K:497:VAL:HG22 | 2.13 | 0.48 |
| 1:M:90:ARG:HD3 | 1:M:174:ARG:O | 2.13 | 0.48 |
| 1:R:273:LYS:CB | 1:T:11:ILE:HB | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:19:ARG:NH1 | 1:T:21:ALA:O | 2.46 | 0.48 |
| 1:T:51:ASN:HA | 1:T:83:ASP:HB3 | 1.94 | 0.48 |
| 1:U:19:ARG:NH1 | 1:U:21:ALA:O | 2.46 | 0.48 |
| 1:V:284:LYS:HE2 | 1:X:7:LEU:HD22 | 1.95 | 0.48 |
| 1:U:11:ILE:HB | 1:W:273:LYS:HB3 | 1.93 | 0.48 |
| 1:A:89:ILE:HG21 | 1:A:177:VAL:HG22 | 1.96 | 0.48 |
| 1:B:456:ARG:NH1 | 2:B:700:FDP:O2P | 2.34 | 0.48 |
| 1:D:212:PHE:HD2 | 1:D:214:ARG:HH21 | 1.62 | 0.48 |
| 1:J:51:ASN:HA | 1:J:83:ASP:HB3 | 1.94 | 0.48 |
| 1:Q:270:PRO:HD2 | 1:Q:273:LYS:HD3 | 1.95 | 0.48 |
| 1:R:482:ASP:H | 1:R:490:ASN:HD21 | 1.61 | 0.48 |
| 1:U:311:ALA:HB3 | 1:W:312:GLU:HG3 | 1.95 | 0.48 |
| 1:V:89:ILE:HG21 | 1:V:177:VAL:HG22 | 1.96 | 0.48 |
| 1:W:193:ASP:CA | 1:W:196:ASP:HB2 | 2.42 | 0.48 |
| 1:X:90:ARG:HD3 | 1:X:174:ARG:O | 2.13 | 0.48 |
| 1:A:90:ARG:HD3 | 1:A:174:ARG:O | 2.14 | 0.48 |
| 1:D:242:HIS:CE1 | 1:F:12:PHE:CE2 | 3.02 | 0.48 |
| 1:F:472:THR:CG2 | 1:F:498:GLU:HA | 2.18 | 0.48 |
| 1:H:483:HIS:CD2 | 1:I:483:HIS:CD2 | 3.01 | 0.48 |
| 1:J:19:ARG:NH1 | 1:J:21:ALA:O | 2.46 | 0.48 |
| 1:H:272:GLU:HG3 | 1:J:352:GLU:HB2 | 1.95 | 0.48 |
| 1:L:19:ARG:NH1 | 1:L:21:ALA:O | 2.46 | 0.48 |
| 1:M:51:ASN:HA | 1:M:83:ASP:HB3 | 1.94 | 0.48 |
| 1:M:376:ALA:HA | 1:N:494:ILE:HD12 | 1.96 | 0.48 |
| 1:Q:482:ASP:H | 1:Q:490:ASN:HD21 | 1.61 | 0.48 |
| 1:U:297:GLN:HB3 | 1:W:310:ARG:H | 1.77 | 0.48 |
| 1:W:90:ARG:HD3 | 1:W:174:ARG:O | 2.13 | 0.48 |
| 1:E:90:ARG:HD3 | 1:E:174:ARG:O | 2.13 | 0.48 |
| 1:E:212:PHE:HD2 | 1:E:214:ARG:HH21 | 1.62 | 0.48 |
| 1:F:89:ILE:HG21 | 1:F:177:VAL:HG22 | 1.96 | 0.48 |
| 1:G:193:ASP:CA | 1:G:196:ASP:HB2 | 2.41 | 0.48 |
| 1:H:89:ILE:HG21 | 1:H:177:VAL:HG22 | 1.96 | 0.48 |
| 1:I:195:VAL:CG2 | 1:N:496:LEU:HG | 2.43 | 0.48 |
| 1:C:390:GLU:O | 1:P:372:ILE:HG13 | 2.14 | 0.48 |
| 1:Q:212:PHE:HD2 | 1:Q:214:ARG:HH21 | 1.62 | 0.48 |
| 1:Q:276:VAL:CG1 | 1:S:9:LEU:HB3 | 2.43 | 0.48 |
| 1:Q:379:ALA:CB | 1:R:390:GLU:OE1 | 2.62 | 0.48 |
| 1:V:279:LYS:HB3 | 1:X:6:ASN:OD1 | 2.13 | 0.48 |
| 1:W:372:ILE:HD11 | 1:X:390:GLU:HG2 | 1.96 | 0.48 |
| 1:V:9:LEU:CB | 1:X:280:ILE:HD11 | 2.42 | 0.48 |
| 1:B:402:THR:OG1 | 1:B:404:ARG:HB2 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:471:GLN:O | 1:D:497:VAL:HG22 | 2.13 | 0.48 |
| 1:I:193:ASP:CA | 1:I:196:ASP:HB2 | 2.41 | 0.48 |
| 1:K:272:GLU:CG | 1:M:352:GLU:HG2 | 2.44 | 0.48 |
| 1:M:49:ARG:NE | 1:M:83:ASP:OD2 | 2.33 | 0.48 |
| 1:M:373:PRO:CA | 1:N:390:GLU:O | 2.46 | 0.48 |
| 1:N:90:ARG:HD3 | 1:N:174:ARG:O | 2.13 | 0.48 |
| 1:Q:193:ASP:O | 1:Q:196:ASP:HB2 | 2.14 | 0.48 |
| 1:R:51:ASN:HA | 1:R:83:ASP:HB3 | 1.94 | 0.48 |
| 1:Q:297:GLN:CD | 1:S:310:ARG:HG2 | 2.24 | 0.48 |
| 1:S:372:ILE:CG1 | 1:T:390:GLU:CG | 2.91 | 0.48 |
| 1:S:372:ILE:HG23 | 1:T:390:GLU:C | 2.33 | 0.48 |
| 1:U:89:ILE:HG21 | 1:U:177:VAL:HG22 | 1.96 | 0.48 |
| 1:V:212:PHE:HD2 | 1:V:214:ARG:HH21 | 1.62 | 0.48 |
| 1:W:471:GLN:O | 1:W:497:VAL:HG22 | 2.13 | 0.48 |
| 1:X:212:PHE:HD2 | 1:X:214:ARG:HH21 | 1.62 | 0.48 |
| 1:X:471:GLN:O | 1:X:497:VAL:HG22 | 2.13 | 0.48 |
| 1:E:402:THR:OG1 | 1:E:404:ARG:HB2 | 2.14 | 0.48 |
| 1:F:270:PRO:O | 1:F:273:LYS:HB2 | 2.14 | 0.48 |
| 1:F:390:GLU:HG2 | 1:G:372:ILE:HD11 | 1.94 | 0.48 |
| 1:G:193:ASP:O | 1:G:196:ASP:HB2 | 2.14 | 0.48 |
| 1:I:402:THR:OG1 | 1:I:404:ARG:HB2 | 2.14 | 0.48 |
| 1:J:402:THR:OG1 | 1:J:404:ARG:HB2 | 2.14 | 0.48 |
| 1:J:482:ASP:H | 1:J:490:ASN:HD21 | 1.61 | 0.48 |
| 1:M:212:PHE:HD2 | 1:M:214:ARG:HH21 | 1.62 | 0.48 |
| 1:O:49:ARG:NE | 1:O:83:ASP:OD2 | 2.33 | 0.48 |
| 1:P:270:PRO:O | 1:P:273:LYS:HB2 | 2.14 | 0.48 |
| 1:Q:311:ALA:CB | 1:S:312:GLU:HA | 2.43 | 0.48 |
| 1:T:49:ARG:NE | 1:T:83:ASP:OD2 | 2.33 | 0.48 |
| 1:T:89:ILE:HG21 | 1:T:177:VAL:HG22 | 1.96 | 0.48 |
| 1:V:12:PHE:CD2 | 1:V:12:PHE:N | 2.79 | 0.48 |
| 1:V:402:THR:OG1 | 1:V:404:ARG:HB2 | 2.14 | 0.48 |
| 1:X:19:ARG:NH1 | 1:X:21:ALA:O | 2.46 | 0.48 |
| 1:G:212:PHE:HD2 | 1:G:214:ARG:HH21 | 1.62 | 0.48 |
| 1:I:471:GLN:O | 1:I:497:VAL:HG22 | 2.13 | 0.48 |
| 1:J:212:PHE:HD2 | 1:J:214:ARG:HH21 | 1.62 | 0.48 |
| 1:K:19:ARG:NH1 | 1:K:21:ALA:O | 2.46 | 0.48 |
| 1:M:193:ASP:O | 1:M:196:ASP:HB2 | 2.14 | 0.48 |
| 1:N:471:GLN:O | 1:N:497:VAL:HG22 | 2.13 | 0.48 |
| 1:O:193:ASP:O | 1:O:196:ASP:HB2 | 2.14 | 0.48 |
| 1:P:402:THR:OG1 | 1:P:404:ARG:HB2 | 2.14 | 0.48 |
| 1:P:51:ASN:HA | 1:P:83:ASP:HB3 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:19:ARG:NH1 | 1:R:21:ALA:O | 2.46 | 0.48 |
| 1:S:193:ASP:O | 1:S:196:ASP:HB2 | 2.14 | 0.48 |
| 1:R:297:GLN:CD | 1:T:310:ARG:HG2 | 2.34 | 0.48 |
| 1:D:270:PRO:HD2 | 1:D:273:LYS:HD3 | 1.95 | 0.47 |
| 1:D:402:THR:OG1 | 1:D:404:ARG:HB2 | 2.14 | 0.47 |
| 1:E:89:ILE:HG21 | 1:E:177:VAL:HG22 | 1.96 | 0.47 |
| 1:H:311:ALA:O | 1:J:311:ALA:O | 2.31 | 0.47 |
| 1:I:11:ILE:HG12 | 1:I:12:PHE:CD2 | 2.47 | 0.47 |
| 1:J:193:ASP:O | 1:J:196:ASP:HB2 | 2.14 | 0.47 |
| 1:J:270:PRO:O | 1:J:273:LYS:HB2 | 2.14 | 0.47 |
| 1:L:273:LYS:HG2 | 1:N:11:ILE:CA | 2.44 | 0.47 |
| 1:L:372:ILE:HD12 | 1:L:374:MET:HG3 | 1.96 | 0.47 |
| 1:O:89:ILE:HG21 | 1:O:177:VAL:HG22 | 1.96 | 0.47 |
| 1:Q:19:ARG:NH1 | 1:Q:21:ALA:O | 2.46 | 0.47 |
| 1:Q:402:THR:OG1 | 1:Q:404:ARG:HB2 | 2.14 | 0.47 |
| 1:S:19:ARG:NH1 | 1:S:21:ALA:O | 2.46 | 0.47 |
| 1:S:402:THR:OG1 | 1:S:404:ARG:HB2 | 2.14 | 0.47 |
| 1:V:90:ARG:HD3 | 1:V:174:ARG:O | 2.13 | 0.47 |
| 1:X:193:ASP:O | 1:X:196:ASP:HB2 | 2.14 | 0.47 |
| 1:X:402:THR:OG1 | 1:X:404:ARG:HB2 | 2.14 | 0.47 |
| 1:X:89:ILE:HG21 | 1:X:177:VAL:HG22 | 1.96 | 0.47 |
| 1:B:89:ILE:HG21 | 1:B:177:VAL:HG22 | 1.96 | 0.47 |
| 1:C:49:ARG:NE | 1:C:83:ASP:OD2 | 2.33 | 0.47 |
| 1:H:371:HIS:C | 1:H:372:ILE:HD13 | 2.34 | 0.47 |
| 1:N:89:ILE:HG21 | 1:N:177:VAL:HG22 | 1.95 | 0.47 |
| 1:R:471:GLN:O | 1:R:497:VAL:HG22 | 2.13 | 0.47 |
| 1:S:384:ALA:O | 1:S:387:SER:HB2 | 2.14 | 0.47 |
| 1:U:193:ASP:O | 1:U:196:ASP:HB2 | 2.14 | 0.47 |
| 1:A:193:ASP:O | 1:A:196:ASP:HB2 | 2.14 | 0.47 |
| 1:A:471:GLN:O | 1:A:497:VAL:HG22 | 2.13 | 0.47 |
| 1:C:402:THR:OG1 | 1:C:404:ARG:HB2 | 2.14 | 0.47 |
| 1:D:472:THR:CG2 | 1:D:498:GLU:HA | 2.18 | 0.47 |
| 1:K:193:ASP:CA | 1:K:196:ASP:HB2 | 2.41 | 0.47 |
| 1:K:270:PRO:HD2 | 1:K:273:LYS:HD3 | 1.95 | 0.47 |
| 1:L:89:ILE:HG21 | 1:L:177:VAL:HG22 | 1.95 | 0.47 |
| 1:O:315:ASP:CB | 1:P:311:ALA:HA | 2.42 | 0.47 |
| 1:O:365:SER:CB | 1:P:3:LEU:HD12 | 2.45 | 0.47 |
| 1:R:212:PHE:HD2 | 1:R:214:ARG:HH21 | 1.62 | 0.47 |
| 1:T:193:ASP:O | 1:T:196:ASP:HB2 | 2.14 | 0.47 |
| 1:U:6:ASN:OD1 | 1:W:279:LYS:CE | 2.51 | 0.47 |
| 1:C:193:ASP:O | 1:C:196:ASP:HB2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:384:ALA:O | 1:D:387:SER:HB2 | 2.14 | 0.47 |
| 1:E:103:ARG:HG3 | 1:E:167:ASN:HA | 1.97 | 0.47 |
| 1:H:270:PRO:HD2 | 1:H:273:LYS:HD3 | 1.95 | 0.47 |
| 1:I:193:ASP:O | 1:I:196:ASP:HB2 | 2.14 | 0.47 |
| 1:I:482:ASP:H | 1:I:490:ASN:HD21 | 1.61 | 0.47 |
| 1:P:384:ALA:O | 1:P:387:SER:HB2 | 2.15 | 0.47 |
| 1:Q:49:ARG:NE | 1:Q:83:ASP:OD2 | 2.33 | 0.47 |
| 1:T:212:PHE:HD2 | 1:T:214:ARG:HH21 | 1.62 | 0.47 |
| 1:R:11:ILE:HB | 1:T:273:LYS:HG2 | 1.95 | 0.47 |
| 1:T:402:THR:OG1 | 1:T:404:ARG:HB2 | 2.14 | 0.47 |
| 1:W:19:ARG:NH1 | 1:W:21:ALA:O | 2.46 | 0.47 |
| 1:X:482:ASP:H | 1:X:490:ASN:HD21 | 1.61 | 0.47 |
| 1:C:193:ASP:CA | 1:C:196:ASP:HB2 | 2.41 | 0.47 |
| 1:C:90:ARG:HD3 | 1:C:174:ARG:O | 2.13 | 0.47 |
| 1:D:456:ARG:NH1 | 2:D:700:FDP:O2P | 2.34 | 0.47 |
| 1:G:482:ASP:H | 1:G:490:ASN:HD21 | 1.61 | 0.47 |
| 1:H:384:ALA:O | 1:H:387:SER:HB2 | 2.14 | 0.47 |
| 1:J:384:ALA:O | 1:J:387:SER:HB2 | 2.14 | 0.47 |
| 1:O:19:ARG:NH1 | 1:O:21:ALA:O | 2.46 | 0.47 |
| 1:O:310:ARG:NH2 | 1:P:297:GLN:OE1 | 2.47 | 0.47 |
| 1:Q:90:ARG:HD3 | 1:Q:174:ARG:O | 2.14 | 0.47 |
| 1:C:496:LEU:CG | 1:V:195:VAL:CG2 | 2.80 | 0.47 |
| 1:V:193:ASP:O | 1:V:196:ASP:HB2 | 2.14 | 0.47 |
| 1:X:193:ASP:CA | 1:X:196:ASP:HB2 | 2.41 | 0.47 |
| 1:X:384:ALA:O | 1:X:387:SER:HB2 | 2.14 | 0.47 |
| 1:C:384:ALA:O | 1:C:387:SER:HB2 | 2.14 | 0.47 |
| 1:D:90:ARG:HD3 | 1:D:174:ARG:O | 2.13 | 0.47 |
| 1:D:89:ILE:HG21 | 1:D:177:VAL:HG22 | 1.96 | 0.47 |
| 1:F:193:ASP:O | 1:F:196:ASP:HB2 | 2.14 | 0.47 |
| 1:K:482:ASP:H | 1:K:490:ASN:HD21 | 1.61 | 0.47 |
| 1:L:384:ALA:O | 1:L:387:SER:HB2 | 2.14 | 0.47 |
| 1:M:193:ASP:CA | 1:M:196:ASP:HB2 | 2.41 | 0.47 |
| 1:N:193:ASP:O | 1:N:196:ASP:HB2 | 2.14 | 0.47 |
| 1:N:224:LYS:HE3 | 1:N:224:LYS:HB3 | 1.81 | 0.47 |
| 1:O:270:PRO:CG | 1:O:273:LYS:HD2 | 2.45 | 0.47 |
| 1:O:310:ARG:HG2 | 1:P:297:GLN:CB | 2.42 | 0.47 |
| 1:P:212:PHE:HD2 | 1:P:214:ARG:HH21 | 1.62 | 0.47 |
| 1:P:19:ARG:NH1 | 1:P:21:ALA:O | 2.46 | 0.47 |
| 1:S:89:ILE:HG21 | 1:S:177:VAL:HG22 | 1.96 | 0.47 |
| 1:U:270:PRO:HD2 | 1:U:273:LYS:HD3 | 1.95 | 0.47 |
| 1:C:250:SER:HB2 | 1:N:446:LYS:CD | 2.37 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:193:ASP:O | 1:D:196:ASP:HB2 | 2.14 | 0.47 |
| 1:F:384:ALA:O | 1:F:387:SER:HB2 | 2.14 | 0.47 |
| 1:H:193:ASP:O | 1:H:196:ASP:HB2 | 2.14 | 0.47 |
| 1:I:384:ALA:O | 1:I:387:SER:HB2 | 2.14 | 0.47 |
| 1:L:193:ASP:CA | 1:L:196:ASP:HB2 | 2.41 | 0.47 |
| 1:N:402:THR:OG1 | 1:N:404:ARG:HB2 | 2.14 | 0.47 |
| 1:O:384:ALA:O | 1:O:387:SER:HB2 | 2.14 | 0.47 |
| 1:O:482:ASP:H | 1:O:490:ASN:HD21 | 1.61 | 0.47 |
| 1:Q:297:GLN:HB2 | 1:S:310:ARG:HG2 | 1.95 | 0.47 |
| 1:S:493:ARG:HG2 | 1:T:482:ASP:OD2 | 2.15 | 0.47 |
| 1:Q:284:LYS:CG | 1:S:7:LEU:CD2 | 2.90 | 0.47 |
| 1:U:212:PHE:HD2 | 1:U:214:ARG:HH21 | 1.62 | 0.47 |
| 1:U:310:ARG:HB2 | 1:W:297:GLN:HB2 | 1.97 | 0.47 |
| 1:U:372:ILE:HD12 | 1:U:374:MET:HG2 | 1.97 | 0.47 |
| 1:W:212:PHE:HD2 | 1:W:214:ARG:HH21 | 1.62 | 0.47 |
| 1:W:89:ILE:HG21 | 1:W:177:VAL:HG22 | 1.96 | 0.47 |
| 1:G:384:ALA:O | 1:G:387:SER:HB2 | 2.15 | 0.47 |
| 1:G:402:THR:OG1 | 1:G:404:ARG:HB2 | 2.15 | 0.47 |
| 1:G:89:ILE:HG21 | 1:G:177:VAL:HG22 | 1.96 | 0.47 |
| 1:H:270:PRO:CG | 1:H:273:LYS:HD2 | 2.45 | 0.47 |
| 1:J:89:ILE:HG21 | 1:J:177:VAL:HG22 | 1.96 | 0.47 |
| 1:K:193:ASP:O | 1:K:196:ASP:HB2 | 2.14 | 0.47 |
| 1:K:193:ASP:O | 1:K:197:LEU:N | 2.38 | 0.47 |
| 1:L:12:PHE:CD2 | 1:L:12:PHE:N | 2.79 | 0.47 |
| 1:O:212:PHE:HD2 | 1:O:214:ARG:HH21 | 1.62 | 0.47 |
| 1:O:365:SER:HB3 | 1:P:3:LEU:HD12 | 1.95 | 0.47 |
| 1:W:384:ALA:O | 1:W:387:SER:HB2 | 2.14 | 0.47 |
| 1:B:482:ASP:H | 1:B:490:ASN:HD21 | 1.61 | 0.47 |
| 1:E:384:ALA:O | 1:E:387:SER:HB2 | 2.14 | 0.47 |
| 1:F:402:THR:OG1 | 1:F:404:ARG:HB2 | 2.14 | 0.47 |
| 1:H:11:ILE:HG13 | 1:H:12:PHE:HD2 | 1.80 | 0.47 |
| 1:H:242:HIS:NE2 | 1:J:12:PHE:HE2 | 2.11 | 0.47 |
| 1:I:212:PHE:HD2 | 1:I:214:ARG:HH21 | 1.62 | 0.47 |
| 1:I:456:ARG:NH1 | 2:I:700:FDP:O2P | 2.34 | 0.47 |
| 1:J:224:LYS:HB3 | 1:J:224:LYS:HE3 | 1.82 | 0.47 |
| 1:K:90:ARG:HD3 | 1:K:174:ARG:O | 2.13 | 0.47 |
| 1:M:270:PRO:O | 1:M:273:LYS:HB2 | 2.14 | 0.47 |
| 1:P:193:ASP:O | 1:P:196:ASP:HB2 | 2.14 | 0.47 |
| 1:P:49:ARG:NE | 1:P:83:ASP:OD2 | 2.33 | 0.47 |
| 1:R:89:ILE:HG21 | 1:R:177:VAL:HG22 | 1.96 | 0.47 |
| 1:C:89:ILE:HG21 | 1:C:177:VAL:HG22 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:11:ILE:O | 1:F:273:LYS:HE3 | 2.15 | 0.47 |
| 1:D:270:PRO:CG | 1:D:273:LYS:HD2 | 2.45 | 0.47 |
| 1:E:193:ASP:O | 1:E:196:ASP:HB2 | 2.14 | 0.47 |
| 1:F:212:PHE:HD2 | 1:F:214:ARG:HH21 | 1.62 | 0.47 |
| 1:H:193:ASP:CA | 1:H:196:ASP:HB2 | 2.42 | 0.47 |
| 1:K:297:GLN:CB | 1:M:310:ARG:HG2 | 2.44 | 0.47 |
| 1:N:19:ARG:NH1 | 1:N:21:ALA:O | 2.46 | 0.47 |
| 1:Q:89:ILE:HG21 | 1:Q:177:VAL:HG22 | 1.96 | 0.47 |
| 1:U:384:ALA:O | 1:U:387:SER:HB2 | 2.14 | 0.47 |
| 1:V:193:ASP:CA | 1:V:196:ASP:HB2 | 2.41 | 0.47 |
| 1:V:370:GLN:CB | 1:V:374:MET:SD | 3.03 | 0.47 |
| 1:A:270:PRO:CG | 1:A:273:LYS:HD2 | 2.45 | 0.47 |
| 1:A:370:GLN:CB | 1:A:374:MET:SD | 3.03 | 0.47 |
| 1:B:270:PRO:CG | 1:B:273:LYS:HD2 | 2.45 | 0.47 |
| 1:B:384:ALA:O | 1:B:387:SER:HB2 | 2.14 | 0.47 |
| 1:D:373:PRO:HB3 | 1:E:391:THR:HA | 1.97 | 0.47 |
| 1:I:19:ARG:NH1 | 1:I:21:ALA:O | 2.46 | 0.47 |
| 1:L:212:PHE:HD2 | 1:L:214:ARG:HH21 | 1.62 | 0.47 |
| 1:L:231:ARG:HH21 | 1:S:231:ARG:HH21 | 1.62 | 0.47 |
| 1:M:402:THR:OG1 | 1:M:404:ARG:HB2 | 2.14 | 0.47 |
| 1:L:273:LYS:HG2 | 1:N:11:ILE:HB | 1.96 | 0.47 |
| 1:N:384:ALA:O | 1:N:387:SER:HB2 | 2.14 | 0.47 |
| 1:O:11:ILE:HB | 1:P:273:LYS:CB | 2.45 | 0.47 |
| 1:S:270:PRO:O | 1:S:273:LYS:HB2 | 2.14 | 0.47 |
| 1:T:384:ALA:O | 1:T:387:SER:HB2 | 2.14 | 0.47 |
| 1:W:193:ASP:O | 1:W:196:ASP:HB2 | 2.14 | 0.47 |
| 1:A:283:SER:HB3 | 1:I:3:LEU:HD21 | 1.96 | 0.46 |
| 1:A:402:THR:OG1 | 1:A:404:ARG:HB2 | 2.14 | 0.46 |
| 1:B:193:ASP:CA | 1:B:196:ASP:HB2 | 2.41 | 0.46 |
| 1:B:193:ASP:O | 1:B:196:ASP:HB2 | 2.14 | 0.46 |
| 1:C:212:PHE:HD2 | 1:C:214:ARG:HH21 | 1.62 | 0.46 |
| 1:E:12:PHE:N | 1:E:12:PHE:CD2 | 2.79 | 0.46 |
| 1:H:311:ALA:CB | 1:J:312:GLU:HG2 | 2.44 | 0.46 |
| 1:P:482:ASP:H | 1:P:490:ASN:HD21 | 1.61 | 0.46 |
| 1:U:193:ASP:CA | 1:U:196:ASP:HB2 | 2.41 | 0.46 |
| 1:A:384:ALA:O | 1:A:387:SER:HB2 | 2.14 | 0.46 |
| 1:B:311:ALA:HA | 1:C:315:ASP:HB2 | 1.97 | 0.46 |
| 1:D:272:GLU:HG3 | 1:F:352:GLU:HB2 | 1.97 | 0.46 |
| 1:L:193:ASP:O | 1:L:196:ASP:HB2 | 2.14 | 0.46 |
| 1:M:384:ALA:O | 1:M:387:SER:HB2 | 2.14 | 0.46 |
| 1:O:424:ARG:CG | 1:O:424:ARG:NH1 | 2.41 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:193:ASP:CA | 1:P:196:ASP:HB2 | 2.42 | 0.46 |
| 1:Q:284:LYS:CG | 1:S:7:LEU:HD22 | 2.46 | 0.46 |
| 1:T:372:ILE:HD12 | 1:T:374:MET:CG | 2.46 | 0.46 |
| 1:V:384:ALA:O | 1:V:387:SER:HB2 | 2.14 | 0.46 |
| 1:X:370:GLN:CB | 1:X:374:MET:SD | 3.03 | 0.46 |
| 1:A:273:LYS:NZ | 1:I:352:GLU:OE1 | 2.48 | 0.46 |
| 1:C:270:PRO:CG | 1:C:273:LYS:HD2 | 2.45 | 0.46 |
| 1:A:369:LEU:CD1 | 1:I:3:LEU:HD13 | 2.45 | 0.46 |
| 1:K:372:ILE:HD12 | 1:K:374:MET:CG | 2.46 | 0.46 |
| 1:I:229:LYS:CG | 1:M:487:GLY:HA3 | 2.25 | 0.46 |
| 1:Q:370:GLN:CB | 1:Q:374:MET:SD | 3.03 | 0.46 |
| 1:R:11:ILE:HG13 | 1:R:12:PHE:HD2 | 1.72 | 0.46 |
| 1:R:193:ASP:O | 1:R:196:ASP:HB2 | 2.14 | 0.46 |
| 1:R:297:GLN:HB3 | 1:R:297:GLN:HE21 | 1.50 | 0.46 |
| 1:R:384:ALA:O | 1:R:387:SER:HB2 | 2.15 | 0.46 |
| 1:W:270:PRO:O | 1:W:273:LYS:HB2 | 2.14 | 0.46 |
| 1:A:372:ILE:HD11 | 1:A:374:MET:HE2 | 1.96 | 0.46 |
| 1:B:276:VAL:CG1 | 1:C:9:LEU:HB3 | 2.45 | 0.46 |
| 1:B:370:GLN:CB | 1:B:374:MET:SD | 3.03 | 0.46 |
| 1:E:370:GLN:CB | 1:E:374:MET:SD | 3.03 | 0.46 |
| 1:E:297:GLN:HB2 | 1:G:310:ARG:CG | 2.46 | 0.46 |
| 1:K:212:PHE:HD2 | 1:K:214:ARG:HH21 | 1.62 | 0.46 |
| 1:K:270:PRO:CG | 1:K:273:LYS:HD2 | 2.45 | 0.46 |
| 1:K:384:ALA:O | 1:K:387:SER:HB2 | 2.14 | 0.46 |
| 1:K:390:GLU:HG2 | 1:L:374:MET:CE | 2.45 | 0.46 |
| 1:M:391:THR:HA | 1:N:373:PRO:CB | 2.45 | 0.46 |
| 1:O:311:ALA:HB3 | 1:P:312:GLU:HG3 | 1.97 | 0.46 |
| 1:Q:270:PRO:CG | 1:Q:273:LYS:HD2 | 2.45 | 0.46 |
| 1:Q:384:ALA:O | 1:Q:387:SER:HB2 | 2.14 | 0.46 |
| 1:X:372:ILE:HD12 | 1:X:374:MET:CG | 2.46 | 0.46 |
| 1:B:212:PHE:HD2 | 1:B:214:ARG:HH21 | 1.62 | 0.46 |
| 1:E:19:ARG:NH1 | 1:E:21:ALA:O | 2.46 | 0.46 |
| 1:H:372:ILE:HG13 | 1:I:390:GLU:O | 2.15 | 0.46 |
| 1:J:372:ILE:HD12 | 1:J:374:MET:CG | 2.46 | 0.46 |
| 1:N:193:ASP:CA | 1:N:196:ASP:HB2 | 2.42 | 0.46 |
| 1:N:372:ILE:HD12 | 1:N:372:ILE:HA | 1.73 | 0.46 |
| 1:O:370:GLN:CB | 1:O:374:MET:SD | 3.03 | 0.46 |
| 1:T:364:ASN:O | 1:T:368:LYS:HG2 | 2.16 | 0.46 |
| 1:T:482:ASP:H | 1:T:490:ASN:HD21 | 1.61 | 0.46 |
| 1:W:372:ILE:HD12 | 1:W:374:MET:CG | 2.46 | 0.46 |
| 1:X:424:ARG:CG | 1:X:424:ARG:NH1 | 2.41 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:391:THR:O | 1:P:373:PRO:HB3 | 2.16 | 0.46 |
| 1:F:370:GLN:CB | 1:F:374:MET:SD | 3.03 | 0.46 |
| 1:L:364:ASN:O | 1:L:368:LYS:HG2 | 2.16 | 0.46 |
| 1:L:273:LYS:HG2 | 1:N:11:ILE:HA | 1.96 | 0.46 |
| 1:N:370:GLN:CB | 1:N:374:MET:SD | 3.03 | 0.46 |
| 1:O:297:GLN:OE1 | 1:P:310:ARG:NH2 | 2.49 | 0.46 |
| 1:O:402:THR:OG1 | 1:O:404:ARG:HB2 | 2.15 | 0.46 |
| 1:R:297:GLN:HB2 | 1:T:310:ARG:CB | 2.36 | 0.46 |
| 1:U:270:PRO:CG | 1:U:273:LYS:HD2 | 2.45 | 0.46 |
| 1:A:362:PHE:HD2 | 1:A:366:ILE:HD12 | 1.81 | 0.46 |
| 1:B:364:ASN:O | 1:B:368:LYS:HG2 | 2.16 | 0.46 |
| 1:C:364:ASN:O | 1:C:368:LYS:HG2 | 2.16 | 0.46 |
| 1:C:370:GLN:CB | 1:C:374:MET:SD | 3.03 | 0.46 |
| 1:D:370:GLN:CB | 1:D:374:MET:SD | 3.03 | 0.46 |
| 1:D:424:ARG:NH1 | 1:D:424:ARG:CG | 2.41 | 0.46 |
| 1:F:19:ARG:NH1 | 1:F:21:ALA:O | 2.46 | 0.46 |
| 1:F:372:ILE:HD12 | 1:F:374:MET:CG | 2.46 | 0.46 |
| 1:G:372:ILE:HD12 | 1:G:374:MET:CG | 2.46 | 0.46 |
| 1:A:12:PHE:HE2 | 1:I:242:HIS:CE1 | 2.34 | 0.46 |
| 1:A:297:GLN:OE1 | 1:I:310:ARG:HG2 | 2.15 | 0.46 |
| 1:H:390:GLU:O | 1:I:373:PRO:CB | 2.63 | 0.46 |
| 1:K:272:GLU:HG3 | 1:M:352:GLU:CB | 2.43 | 0.46 |
| 1:L:276:VAL:CG1 | 1:N:9:LEU:CB | 2.92 | 0.46 |
| 1:L:310:ARG:CZ | 1:N:297:GLN:OE1 | 2.64 | 0.46 |
| 1:N:212:PHE:HD2 | 1:N:214:ARG:HH21 | 1.62 | 0.46 |
| 1:M:483:HIS:HD2 | 1:N:483:HIS:NE2 | 2.13 | 0.46 |
| 1:A:364:ASN:O | 1:A:368:LYS:HG2 | 2.16 | 0.46 |
| 1:B:90:ARG:HD3 | 1:B:174:ARG:O | 2.13 | 0.46 |
| 1:K:364:ASN:O | 1:K:368:LYS:HG2 | 2.16 | 0.46 |
| 1:M:364:ASN:O | 1:M:368:LYS:HG2 | 2.16 | 0.46 |
| 1:O:362:PHE:HD2 | 1:O:366:ILE:HD12 | 1.81 | 0.46 |
| 1:Q:472:THR:CG2 | 1:Q:498:GLU:HA | 2.18 | 0.46 |
| 1:S:212:PHE:HD2 | 1:S:214:ARG:HH21 | 1.62 | 0.46 |
| 1:V:287:VAL:CG2 | 1:X:3:LEU:HD22 | 2.46 | 0.46 |
| 1:V:297:GLN:NE2 | 1:V:300:GLU:HB3 | 2.24 | 0.46 |
| 1:A:472:THR:CG2 | 1:A:498:GLU:HA | 2.18 | 0.46 |
| 1:B:79:ALA:HB2 | 1:B:429:ARG:O | 2.16 | 0.46 |
| 1:E:79:ALA:HB2 | 1:E:429:ARG:O | 2.16 | 0.46 |
| 1:I:364:ASN:O | 1:I:368:LYS:HG2 | 2.16 | 0.46 |
| 1:J:362:PHE:HD2 | 1:J:366:ILE:HD12 | 1.81 | 0.46 |
| 1:M:472:THR:CG2 | 1:M:498:GLU:CA | 2.84 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:79:ALA:HB2 | 1:M:429:ARG:O | 2.16 | 0.46 |
| 1:Q:193:ASP:C | 1:Q:196:ASP:H | 2.20 | 0.46 |
| 1:R:364:ASN:O | 1:R:368:LYS:HG2 | 2.16 | 0.46 |
| 1:W:402:THR:OG1 | 1:W:404:ARG:HB2 | 2.16 | 0.46 |
| 1:A:224:LYS:HB3 | 1:A:224:LYS:HE3 | 1.82 | 0.46 |
| 1:C:362:PHE:HD2 | 1:C:366:ILE:HD12 | 1.81 | 0.46 |
| 1:D:193:ASP:C | 1:D:196:ASP:H | 2.20 | 0.46 |
| 1:E:11:ILE:HG12 | 1:E:12:PHE:CD2 | 2.47 | 0.46 |
| 1:H:212:PHE:HD2 | 1:H:214:ARG:HH21 | 1.62 | 0.46 |
| 1:Q:362:PHE:HD2 | 1:Q:366:ILE:HD12 | 1.81 | 0.46 |
| 1:W:370:GLN:CB | 1:W:374:MET:SD | 3.03 | 0.46 |
| 1:X:364:ASN:O | 1:X:368:LYS:HG2 | 2.16 | 0.46 |
| 1:B:193:ASP:C | 1:B:196:ASP:H | 2.20 | 0.45 |
| 1:C:372:ILE:HD12 | 1:C:374:MET:CG | 2.46 | 0.45 |
| 1:E:372:ILE:HD12 | 1:E:374:MET:CG | 2.46 | 0.45 |
| 1:G:364:ASN:O | 1:G:368:LYS:HG2 | 2.16 | 0.45 |
| 1:F:373:PRO:CB | 1:G:390:GLU:O | 2.64 | 0.45 |
| 1:H:193:ASP:C | 1:H:196:ASP:H | 2.20 | 0.45 |
| 1:H:79:ALA:HB2 | 1:H:429:ARG:O | 2.16 | 0.45 |
| 1:S:362:PHE:HD2 | 1:S:366:ILE:HD12 | 1.81 | 0.45 |
| 1:S:364:ASN:O | 1:S:368:LYS:HG2 | 2.16 | 0.45 |
| 1:V:193:ASP:C | 1:V:196:ASP:H | 2.20 | 0.45 |
| 1:V:79:ALA:HB2 | 1:V:429:ARG:O | 2.16 | 0.45 |
| 1:X:193:ASP:C | 1:X:196:ASP:H | 2.20 | 0.45 |
| 1:A:212:PHE:HD2 | 1:A:214:ARG:HH21 | 1.62 | 0.45 |
| 1:A:372:ILE:HD12 | 1:A:374:MET:CG | 2.46 | 0.45 |
| 1:B:224:LYS:HE3 | 1:B:224:LYS:HB3 | 1.82 | 0.45 |
| 1:D:372:ILE:HD12 | 1:D:374:MET:CG | 2.46 | 0.45 |
| 1:F:362:PHE:HD2 | 1:F:366:ILE:HD12 | 1.81 | 0.45 |
| 1:G:370:GLN:CB | 1:G:374:MET:SD | 3.03 | 0.45 |
| 1:H:297:GLN:HG3 | 1:J:310:ARG:CG | 2.43 | 0.45 |
| 1:H:364:ASN:O | 1:H:368:LYS:HG2 | 2.16 | 0.45 |
| 1:I:79:ALA:HB2 | 1:I:429:ARG:O | 2.16 | 0.45 |
| 1:H:376:ALA:HA | 1:I:494:ILE:HD12 | 1.98 | 0.45 |
| 1:H:352:GLU:OE1 | 1:J:272:GLU:HG2 | 2.16 | 0.45 |
| 1:K:12:PHE:CE2 | 1:M:242:HIS:NE2 | 2.77 | 0.45 |
| 1:L:193:ASP:C | 1:L:196:ASP:H | 2.20 | 0.45 |
| 1:L:272:GLU:C | 1:N:352:GLU:HG2 | 2.36 | 0.45 |
| 1:N:362:PHE:HD2 | 1:N:366:ILE:HD12 | 1.81 | 0.45 |
| 1:Q:456:ARG:NH1 | 2:Q:700:FDP:O2P | 2.34 | 0.45 |
| 1:R:79:ALA:HB2 | 1:R:429:ARG:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:362:PHE:HD2 | 1:T:366:ILE:HD12 | 1.81 | 0.45 |
| 1:V:372:ILE:HD12 | 1:V:374:MET:CG | 2.46 | 0.45 |
| 1:C:168:SER:O | 1:C:169:HIS:HB2 | 2.17 | 0.45 |
| 1:D:364:ASN:O | 1:D:368:LYS:HG2 | 2.16 | 0.45 |
| 1:E:193:ASP:C | 1:E:196:ASP:H | 2.20 | 0.45 |
| 1:E:193:ASP:CA | 1:E:196:ASP:HB2 | 2.41 | 0.45 |
| 1:G:79:ALA:HB2 | 1:G:429:ARG:O | 2.16 | 0.45 |
| 1:I:195:VAL:HG22 | 1:N:496:LEU:CD2 | 2.46 | 0.45 |
| 1:J:364:ASN:O | 1:J:368:LYS:HG2 | 2.16 | 0.45 |
| 1:K:49:ARG:NE | 1:K:83:ASP:OD2 | 2.33 | 0.45 |
| 1:L:168:SER:O | 1:L:169:HIS:HB2 | 2.17 | 0.45 |
| 1:H:496:LEU:HD21 | 1:M:195:VAL:HG23 | 1.97 | 0.45 |
| 1:N:79:ALA:HB2 | 1:N:429:ARG:O | 2.16 | 0.45 |
| 1:O:193:ASP:CA | 1:O:196:ASP:HB2 | 2.41 | 0.45 |
| 1:O:79:ALA:HB2 | 1:O:429:ARG:O | 2.16 | 0.45 |
| 1:C:383:SER:CB | 1:P:383:SER:HB2 | 2.45 | 0.45 |
| 1:Q:79:ALA:HB2 | 1:Q:429:ARG:O | 2.16 | 0.45 |
| 1:S:168:SER:O | 1:S:169:HIS:HB2 | 2.17 | 0.45 |
| 1:Q:272:GLU:HG3 | 1:S:352:GLU:CG | 2.45 | 0.45 |
| 1:U:168:SER:O | 1:U:169:HIS:HB2 | 2.17 | 0.45 |
| 1:A:193:ASP:C | 1:A:196:ASP:H | 2.20 | 0.45 |
| 1:B:280:ILE:CG1 | 1:C:6:ASN:O | 2.64 | 0.45 |
| 1:G:193:ASP:O | 1:G:197:LEU:N | 2.38 | 0.45 |
| 1:N:193:ASP:C | 1:N:196:ASP:H | 2.20 | 0.45 |
| 1:N:364:ASN:O | 1:N:368:LYS:HG2 | 2.16 | 0.45 |
| 1:O:372:ILE:HD12 | 1:O:374:MET:CG | 2.46 | 0.45 |
| 1:P:193:ASP:C | 1:P:196:ASP:H | 2.20 | 0.45 |
| 1:P:364:ASN:O | 1:P:368:LYS:HG2 | 2.16 | 0.45 |
| 1:O:279:LYS:HE3 | 1:P:6:ASN:OD1 | 2.15 | 0.45 |
| 1:Q:372:ILE:HD12 | 1:Q:374:MET:CG | 2.46 | 0.45 |
| 1:S:456:ARG:NH1 | 2:S:700:FDP:O2P | 2.34 | 0.45 |
| 1:V:364:ASN:O | 1:V:368:LYS:HG2 | 2.16 | 0.45 |
| 1:W:79:ALA:HB2 | 1:W:429:ARG:O | 2.16 | 0.45 |
| 1:V:284:LYS:HG2 | 1:X:7:LEU:CD2 | 2.38 | 0.45 |
| 1:D:79:ALA:HB2 | 1:D:429:ARG:O | 2.16 | 0.45 |
| 1:D:272:GLU:CG | 1:F:352:GLU:HG2 | 2.47 | 0.45 |
| 1:F:79:ALA:HB2 | 1:F:429:ARG:O | 2.16 | 0.45 |
| 1:G:168:SER:O | 1:G:169:HIS:HB2 | 2.17 | 0.45 |
| 1:H:311:ALA:CB | 1:J:312:GLU:CA | 2.72 | 0.45 |
| 1:J:370:GLN:CB | 1:J:374:MET:SD | 3.03 | 0.45 |
| 1:K:370:GLN:CB | 1:K:374:MET:SD | 3.03 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:168:SER:O | 1:Q:169:HIS:HB2 | 2.17 | 0.45 |
| 1:R:273:LYS:HD3 | 1:T:11:ILE:C | 2.33 | 0.45 |
| 1:R:362:PHE:HD2 | 1:R:366:ILE:HD12 | 1.81 | 0.45 |
| 1:T:193:ASP:C | 1:T:196:ASP:H | 2.20 | 0.45 |
| 1:U:193:ASP:O | 1:U:197:LEU:N | 2.38 | 0.45 |
| 1:A:79:ALA:HB2 | 1:A:429:ARG:O | 2.16 | 0.45 |
| 1:C:494:ILE:HD12 | 1:P:376:ALA:HA | 1.97 | 0.45 |
| 1:F:456:ARG:NH1 | 2:F:700:FDP:O2P | 2.34 | 0.45 |
| 1:G:193:ASP:C | 1:G:196:ASP:H | 2.20 | 0.45 |
| 1:G:362:PHE:HD2 | 1:G:366:ILE:HD12 | 1.81 | 0.45 |
| 1:H:242:HIS:NE2 | 1:J:12:PHE:CE2 | 2.79 | 0.45 |
| 1:J:193:ASP:C | 1:J:196:ASP:H | 2.20 | 0.45 |
| 1:M:168:SER:O | 1:M:169:HIS:HB2 | 2.17 | 0.45 |
| 1:N:168:SER:O | 1:N:169:HIS:HB2 | 2.17 | 0.45 |
| 1:N:372:ILE:HD12 | 1:N:374:MET:CG | 2.46 | 0.45 |
| 1:O:193:ASP:C | 1:O:196:ASP:H | 2.20 | 0.45 |
| 1:O:11:ILE:O | 1:P:273:LYS:CD | 2.65 | 0.45 |
| 1:S:193:ASP:C | 1:S:196:ASP:H | 2.20 | 0.45 |
| 1:R:311:ALA:CB | 1:T:315:ASP:HB2 | 2.46 | 0.45 |
| 1:U:364:ASN:O | 1:U:368:LYS:HG2 | 2.16 | 0.45 |
| 1:W:362:PHE:HD2 | 1:W:366:ILE:HD12 | 1.81 | 0.45 |
| 1:X:401:ASN:N | 2:X:700:FDP:O5P | 2.50 | 0.45 |
| 1:B:168:SER:O | 1:B:169:HIS:HB2 | 2.17 | 0.45 |
| 1:C:79:ALA:HB2 | 1:C:429:ARG:O | 2.16 | 0.45 |
| 1:D:168:SER:O | 1:D:169:HIS:HB2 | 2.17 | 0.45 |
| 1:E:11:ILE:HG13 | 1:E:12:PHE:HD2 | 1.72 | 0.45 |
| 1:H:315:ASP:CB | 1:J:311:ALA:CA | 2.89 | 0.45 |
| 1:I:168:SER:O | 1:I:169:HIS:HB2 | 2.17 | 0.45 |
| 1:K:362:PHE:HD2 | 1:K:366:ILE:HD12 | 1.81 | 0.45 |
| 1:O:168:SER:O | 1:O:169:HIS:HB2 | 2.17 | 0.45 |
| 1:O:472:THR:CG2 | 1:O:498:GLU:CA | 2.84 | 0.45 |
| 1:R:193:ASP:C | 1:R:196:ASP:H | 2.20 | 0.45 |
| 1:W:193:ASP:C | 1:W:196:ASP:H | 2.20 | 0.45 |
| 1:A:223:ARG:NH1 | 1:A:223:ARG:HG2 | 2.25 | 0.45 |
| 1:F:168:SER:O | 1:F:169:HIS:HB2 | 2.17 | 0.45 |
| 1:F:193:ASP:C | 1:F:196:ASP:H | 2.20 | 0.45 |
| 1:E:242:HIS:NE2 | 1:G:12:PHE:HE2 | 2.15 | 0.45 |
| 1:J:79:ALA:HB2 | 1:J:429:ARG:O | 2.16 | 0.45 |
| 1:P:362:PHE:HD2 | 1:P:366:ILE:HD12 | 1.81 | 0.45 |
| 1:R:311:ALA:HB1 | 1:T:311:ALA:O | 2.16 | 0.45 |
| 1:U:193:ASP:C | 1:U:196:ASP:H | 2.20 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:168:SER:O | 1:V:169:HIS:HB2 | 2.17 | 0.45 |
| 1:C:193:ASP:C | 1:C:196:ASP:H | 2.20 | 0.45 |
| 1:C:178:ASN:OD1 | 1:C:268:GLU:OE2 | 2.35 | 0.45 |
| 1:H:270:PRO:CG | 1:H:273:LYS:CD | 2.94 | 0.45 |
| 1:I:193:ASP:C | 1:I:196:ASP:H | 2.20 | 0.45 |
| 1:L:178:ASN:OD1 | 1:L:268:GLU:OE2 | 2.35 | 0.45 |
| 1:L:272:GLU:O | 1:N:352:GLU:HG2 | 2.17 | 0.45 |
| 1:K:297:GLN:OE1 | 1:M:310:ARG:CZ | 2.65 | 0.45 |
| 1:O:372:ILE:HD11 | 1:O:374:MET:HE2 | 1.98 | 0.45 |
| 1:S:79:ALA:HB2 | 1:S:429:ARG:O | 2.16 | 0.45 |
| 1:S:494:ILE:HD12 | 1:T:376:ALA:CB | 2.44 | 0.45 |
| 1:U:188:ALA:CB | 1:U:218:GLN:HG2 | 2.21 | 0.45 |
| 1:U:372:ILE:HA | 1:U:372:ILE:HD12 | 1.78 | 0.45 |
| 1:V:273:LYS:CG | 1:X:11:ILE:HB | 2.47 | 0.45 |
| 1:V:9:LEU:HB2 | 1:X:280:ILE:CD1 | 2.42 | 0.45 |
| 1:W:364:ASN:O | 1:W:368:LYS:HG2 | 2.16 | 0.45 |
| 1:X:178:ASN:OD1 | 1:X:268:GLU:OE2 | 2.35 | 0.45 |
| 1:F:364:ASN:O | 1:F:368:LYS:HG2 | 2.16 | 0.45 |
| 1:F:372:ILE:HA | 1:F:372:ILE:HD12 | 1.73 | 0.45 |
| 1:H:9:LEU:CB | 1:J:276:VAL:HG13 | 2.46 | 0.45 |
| 1:P:178:ASN:OD1 | 1:P:268:GLU:OE2 | 2.35 | 0.45 |
| 1:Q:11:ILE:CB | 1:S:273:LYS:HG2 | 2.46 | 0.45 |
| 1:W:168:SER:O | 1:W:169:HIS:HB2 | 2.17 | 0.45 |
| 1:B:362:PHE:HD2 | 1:B:366:ILE:HD12 | 1.81 | 0.44 |
| 1:D:224:LYS:HB3 | 1:D:224:LYS:HE3 | 1.82 | 0.44 |
| 1:E:364:ASN:O | 1:E:368:LYS:HG2 | 2.16 | 0.44 |
| 1:H:311:ALA:HB3 | 1:J:312:GLU:HG2 | 1.98 | 0.44 |
| 1:I:178:ASN:OD1 | 1:I:268:GLU:OE2 | 2.35 | 0.44 |
| 1:I:362:PHE:HD2 | 1:I:366:ILE:HD12 | 1.81 | 0.44 |
| 1:N:178:ASN:OD1 | 1:N:268:GLU:OE2 | 2.35 | 0.44 |
| 1:Q:352:GLU:HG2 | 1:S:272:GLU:O | 2.16 | 0.44 |
| 1:P:487:GLY:N | 1:V:229:LYS:HE3 | 2.29 | 0.44 |
| 1:U:372:ILE:CG1 | 1:V:390:GLU:O | 2.65 | 0.44 |
| 1:C:270:PRO:CG | 1:C:273:LYS:CD | 2.94 | 0.44 |
| 1:D:178:ASN:OD1 | 1:D:268:GLU:OE2 | 2.35 | 0.44 |
| 1:E:283:SER:OG | 1:G:3:LEU:CD2 | 2.64 | 0.44 |
| 1:G:372:ILE:HD12 | 1:G:372:ILE:HA | 1.73 | 0.44 |
| 1:H:362:PHE:HD2 | 1:H:366:ILE:HD12 | 1.81 | 0.44 |
| 1:J:17:ASN:HD22 | 1:J:17:ASN:C | 2.21 | 0.44 |
| 1:M:472:THR:CG2 | 1:M:498:GLU:HA | 2.18 | 0.44 |
| 1:Q:178:ASN:OD1 | 1:Q:268:GLU:OE2 | 2.35 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:193:ASP:CA | 1:S:196:ASP:HB2 | 2.42 | 0.44 |
| 1:T:188:ALA:CB | 1:T:218:GLN:HG2 | 2.21 | 0.44 |
| 1:U:491:GLN:OE1 | 1:U:493:ARG:HD2 | 2.18 | 0.44 |
| 1:U:390:GLU:HG2 | 1:V:374:MET:HE2 | 1.99 | 0.44 |
| 1:B:372:ILE:HD12 | 1:B:374:MET:CG | 2.46 | 0.44 |
| 1:D:17:ASN:C | 1:D:17:ASN:HD22 | 2.21 | 0.44 |
| 1:F:178:ASN:OD1 | 1:F:268:GLU:OE2 | 2.35 | 0.44 |
| 1:J:491:GLN:OE1 | 1:J:493:ARG:HD2 | 2.18 | 0.44 |
| 1:K:193:ASP:C | 1:K:196:ASP:H | 2.20 | 0.44 |
| 1:K:491:GLN:OE1 | 1:K:493:ARG:HD2 | 2.18 | 0.44 |
| 1:L:17:ASN:C | 1:L:17:ASN:HD22 | 2.21 | 0.44 |
| 1:M:483:HIS:CD2 | 1:N:483:HIS:NE2 | 2.85 | 0.44 |
| 1:O:178:ASN:OD1 | 1:O:268:GLU:OE2 | 2.35 | 0.44 |
| 1:Q:270:PRO:CG | 1:Q:273:LYS:CD | 2.94 | 0.44 |
| 1:T:168:SER:O | 1:T:169:HIS:HB2 | 2.17 | 0.44 |
| 1:S:376:ALA:HB1 | 1:T:494:ILE:HB | 1.99 | 0.44 |
| 1:V:17:ASN:C | 1:V:17:ASN:HD22 | 2.21 | 0.44 |
| 1:X:362:PHE:HD2 | 1:X:366:ILE:HD12 | 1.81 | 0.44 |
| 1:X:79:ALA:HB2 | 1:X:429:ARG:O | 2.16 | 0.44 |
| 1:A:17:ASN:HD22 | 1:A:17:ASN:C | 2.21 | 0.44 |
| 1:B:178:ASN:OD1 | 1:B:268:GLU:OE2 | 2.35 | 0.44 |
| 1:C:17:ASN:C | 1:C:17:ASN:HD22 | 2.21 | 0.44 |
| 1:K:79:ALA:HB2 | 1:K:429:ARG:O | 2.17 | 0.44 |
| 1:M:193:ASP:C | 1:M:196:ASP:H | 2.20 | 0.44 |
| 1:M:373:PRO:HB3 | 1:N:391:THR:CA | 2.45 | 0.44 |
| 1:O:398:VAL:HG13 | 1:O:479:ILE:HB | 2.00 | 0.44 |
| 1:P:168:SER:O | 1:P:169:HIS:HB2 | 2.17 | 0.44 |
| 1:T:178:ASN:OD1 | 1:T:268:GLU:OE2 | 2.35 | 0.44 |
| 1:R:284:LYS:CG | 1:T:7:LEU:HD21 | 2.38 | 0.44 |
| 1:U:362:PHE:HD2 | 1:U:366:ILE:HD12 | 1.81 | 0.44 |
| 1:V:178:ASN:OD1 | 1:V:268:GLU:OE2 | 2.35 | 0.44 |
| 1:X:17:ASN:HD22 | 1:X:17:ASN:C | 2.21 | 0.44 |
| 1:B:372:ILE:HD11 | 1:B:374:MET:HE1 | 1.98 | 0.44 |
| 1:B:280:ILE:HD11 | 1:C:9:LEU:HB2 | 1.99 | 0.44 |
| 1:J:178:ASN:OD1 | 1:J:268:GLU:OE2 | 2.35 | 0.44 |
| 1:K:372:ILE:HD11 | 1:K:374:MET:HE2 | 2.00 | 0.44 |
| 1:K:391:THR:C | 1:L:373:PRO:HB3 | 2.37 | 0.44 |
| 1:L:491:GLN:OE1 | 1:L:493:ARG:HD2 | 2.18 | 0.44 |
| 1:M:483:HIS:NE2 | 1:N:483:HIS:CD2 | 2.86 | 0.44 |
| 1:L:3:LEU:HD23 | 1:N:283:SER:HB3 | 1.98 | 0.44 |
| 1:N:451:GLU:H | 1:N:451:GLU:HG2 | 1.59 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:6:ASN:OD1 | 1:P:279:LYS:CE | 2.54 | 0.44 |
| 1:P:224:LYS:HB3 | 1:P:224:LYS:HE3 | 1.82 | 0.44 |
| 1:R:491:GLN:OE1 | 1:R:493:ARG:HD2 | 2.18 | 0.44 |
| 1:U:79:ALA:HB2 | 1:U:429:ARG:O | 2.16 | 0.44 |
| 1:V:362:PHE:HD2 | 1:V:366:ILE:HD12 | 1.81 | 0.44 |
| 1:V:491:GLN:OE1 | 1:V:493:ARG:HD2 | 2.18 | 0.44 |
| 1:U:11:ILE:HG13 | 1:W:273:LYS:HD3 | 1.99 | 0.44 |
| 1:A:168:SER:O | 1:A:169:HIS:HB2 | 2.17 | 0.44 |
| 1:A:178:ASN:OD1 | 1:A:268:GLU:OE2 | 2.35 | 0.44 |
| 1:B:398:VAL:HG13 | 1:B:479:ILE:HB | 2.00 | 0.44 |
| 1:D:491:GLN:HG3 | 1:E:491:GLN:HG3 | 1.99 | 0.44 |
| 1:E:491:GLN:OE1 | 1:E:493:ARG:HD2 | 2.18 | 0.44 |
| 1:J:168:SER:O | 1:J:169:HIS:HB2 | 2.17 | 0.44 |
| 1:K:17:ASN:C | 1:K:17:ASN:HD22 | 2.21 | 0.44 |
| 1:L:79:ALA:HB2 | 1:L:429:ARG:O | 2.16 | 0.44 |
| 1:O:352:GLU:HB2 | 1:P:272:GLU:HG3 | 1.99 | 0.44 |
| 1:P:17:ASN:C | 1:P:17:ASN:HD22 | 2.21 | 0.44 |
| 1:P:79:ALA:HB2 | 1:P:429:ARG:O | 2.16 | 0.44 |
| 1:Q:383:SER:CB | 1:R:383:SER:HB2 | 2.46 | 0.44 |
| 1:Q:374:MET:HE2 | 1:R:390:GLU:HG2 | 1.99 | 0.44 |
| 1:U:372:ILE:HD12 | 1:U:374:MET:HG3 | 1.99 | 0.44 |
| 1:V:372:ILE:HD12 | 1:V:372:ILE:HA | 1.73 | 0.44 |
| 1:X:372:ILE:HA | 1:X:372:ILE:HD12 | 1.73 | 0.44 |
| 1:X:491:GLN:OE1 | 1:X:493:ARG:HD2 | 2.18 | 0.44 |
| 1:D:362:PHE:HD2 | 1:D:366:ILE:HD12 | 1.81 | 0.44 |
| 1:D:398:VAL:HG13 | 1:D:479:ILE:HB | 2.00 | 0.44 |
| 1:E:398:VAL:HG13 | 1:E:479:ILE:HB | 2.00 | 0.44 |
| 1:H:17:ASN:C | 1:H:17:ASN:HD22 | 2.21 | 0.44 |
| 1:H:491:GLN:OE1 | 1:H:493:ARG:HD2 | 2.18 | 0.44 |
| 1:J:101:MET:HE1 | 1:J:124:PHE:CE1 | 2.53 | 0.44 |
| 1:K:168:SER:O | 1:K:169:HIS:HB2 | 2.17 | 0.44 |
| 1:L:401:ASN:N | 2:L:700:FDP:O5P | 2.50 | 0.44 |
| 1:O:17:ASN:HD22 | 1:O:17:ASN:C | 2.21 | 0.44 |
| 1:O:364:ASN:O | 1:O:368:LYS:HG2 | 2.16 | 0.44 |
| 1:P:424:ARG:CG | 1:P:424:ARG:NH1 | 2.41 | 0.44 |
| 1:Q:297:GLN:HB2 | 1:S:310:ARG:HB2 | 2.00 | 0.44 |
| 1:Q:364:ASN:O | 1:Q:368:LYS:HG2 | 2.16 | 0.44 |
| 1:T:3:LEU:HD23 | 1:T:4:ALA:N | 2.24 | 0.44 |
| 1:T:491:GLN:OE1 | 1:T:493:ARG:HD2 | 2.18 | 0.44 |
| 1:T:79:ALA:HB2 | 1:T:429:ARG:O | 2.16 | 0.44 |
| 1:U:17:ASN:HD22 | 1:U:17:ASN:C | 2.21 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:178:ASN:OD1 | 1:W:268:GLU:OE2 | 2.35 | 0.44 |
| 1:W:398:VAL:HG13 | 1:W:479:ILE:HB | 2.00 | 0.44 |
| 1:E:17:ASN:C | 1:E:17:ASN:HD22 | 2.21 | 0.44 |
| 1:E:362:PHE:HD2 | 1:E:366:ILE:HD12 | 1.81 | 0.44 |
| 1:H:312:GLU:CG | 1:J:311:ALA:HB3 | 2.48 | 0.44 |
| 1:J:398:VAL:HG13 | 1:J:479:ILE:HB | 2.00 | 0.44 |
| 1:L:352:GLU:HG2 | 1:N:272:GLU:C | 2.38 | 0.44 |
| 1:O:401:ASN:N | 2:O:700:FDP:O5P | 2.50 | 0.44 |
| 1:Q:451:GLU:H | 1:Q:451:GLU:HG2 | 1.59 | 0.44 |
| 1:Q:491:GLN:OE1 | 1:Q:493:ARG:HD2 | 2.18 | 0.44 |
| 1:W:17:ASN:HD22 | 1:W:17:ASN:C | 2.21 | 0.44 |
| 1:W:49:ARG:NE | 1:W:83:ASP:OD2 | 2.33 | 0.44 |
| 1:X:168:SER:O | 1:X:169:HIS:HB2 | 2.17 | 0.44 |
| 1:C:491:GLN:OE1 | 1:C:493:ARG:HD2 | 2.18 | 0.44 |
| 1:D:491:GLN:OE1 | 1:D:493:ARG:HD2 | 2.18 | 0.44 |
| 1:D:6:ASN:OD1 | 1:F:279:LYS:HE3 | 2.17 | 0.44 |
| 1:H:398:VAL:HG13 | 1:H:479:ILE:HB | 2.00 | 0.44 |
| 1:K:101:MET:HE1 | 1:K:124:PHE:CE1 | 2.53 | 0.44 |
| 1:K:178:ASN:OD1 | 1:K:268:GLU:OE2 | 2.35 | 0.44 |
| 1:M:362:PHE:HD2 | 1:M:366:ILE:HD12 | 1.81 | 0.44 |
| 1:M:491:GLN:OE1 | 1:M:493:ARG:HD2 | 2.18 | 0.44 |
| 1:C:483:HIS:CD2 | 1:P:483:HIS:CD2 | 3.06 | 0.44 |
| 1:Q:17:ASN:HD22 | 1:Q:17:ASN:C | 2.21 | 0.44 |
| 1:U:472:THR:CG2 | 1:U:498:GLU:CA | 2.84 | 0.44 |
| 1:W:401:ASN:N | 2:W:700:FDP:O5P | 2.50 | 0.44 |
| 1:B:491:GLN:OE1 | 1:B:493:ARG:HD2 | 2.18 | 0.43 |
| 1:D:242:HIS:HE1 | 1:F:12:PHE:CE2 | 2.36 | 0.43 |
| 1:F:17:ASN:HD22 | 1:F:17:ASN:C | 2.21 | 0.43 |
| 1:G:178:ASN:OD1 | 1:G:268:GLU:OE2 | 2.35 | 0.43 |
| 1:H:168:SER:O | 1:H:169:HIS:HB2 | 2.17 | 0.43 |
| 1:H:178:ASN:OD1 | 1:H:268:GLU:OE2 | 2.35 | 0.43 |
| 1:K:270:PRO:CG | 1:K:273:LYS:CD | 2.94 | 0.43 |
| 1:M:17:ASN:HD22 | 1:M:17:ASN:C | 2.21 | 0.43 |
| 1:R:178:ASN:OD1 | 1:R:268:GLU:OE2 | 2.35 | 0.43 |
| 1:R:193:ASP:CA | 1:R:196:ASP:HB2 | 2.41 | 0.43 |
| 1:R:371:HIS:CD2 | 1:R:373:PRO:O | 2.71 | 0.43 |
| 1:S:178:ASN:OD1 | 1:S:268:GLU:OE2 | 2.35 | 0.43 |
| 1:X:398:VAL:HG13 | 1:X:479:ILE:HB | 2.00 | 0.43 |
| 1:A:369:LEU:HD12 | 1:I:3:LEU:HD13 | 2.00 | 0.43 |
| 1:B:17:ASN:HD22 | 1:B:17:ASN:C | 2.21 | 0.43 |
| 1:E:310:ARG:HG2 | 1:G:297:GLN:OE1 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:398:VAL:HG13 | 1:G:479:ILE:HB | 2.00 | 0.43 |
| 1:G:491:GLN:OE1 | 1:G:493:ARG:HD2 | 2.18 | 0.43 |
| 1:L:362:PHE:HD2 | 1:L:366:ILE:HD12 | 1.81 | 0.43 |
| 1:O:372:ILE:HA | 1:O:372:ILE:HD12 | 1.73 | 0.43 |
| 1:R:168:SER:O | 1:R:169:HIS:HB2 | 2.17 | 0.43 |
| 1:R:272:GLU:HG2 | 1:T:352:GLU:CD | 2.39 | 0.43 |
| 1:S:17:ASN:C | 1:S:17:ASN:HD22 | 2.21 | 0.43 |
| 1:W:491:GLN:OE1 | 1:W:493:ARG:HD2 | 2.18 | 0.43 |
| 1:A:372:ILE:HA | 1:A:372:ILE:HD12 | 1.73 | 0.43 |
| 1:A:398:VAL:HG13 | 1:A:479:ILE:HB | 2.00 | 0.43 |
| 1:D:273:LYS:HG2 | 1:F:11:ILE:HB | 1.99 | 0.43 |
| 1:E:311:ALA:CB | 1:G:312:GLU:HA | 2.47 | 0.43 |
| 1:P:491:GLN:OE1 | 1:P:493:ARG:HD2 | 2.18 | 0.43 |
| 1:T:3:LEU:CD2 | 1:T:4:ALA:N | 2.80 | 0.43 |
| 1:A:270:PRO:CG | 1:A:273:LYS:CD | 2.94 | 0.43 |
| 1:B:372:ILE:HD12 | 1:B:372:ILE:HA | 1.73 | 0.43 |
| 1:B:3:LEU:HD13 | 1:C:369:LEU:CD1 | 2.48 | 0.43 |
| 1:C:398:VAL:HG13 | 1:C:479:ILE:HB | 2.00 | 0.43 |
| 1:E:272:GLU:CB | 1:G:352:GLU:HG2 | 2.49 | 0.43 |
| 1:K:11:ILE:HB | 1:M:273:LYS:CG | 2.43 | 0.43 |
| 1:M:178:ASN:OD1 | 1:M:268:GLU:OE2 | 2.35 | 0.43 |
| 1:N:398:VAL:HG13 | 1:N:479:ILE:HB | 2.00 | 0.43 |
| 1:Q:224:LYS:HB3 | 1:Q:224:LYS:HE3 | 1.81 | 0.43 |
| 1:Q:398:VAL:HG13 | 1:Q:479:ILE:HB | 2.00 | 0.43 |
| 1:R:402:THR:OG1 | 1:R:404:ARG:HB2 | 2.19 | 0.43 |
| 1:T:17:ASN:HD22 | 1:T:17:ASN:C | 2.21 | 0.43 |
| 1:U:178:ASN:OD1 | 1:U:268:GLU:OE2 | 2.35 | 0.43 |
| 1:A:491:GLN:OE1 | 1:A:493:ARG:HD2 | 2.18 | 0.43 |
| 1:B:272:GLU:O | 1:C:352:GLU:CG | 2.66 | 0.43 |
| 1:E:168:SER:O | 1:E:169:HIS:HB2 | 2.17 | 0.43 |
| 1:I:491:GLN:OE1 | 1:I:493:ARG:HD2 | 2.18 | 0.43 |
| 1:N:491:GLN:OE1 | 1:N:493:ARG:HD2 | 2.18 | 0.43 |
| 1:R:276:VAL:CG1 | 1:T:9:LEU:HB2 | 2.45 | 0.43 |
| 1:V:273:LYS:HD3 | 1:X:11:ILE:HB | 1.99 | 0.43 |
| 1:V:287:VAL:HG23 | 1:X:3:LEU:HD21 | 2.00 | 0.43 |
| 1:W:390:GLU:HG2 | 1:X:374:MET:HE2 | 1.99 | 0.43 |
| 1:C:496:LEU:CD2 | 1:V:195:VAL:CG2 | 2.93 | 0.43 |
| 1:E:101:MET:HE1 | 1:E:124:PHE:CE1 | 2.54 | 0.43 |
| 1:I:17:ASN:C | 1:I:17:ASN:HD22 | 2.21 | 0.43 |
| 1:I:487:GLY:HA2 | 1:M:229:LYS:CD | 2.42 | 0.43 |
| 1:O:451:GLU:HG2 | 1:O:451:GLU:H | 1.59 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:491:GLN:OE1 | 1:O:493:ARG:HD2 | 2.18 | 0.43 |
| 1:R:280:ILE:HD11 | 1:T:9:LEU:CB | 2.40 | 0.43 |
| 1:R:424:ARG:NH1 | 1:R:424:ARG:CG | 2.41 | 0.43 |
| 1:R:398:VAL:HG13 | 1:R:479:ILE:HB | 2.00 | 0.43 |
| 1:S:398:VAL:HG13 | 1:S:479:ILE:HB | 2.00 | 0.43 |
| 1:E:178:ASN:OD1 | 1:E:268:GLU:OE2 | 2.35 | 0.43 |
| 1:F:398:VAL:HG13 | 1:F:479:ILE:HB | 2.00 | 0.43 |
| 1:I:224:LYS:HE3 | 1:I:224:LYS:HB3 | 1.81 | 0.43 |
| 1:L:398:VAL:HG13 | 1:L:479:ILE:HB | 2.00 | 0.43 |
| 1:M:398:VAL:HG13 | 1:M:479:ILE:HB | 2.00 | 0.43 |
| 1:N:17:ASN:C | 1:N:17:ASN:HD22 | 2.21 | 0.43 |
| 1:O:429:ARG:O | 1:O:432:ASN:HB2 | 2.19 | 0.43 |
| 1:U:402:THR:OG1 | 1:U:404:ARG:HB2 | 2.18 | 0.43 |
| 1:V:287:VAL:HG23 | 1:X:3:LEU:HD22 | 2.01 | 0.43 |
| 1:F:491:GLN:OE1 | 1:F:493:ARG:HD2 | 2.18 | 0.43 |
| 1:G:224:LYS:HB3 | 1:G:224:LYS:HE3 | 1.82 | 0.43 |
| 1:G:429:ARG:O | 1:G:432:ASN:HB2 | 2.19 | 0.43 |
| 1:F:483:HIS:CD2 | 1:G:483:HIS:NE2 | 2.86 | 0.43 |
| 1:H:401:ASN:N | 2:H:700:FDP:O5P | 2.50 | 0.43 |
| 1:K:283:SER:HB3 | 1:M:3:LEU:CD2 | 2.49 | 0.43 |
| 1:L:279:LYS:HB3 | 1:N:6:ASN:CG | 2.39 | 0.43 |
| 1:T:429:ARG:O | 1:T:432:ASN:HB2 | 2.19 | 0.43 |
| 1:T:398:VAL:HG13 | 1:T:479:ILE:HB | 2.00 | 0.43 |
| 1:G:17:ASN:C | 1:G:17:ASN:HD22 | 2.21 | 0.43 |
| 1:J:429:ARG:O | 1:J:432:ASN:HB2 | 2.19 | 0.43 |
| 1:L:293:ILE:HG12 | 1:L:326:CYS:HB2 | 2.01 | 0.43 |
| 1:S:429:ARG:O | 1:S:432:ASN:HB2 | 2.19 | 0.43 |
| 1:S:491:GLN:OE1 | 1:S:493:ARG:HD2 | 2.18 | 0.43 |
| 1:V:424:ARG:NH1 | 1:V:424:ARG:CG | 2.41 | 0.43 |
| 1:W:293:ILE:HG12 | 1:W:326:CYS:HB2 | 2.01 | 0.43 |
| 1:C:429:ARG:O | 1:C:432:ASN:HB2 | 2.19 | 0.43 |
| 1:D:188:ALA:CB | 1:D:218:GLN:HG2 | 2.21 | 0.43 |
| 1:D:429:ARG:O | 1:D:432:ASN:HB2 | 2.19 | 0.43 |
| 1:H:293:ILE:HG12 | 1:H:326:CYS:HB2 | 2.01 | 0.43 |
| 1:K:6:ASN:OD1 | 1:M:279:LYS:HE3 | 2.18 | 0.43 |
| 1:L:276:VAL:HG13 | 1:N:9:LEU:HD13 | 2.01 | 0.43 |
| 1:O:377:ASP:OD2 | 1:O:377:ASP:N | 2.52 | 0.43 |
| 1:P:293:ILE:HG12 | 1:P:326:CYS:HB2 | 2.01 | 0.43 |
| 1:C:373:PRO:HD3 | 1:P:392:LYS:HD2 | 2.01 | 0.43 |
| 1:R:371:HIS:C | 1:R:372:ILE:HD13 | 2.39 | 0.43 |
| 1:S:451:GLU:HG2 | 1:S:451:GLU:H | 1.59 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:242:HIS:CE1 | 1:T:12:PHE:CE2 | 3.07 | 0.43 |
| 1:V:293:ILE:HG12 | 1:V:326:CYS:HB2 | 2.01 | 0.43 |
| 1:V:79:ALA:HA | 1:V:429:ARG:HB3 | 2.01 | 0.43 |
| 1:W:362:PHE:O | 1:W:366:ILE:HD12 | 2.19 | 0.43 |
| 1:W:429:ARG:O | 1:W:432:ASN:HB2 | 2.19 | 0.43 |
| 1:V:272:GLU:CB | 1:X:352:GLU:HG2 | 2.49 | 0.43 |
| 1:B:79:ALA:HA | 1:B:429:ARG:HB3 | 2.01 | 0.42 |
| 1:E:377:ASP:OD2 | 1:E:377:ASP:N | 2.52 | 0.42 |
| 1:F:362:PHE:O | 1:F:366:ILE:HD12 | 2.19 | 0.42 |
| 1:K:398:VAL:HG13 | 1:K:479:ILE:HB | 2.00 | 0.42 |
| 1:H:498:GLU:HG2 | 1:M:195:VAL:HG11 | 2.01 | 0.42 |
| 1:M:390:GLU:HA | 1:N:372:ILE:HG13 | 2.01 | 0.42 |
| 1:P:362:PHE:O | 1:P:366:ILE:HD12 | 2.19 | 0.42 |
| 1:P:429:ARG:O | 1:P:432:ASN:HB2 | 2.19 | 0.42 |
| 1:Q:297:GLN:OE1 | 1:S:310:ARG:CZ | 2.67 | 0.42 |
| 1:U:138:GLY:HA2 | 1:U:151:GLN:HE21 | 1.84 | 0.42 |
| 1:U:279:LYS:HE3 | 1:W:6:ASN:OD1 | 2.19 | 0.42 |
| 1:U:398:VAL:HG13 | 1:U:479:ILE:HB | 2.00 | 0.42 |
| 1:X:293:ILE:HG12 | 1:X:326:CYS:HB2 | 2.01 | 0.42 |
| 1:A:429:ARG:O | 1:A:432:ASN:HB2 | 2.19 | 0.42 |
| 1:A:6:ASN:O | 1:I:280:ILE:HG12 | 2.19 | 0.42 |
| 1:E:429:ARG:O | 1:E:432:ASN:HB2 | 2.19 | 0.42 |
| 1:F:212:PHE:CD2 | 1:F:214:ARG:NE | 2.88 | 0.42 |
| 1:F:472:THR:CG2 | 1:F:498:GLU:CA | 2.84 | 0.42 |
| 1:G:79:ALA:HA | 1:G:429:ARG:HB3 | 2.02 | 0.42 |
| 1:H:138:GLY:HA2 | 1:H:151:GLN:HE21 | 1.85 | 0.42 |
| 1:H:312:GLU:HG3 | 1:J:311:ALA:HB3 | 2.00 | 0.42 |
| 1:H:451:GLU:HG2 | 1:H:451:GLU:H | 1.59 | 0.42 |
| 1:H:496:LEU:HG | 1:M:195:VAL:HG21 | 1.89 | 0.42 |
| 1:H:79:ALA:HA | 1:H:429:ARG:HB3 | 2.01 | 0.42 |
| 1:K:293:ILE:HG12 | 1:K:326:CYS:HB2 | 2.01 | 0.42 |
| 1:K:451:GLU:H | 1:K:451:GLU:HG2 | 1.59 | 0.42 |
| 1:L:362:PHE:O | 1:L:366:ILE:HD12 | 2.19 | 0.42 |
| 1:M:293:ILE:HG12 | 1:M:326:CYS:HB2 | 2.01 | 0.42 |
| 1:O:79:ALA:HA | 1:O:429:ARG:HB3 | 2.01 | 0.42 |
| 1:P:138:GLY:HA2 | 1:P:151:GLN:HE21 | 1.84 | 0.42 |
| 1:R:17:ASN:C | 1:R:17:ASN:HD22 | 2.21 | 0.42 |
| 1:S:293:ILE:HG12 | 1:S:326:CYS:HB2 | 2.01 | 0.42 |
| 1:T:224:LYS:HB3 | 1:T:224:LYS:HE3 | 1.81 | 0.42 |
| 1:T:474:ASP:O | 1:T:497:VAL:HG13 | 2.20 | 0.42 |
| 1:U:293:ILE:HG12 | 1:U:326:CYS:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:451:GLU:HG2 | 1:U:451:GLU:H | 1.59 | 0.42 |
| 1:U:6:ASN:CG | 1:W:279:LYS:HE3 | 2.36 | 0.42 |
| 1:W:79:ALA:HA | 1:W:429:ARG:HB3 | 2.01 | 0.42 |
| 1:C:138:GLY:HA2 | 1:C:151:GLN:HE21 | 1.85 | 0.42 |
| 1:C:293:ILE:HG12 | 1:C:326:CYS:HB2 | 2.01 | 0.42 |
| 1:H:362:PHE:O | 1:H:366:ILE:HD12 | 2.19 | 0.42 |
| 1:M:491:GLN:HG3 | 1:N:491:GLN:CG | 2.47 | 0.42 |
| 1:N:293:ILE:HG12 | 1:N:326:CYS:HB2 | 2.01 | 0.42 |
| 1:N:362:PHE:O | 1:N:366:ILE:HD12 | 2.19 | 0.42 |
| 1:P:398:VAL:HG13 | 1:P:479:ILE:HB | 2.00 | 0.42 |
| 1:Q:242:HIS:NE2 | 1:S:12:PHE:CE2 | 2.85 | 0.42 |
| 1:Q:310:ARG:HG2 | 1:S:297:GLN:HB2 | 2.00 | 0.42 |
| 1:T:212:PHE:CD2 | 1:T:214:ARG:NE | 2.88 | 0.42 |
| 1:T:472:THR:CG2 | 1:T:498:GLU:CA | 2.84 | 0.42 |
| 1:T:79:ALA:HA | 1:T:429:ARG:HB3 | 2.01 | 0.42 |
| 1:V:212:PHE:CD2 | 1:V:214:ARG:NE | 2.88 | 0.42 |
| 1:V:429:ARG:O | 1:V:432:ASN:HB2 | 2.19 | 0.42 |
| 1:B:352:GLU:HG2 | 1:C:272:GLU:O | 2.18 | 0.42 |
| 1:C:377:ASP:OD2 | 1:C:377:ASP:N | 2.52 | 0.42 |
| 1:E:293:ILE:HG12 | 1:E:326:CYS:HB2 | 2.01 | 0.42 |
| 1:E:362:PHE:O | 1:E:366:ILE:HD12 | 2.19 | 0.42 |
| 1:E:49:ARG:NE | 1:E:83:ASP:OD2 | 2.33 | 0.42 |
| 1:F:483:HIS:NE2 | 1:G:483:HIS:CD2 | 2.86 | 0.42 |
| 1:G:212:PHE:CD2 | 1:G:214:ARG:NE | 2.88 | 0.42 |
| 1:I:293:ILE:HG12 | 1:I:326:CYS:HB2 | 2.01 | 0.42 |
| 1:I:429:ARG:O | 1:I:432:ASN:HB2 | 2.19 | 0.42 |
| 1:K:12:PHE:HE2 | 1:M:242:HIS:NE2 | 2.08 | 0.42 |
| 1:M:362:PHE:O | 1:M:366:ILE:HD12 | 2.19 | 0.42 |
| 1:N:429:ARG:O | 1:N:432:ASN:HB2 | 2.19 | 0.42 |
| 1:R:429:ARG:O | 1:R:432:ASN:HB2 | 2.19 | 0.42 |
| 1:S:362:PHE:O | 1:S:366:ILE:HD12 | 2.19 | 0.42 |
| 1:S:474:ASP:O | 1:S:497:VAL:HG13 | 2.20 | 0.42 |
| 1:Q:276:VAL:HG13 | 1:S:9:LEU:HB3 | 2.02 | 0.42 |
| 1:T:293:ILE:HG12 | 1:T:326:CYS:HB2 | 2.01 | 0.42 |
| 1:U:377:ASP:N | 1:U:377:ASP:OD2 | 2.52 | 0.42 |
| 1:U:491:GLN:HG3 | 1:V:491:GLN:HG3 | 2.01 | 0.42 |
| 1:U:79:ALA:HA | 1:U:429:ARG:HB3 | 2.01 | 0.42 |
| 1:V:276:VAL:HG13 | 1:X:9:LEU:CD1 | 2.48 | 0.42 |
| 1:U:372:ILE:CD1 | 1:V:390:GLU:HG2 | 2.45 | 0.42 |
| 1:V:398:VAL:HG13 | 1:V:479:ILE:HB | 2.00 | 0.42 |
| 1:A:352:GLU:HG2 | 1:I:272:GLU:CG | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:79:ALA:HA | 1:A:429:ARG:HB3 | 2.01 | 0.42 |
| 1:B:138:GLY:HA2 | 1:B:151:GLN:HE21 | 1.85 | 0.42 |
| 1:B:429:ARG:O | 1:B:432:ASN:HB2 | 2.19 | 0.42 |
| 1:D:138:GLY:HA2 | 1:D:151:GLN:HE21 | 1.85 | 0.42 |
| 1:D:79:ALA:HA | 1:D:429:ARG:HB3 | 2.01 | 0.42 |
| 1:F:138:GLY:HA2 | 1:F:151:GLN:HE21 | 1.84 | 0.42 |
| 1:H:297:GLN:HB2 | 1:J:310:ARG:HB2 | 1.99 | 0.42 |
| 1:H:429:ARG:O | 1:H:432:ASN:HB2 | 2.19 | 0.42 |
| 1:I:398:VAL:HG13 | 1:I:479:ILE:HB | 2.00 | 0.42 |
| 1:J:79:ALA:HA | 1:J:429:ARG:HB3 | 2.01 | 0.42 |
| 1:K:474:ASP:O | 1:K:497:VAL:HG13 | 2.20 | 0.42 |
| 1:L:474:ASP:O | 1:L:497:VAL:HG13 | 2.20 | 0.42 |
| 1:N:474:ASP:O | 1:N:497:VAL:HG13 | 2.20 | 0.42 |
| 1:O:212:PHE:CD2 | 1:O:214:ARG:NE | 2.88 | 0.42 |
| 1:O:474:ASP:O | 1:O:497:VAL:HG13 | 2.20 | 0.42 |
| 1:R:138:GLY:HA2 | 1:R:151:GLN:HE21 | 1.85 | 0.42 |
| 1:R:212:PHE:CD2 | 1:R:214:ARG:NE | 2.88 | 0.42 |
| 1:R:377:ASP:OD2 | 1:R:377:ASP:N | 2.52 | 0.42 |
| 1:U:270:PRO:CG | 1:U:273:LYS:CD | 2.94 | 0.42 |
| 1:V:224:LYS:HE3 | 1:V:224:LYS:HB3 | 1.81 | 0.42 |
| 1:W:138:GLY:HA2 | 1:W:151:GLN:HE21 | 1.84 | 0.42 |
| 1:D:270:PRO:CG | 1:D:273:LYS:CD | 2.94 | 0.42 |
| 1:G:293:ILE:HG12 | 1:G:326:CYS:HB2 | 2.01 | 0.42 |
| 1:H:212:PHE:CD2 | 1:H:214:ARG:NE | 2.88 | 0.42 |
| 1:J:474:ASP:O | 1:J:497:VAL:HG13 | 2.20 | 0.42 |
| 1:K:312:GLU:HA | 1:M:311:ALA:CB | 2.35 | 0.42 |
| 1:K:377:ASP:OD2 | 1:K:377:ASP:N | 2.52 | 0.42 |
| 1:L:79:ALA:HA | 1:L:429:ARG:HB3 | 2.01 | 0.42 |
| 1:M:429:ARG:O | 1:M:432:ASN:HB2 | 2.19 | 0.42 |
| 1:R:79:ALA:HA | 1:R:429:ARG:HB3 | 2.01 | 0.42 |
| 1:S:79:ALA:HA | 1:S:429:ARG:HB3 | 2.01 | 0.42 |
| 1:T:138:GLY:HA2 | 1:T:151:GLN:HE21 | 1.85 | 0.42 |
| 1:V:472:THR:CG2 | 1:V:498:GLU:HA | 2.18 | 0.42 |
| 1:W:372:ILE:HD11 | 1:W:374:MET:HE1 | 2.01 | 0.42 |
| 1:X:212:PHE:CD2 | 1:X:214:ARG:NE | 2.88 | 0.42 |
| 1:F:429:ARG:O | 1:F:432:ASN:HB2 | 2.19 | 0.42 |
| 1:H:424:ARG:CG | 1:H:424:ARG:NH1 | 2.41 | 0.42 |
| 1:J:362:PHE:O | 1:J:366:ILE:HD12 | 2.19 | 0.42 |
| 1:K:362:PHE:O | 1:K:366:ILE:HD12 | 2.20 | 0.42 |
| 1:K:372:ILE:HD12 | 1:K:372:ILE:HA | 1.73 | 0.42 |
| 1:K:79:ALA:HA | 1:K:429:ARG:HB3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:424:ARG:NH1 | 1:M:424:ARG:CG | 2.41 | 0.42 |
| 1:M:79:ALA:HA | 1:M:429:ARG:HB3 | 2.02 | 0.42 |
| 1:M:474:ASP:O | 1:M:497:VAL:HG13 | 2.20 | 0.42 |
| 1:L:283:SER:CA | 1:N:3:LEU:HD21 | 2.49 | 0.42 |
| 1:T:53:SER:HA | 1:T:85:LYS:CG | 2.50 | 0.42 |
| 1:V:11:ILE:HD12 | 1:X:269:ILE:HG12 | 2.02 | 0.42 |
| 1:X:79:ALA:HA | 1:X:429:ARG:HB3 | 2.01 | 0.42 |
| 1:B:276:VAL:HG13 | 1:C:9:LEU:CB | 2.49 | 0.42 |
| 1:E:3:LEU:HD13 | 1:G:369:LEU:HD12 | 2.01 | 0.42 |
| 1:F:474:ASP:O | 1:F:497:VAL:HG13 | 2.20 | 0.42 |
| 1:J:138:GLY:HA2 | 1:J:151:GLN:HE21 | 1.85 | 0.42 |
| 1:L:212:PHE:CD2 | 1:L:214:ARG:NE | 2.88 | 0.42 |
| 1:L:224:LYS:HE3 | 1:L:224:LYS:HB3 | 1.82 | 0.42 |
| 1:O:362:PHE:O | 1:O:366:ILE:HD12 | 2.19 | 0.42 |
| 1:O:263:GLY:HA2 | 1:P:310:ARG:HH11 | 1.84 | 0.42 |
| 1:P:53:SER:HA | 1:P:85:LYS:CG | 2.50 | 0.42 |
| 1:Q:270:PRO:CB | 1:Q:273:LYS:HD2 | 2.50 | 0.42 |
| 1:S:189:VAL:HG13 | 1:S:193:ASP:HB2 | 2.02 | 0.42 |
| 1:L:487:GLY:CA | 1:S:229:LYS:CD | 2.94 | 0.42 |
| 1:R:11:ILE:O | 1:T:273:LYS:HE3 | 2.20 | 0.42 |
| 1:U:424:ARG:NH1 | 1:U:424:ARG:CG | 2.41 | 0.42 |
| 1:U:429:ARG:O | 1:U:432:ASN:HB2 | 2.19 | 0.42 |
| 1:A:189:VAL:HG13 | 1:A:193:ASP:HB2 | 2.02 | 0.42 |
| 1:A:293:ILE:HG12 | 1:A:326:CYS:HB2 | 2.01 | 0.42 |
| 1:A:371:HIS:O | 1:A:374:MET:CG | 2.57 | 0.42 |
| 1:B:293:ILE:HG12 | 1:B:326:CYS:HB2 | 2.01 | 0.42 |
| 1:C:53:SER:HA | 1:C:85:LYS:CG | 2.50 | 0.42 |
| 1:D:270:PRO:CB | 1:D:273:LYS:HD2 | 2.50 | 0.42 |
| 1:E:138:GLY:HA2 | 1:E:151:GLN:HE21 | 1.85 | 0.42 |
| 1:G:362:PHE:O | 1:G:366:ILE:HD12 | 2.19 | 0.42 |
| 1:I:362:PHE:O | 1:I:366:ILE:HD12 | 2.19 | 0.42 |
| 1:I:372:ILE:HD12 | 1:I:374:MET:HG3 | 2.00 | 0.42 |
| 1:J:189:VAL:HG13 | 1:J:193:ASP:HB2 | 2.02 | 0.42 |
| 1:K:401:ASN:N | 2:K:700:FDP:O5P | 2.50 | 0.42 |
| 1:N:79:ALA:HA | 1:N:429:ARG:HB3 | 2.01 | 0.42 |
| 1:P:474:ASP:O | 1:P:497:VAL:HG13 | 2.20 | 0.42 |
| 1:Q:429:ARG:O | 1:Q:432:ASN:HB2 | 2.19 | 0.42 |
| 1:Q:79:ALA:HA | 1:Q:429:ARG:HB3 | 2.01 | 0.42 |
| 1:R:272:GLU:HB2 | 1:T:352:GLU:HG2 | 1.94 | 0.42 |
| 1:U:362:PHE:O | 1:U:366:ILE:HD12 | 2.19 | 0.42 |
| 1:W:189:VAL:HG13 | 1:W:193:ASP:HB2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:212:PHE:CD2 | 1:W:214:ARG:NE | 2.88 | 0.42 |
| 1:A:270:PRO:CB | 1:A:273:LYS:HD2 | 2.50 | 0.42 |
| 1:B:362:PHE:O | 1:B:366:ILE:HD12 | 2.19 | 0.42 |
| 1:B:373:PRO:HB3 | 1:O:391:THR:CA | 2.49 | 0.42 |
| 1:C:474:ASP:O | 1:C:497:VAL:HG13 | 2.20 | 0.42 |
| 1:D:293:ILE:HG12 | 1:D:326:CYS:HB2 | 2.01 | 0.42 |
| 1:D:372:ILE:HD11 | 1:D:374:MET:HE1 | 2.01 | 0.42 |
| 1:E:53:SER:HA | 1:E:85:LYS:CG | 2.50 | 0.42 |
| 1:F:371:HIS:O | 1:F:374:MET:CG | 2.57 | 0.42 |
| 1:H:402:THR:OG1 | 1:H:404:ARG:HB2 | 2.20 | 0.42 |
| 1:M:189:VAL:HG13 | 1:M:193:ASP:HB2 | 2.02 | 0.42 |
| 1:O:53:SER:HA | 1:O:85:LYS:CG | 2.50 | 0.42 |
| 1:P:401:ASN:N | 2:P:700:FDP:O5P | 2.50 | 0.42 |
| 1:U:352:GLU:CG | 1:W:272:GLU:CG | 2.98 | 0.42 |
| 1:V:138:GLY:HA2 | 1:V:151:GLN:HE21 | 1.85 | 0.42 |
| 1:W:474:ASP:O | 1:W:497:VAL:HG13 | 2.20 | 0.42 |
| 1:B:212:PHE:CD2 | 1:B:214:ARG:NE | 2.88 | 0.41 |
| 1:B:53:SER:HA | 1:B:85:LYS:CG | 2.50 | 0.41 |
| 1:C:212:PHE:CD2 | 1:C:214:ARG:NE | 2.88 | 0.41 |
| 1:C:270:PRO:CB | 1:C:273:LYS:HD2 | 2.50 | 0.41 |
| 1:C:79:ALA:HA | 1:C:429:ARG:HB3 | 2.01 | 0.41 |
| 1:D:362:PHE:O | 1:D:366:ILE:HD12 | 2.19 | 0.41 |
| 1:F:293:ILE:HG12 | 1:F:326:CYS:HB2 | 2.01 | 0.41 |
| 1:G:53:SER:HA | 1:G:85:LYS:CG | 2.50 | 0.41 |
| 1:H:53:SER:HA | 1:H:85:LYS:CG | 2.50 | 0.41 |
| 1:L:311:ALA:HA | 1:N:315:ASP:HB2 | 2.01 | 0.41 |
| 1:L:472:THR:CG2 | 1:L:498:GLU:CA | 2.84 | 0.41 |
| 1:M:138:GLY:HA2 | 1:M:151:GLN:HE21 | 1.85 | 0.41 |
| 1:P:212:PHE:CD2 | 1:P:214:ARG:NE | 2.88 | 0.41 |
| 1:P:371:HIS:C | 1:P:372:ILE:HD13 | 2.40 | 0.41 |
| 1:Q:474:ASP:O | 1:Q:497:VAL:HG13 | 2.20 | 0.41 |
| 1:S:138:GLY:HA2 | 1:S:151:GLN:HE21 | 1.84 | 0.41 |
| 1:U:11:ILE:HB | 1:W:273:LYS:CD | 2.42 | 0.41 |
| 1:U:212:PHE:CD2 | 1:U:214:ARG:NE | 2.88 | 0.41 |
| 1:U:311:ALA:HB3 | 1:W:312:GLU:CG | 2.49 | 0.41 |
| 1:X:362:PHE:O | 1:X:366:ILE:HD12 | 2.19 | 0.41 |
| 1:D:474:ASP:O | 1:D:497:VAL:HG13 | 2.20 | 0.41 |
| 1:E:272:GLU:HG3 | 1:G:352:GLU:CB | 2.50 | 0.41 |
| 1:I:474:ASP:O | 1:I:497:VAL:HG13 | 2.20 | 0.41 |
| 1:L:429:ARG:O | 1:L:432:ASN:HB2 | 2.19 | 0.41 |
| 1:K:242:HIS:NE2 | 1:M:12:PHE:CE2 | 2.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:284:LYS:CG | 1:N:7:LEU:HD22 | 2.50 | 0.41 |
| 1:O:135:VAL:HG12 | 1:O:136:ARG:N | 2.35 | 0.41 |
| 1:O:293:ILE:HG12 | 1:O:326:CYS:HB2 | 2.01 | 0.41 |
| 1:O:315:ASP:HB2 | 1:P:311:ALA:CA | 2.48 | 0.41 |
| 1:P:189:VAL:HG13 | 1:P:193:ASP:HB2 | 2.02 | 0.41 |
| 1:P:79:ALA:HA | 1:P:429:ARG:HB3 | 2.02 | 0.41 |
| 1:Q:293:ILE:HG12 | 1:Q:326:CYS:HB2 | 2.01 | 0.41 |
| 1:Q:362:PHE:O | 1:Q:366:ILE:HD12 | 2.19 | 0.41 |
| 1:R:362:PHE:O | 1:R:366:ILE:HD12 | 2.19 | 0.41 |
| 1:X:474:ASP:O | 1:X:497:VAL:HG13 | 2.20 | 0.41 |
| 1:A:138:GLY:HA2 | 1:A:151:GLN:HE21 | 1.85 | 0.41 |
| 1:A:362:PHE:O | 1:A:366:ILE:HD12 | 2.19 | 0.41 |
| 1:B:188:ALA:CB | 1:B:218:GLN:HG2 | 2.21 | 0.41 |
| 1:B:270:PRO:CB | 1:B:273:LYS:HD2 | 2.50 | 0.41 |
| 1:B:474:ASP:O | 1:B:497:VAL:HG13 | 2.20 | 0.41 |
| 1:C:223:ARG:NH1 | 1:C:223:ARG:HG2 | 2.26 | 0.41 |
| 1:E:189:VAL:HG13 | 1:E:193:ASP:HB2 | 2.02 | 0.41 |
| 1:E:474:ASP:O | 1:E:497:VAL:HG13 | 2.20 | 0.41 |
| 1:G:189:VAL:HG13 | 1:G:193:ASP:HB2 | 2.02 | 0.41 |
| 1:H:189:VAL:HG13 | 1:H:193:ASP:HB2 | 2.02 | 0.41 |
| 1:H:296:THR:O | 1:J:310:ARG:HG3 | 2.20 | 0.41 |
| 1:I:53:SER:HA | 1:I:85:LYS:CG | 2.50 | 0.41 |
| 1:K:212:PHE:CD2 | 1:K:214:ARG:NE | 2.88 | 0.41 |
| 1:L:53:SER:HA | 1:L:85:LYS:CG | 2.50 | 0.41 |
| 1:N:138:GLY:HA2 | 1:N:151:GLN:HE21 | 1.85 | 0.41 |
| 1:O:101:MET:HE1 | 1:O:124:PHE:CE1 | 2.55 | 0.41 |
| 1:O:270:PRO:CB | 1:O:273:LYS:HD2 | 2.50 | 0.41 |
| 1:Q:212:PHE:CD2 | 1:Q:214:ARG:NE | 2.88 | 0.41 |
| 1:Q:390:GLU:O | 1:R:372:ILE:HG13 | 2.20 | 0.41 |
| 1:R:474:ASP:O | 1:R:497:VAL:HG13 | 2.20 | 0.41 |
| 1:U:474:ASP:O | 1:U:497:VAL:HG13 | 2.20 | 0.41 |
| 1:V:401:ASN:N | 2:V:700:FDP:O5P | 2.50 | 0.41 |
| 1:X:138:GLY:HA2 | 1:X:151:GLN:HE21 | 1.84 | 0.41 |
| 1:F:189:VAL:HG13 | 1:F:193:ASP:HB2 | 2.02 | 0.41 |
| 1:G:474:ASP:O | 1:G:497:VAL:HG13 | 2.20 | 0.41 |
| 1:I:212:PHE:CD2 | 1:I:214:ARG:NE | 2.88 | 0.41 |
| 1:I:79:ALA:HA | 1:I:429:ARG:HB3 | 2.01 | 0.41 |
| 1:J:293:ILE:HG12 | 1:J:326:CYS:HB2 | 2.01 | 0.41 |
| 1:K:297:GLN:HB2 | 1:M:310:ARG:HB2 | 2.01 | 0.41 |
| 1:N:189:VAL:HG13 | 1:N:193:ASP:HB2 | 2.02 | 0.41 |
| 1:P:214:ARG:HH11 | 1:P:214:ARG:HG3 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:467:LYS:HE2 | 1:Q:467:LYS:HB3 | 1.86 | 0.41 |
| 1:T:362:PHE:O | 1:T:366:ILE:HD12 | 2.19 | 0.41 |
| 1:S:491:GLN:NE2 | 1:T:491:GLN:NE2 | 2.68 | 0.41 |
| 1:U:214:ARG:HH11 | 1:U:214:ARG:HG3 | 1.86 | 0.41 |
| 1:V:189:VAL:HG13 | 1:V:193:ASP:HB2 | 2.02 | 0.41 |
| 1:B:214:ARG:HG3 | 1:B:214:ARG:HH11 | 1.86 | 0.41 |
| 1:B:49:ARG:NE | 1:B:83:ASP:OD2 | 2.33 | 0.41 |
| 1:C:214:ARG:HH11 | 1:C:214:ARG:HG3 | 1.86 | 0.41 |
| 1:C:362:PHE:O | 1:C:366:ILE:HD12 | 2.20 | 0.41 |
| 1:H:474:ASP:O | 1:H:497:VAL:HG13 | 2.20 | 0.41 |
| 1:K:138:GLY:HA2 | 1:K:151:GLN:HE21 | 1.84 | 0.41 |
| 1:K:429:ARG:O | 1:K:432:ASN:HB2 | 2.19 | 0.41 |
| 1:L:138:GLY:HA2 | 1:L:151:GLN:HE21 | 1.84 | 0.41 |
| 1:N:101:MET:HE1 | 1:N:124:PHE:CE1 | 2.55 | 0.41 |
| 1:N:212:PHE:CD2 | 1:N:214:ARG:NE | 2.88 | 0.41 |
| 1:T:424:ARG:NH1 | 1:T:424:ARG:CG | 2.41 | 0.41 |
| 1:U:189:VAL:HG13 | 1:U:193:ASP:HB2 | 2.02 | 0.41 |
| 1:V:362:PHE:O | 1:V:366:ILE:HD12 | 2.19 | 0.41 |
| 1:W:223:ARG:HG2 | 1:W:223:ARG:NH1 | 2.25 | 0.41 |
| 1:H:310:ARG:H | 1:J:297:GLN:HB3 | 1.86 | 0.41 |
| 1:K:270:PRO:CB | 1:K:273:LYS:HD2 | 2.50 | 0.41 |
| 1:L:310:ARG:NH2 | 1:N:297:GLN:OE1 | 2.53 | 0.41 |
| 1:P:377:ASP:OD2 | 1:P:377:ASP:N | 2.52 | 0.41 |
| 1:U:311:ALA:CB | 1:W:312:GLU:CG | 2.99 | 0.41 |
| 1:V:474:ASP:O | 1:V:497:VAL:HG13 | 2.20 | 0.41 |
| 1:W:53:SER:HA | 1:W:85:LYS:CG | 2.50 | 0.41 |
| 1:X:429:ARG:O | 1:X:432:ASN:HB2 | 2.19 | 0.41 |
| 1:B:272:GLU:CG | 1:C:352:GLU:CB | 2.98 | 0.41 |
| 1:E:79:ALA:HA | 1:E:429:ARG:HB3 | 2.01 | 0.41 |
| 1:F:214:ARG:HG3 | 1:F:214:ARG:HH11 | 1.86 | 0.41 |
| 1:F:79:ALA:HA | 1:F:429:ARG:HB3 | 2.01 | 0.41 |
| 1:G:138:GLY:HA2 | 1:G:151:GLN:HE21 | 1.85 | 0.41 |
| 1:F:373:PRO:HB2 | 1:G:391:THR:HA | 1.95 | 0.41 |
| 1:H:270:PRO:CB | 1:H:273:LYS:HD2 | 2.50 | 0.41 |
| 1:I:138:GLY:HA2 | 1:I:151:GLN:HE21 | 1.84 | 0.41 |
| 1:A:272:GLU:HA | 1:I:313:VAL:CG1 | 2.51 | 0.41 |
| 1:I:451:GLU:HG2 | 1:I:451:GLU:H | 1.59 | 0.41 |
| 1:J:212:PHE:CD2 | 1:J:214:ARG:NE | 2.88 | 0.41 |
| 1:H:310:ARG:H | 1:J:297:GLN:CB | 2.34 | 0.41 |
| 1:K:214:ARG:HH11 | 1:K:214:ARG:HG3 | 1.86 | 0.41 |
| 1:K:283:SER:OG | 1:M:3:LEU:HD23 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:402:THR:OG1 | 1:L:404:ARG:HB2 | 2.20 | 0.41 |
| 1:O:214:ARG:HG3 | 1:O:214:ARG:HH11 | 1.86 | 0.41 |
| 1:P:467:LYS:HB3 | 1:P:467:LYS:HE2 | 1.87 | 0.41 |
| 1:V:53:SER:HA | 1:V:85:LYS:CG | 2.50 | 0.41 |
| 1:U:315:ASP:CB | 1:W:311:ALA:CB | 2.99 | 0.41 |
| 1:X:189:VAL:HG13 | 1:X:193:ASP:HB2 | 2.02 | 0.41 |
| 1:X:214:ARG:HH11 | 1:X:214:ARG:HG3 | 1.86 | 0.41 |
| 1:D:214:ARG:HG3 | 1:D:214:ARG:HH11 | 1.86 | 0.41 |
| 1:G:214:ARG:HH11 | 1:G:214:ARG:HG3 | 1.86 | 0.41 |
| 1:K:189:VAL:HG13 | 1:K:193:ASP:HB2 | 2.02 | 0.41 |
| 1:N:472:THR:CG2 | 1:N:498:GLU:CA | 2.84 | 0.41 |
| 1:N:53:SER:HA | 1:N:85:LYS:CG | 2.50 | 0.41 |
| 1:O:138:GLY:HA2 | 1:O:151:GLN:HE21 | 1.84 | 0.41 |
| 1:O:224:LYS:HB3 | 1:O:224:LYS:HE3 | 1.82 | 0.41 |
| 1:Q:444:ALA:O | 1:Q:448:GLY:N | 2.54 | 0.41 |
| 1:R:293:ILE:HG12 | 1:R:326:CYS:HB2 | 2.01 | 0.41 |
| 1:R:279:LYS:CE | 1:T:6:ASN:OD1 | 2.63 | 0.41 |
| 1:U:376:ALA:HA | 1:V:494:ILE:HD12 | 2.03 | 0.41 |
| 1:A:214:ARG:HH11 | 1:A:214:ARG:HG3 | 1.86 | 0.41 |
| 1:A:474:ASP:O | 1:A:497:VAL:HG13 | 2.20 | 0.41 |
| 1:E:212:PHE:CD2 | 1:E:214:ARG:NE | 2.88 | 0.41 |
| 1:I:189:VAL:HG13 | 1:I:193:ASP:HB2 | 2.02 | 0.41 |
| 1:H:390:GLU:O | 1:I:373:PRO:HB3 | 2.21 | 0.41 |
| 1:I:444:ALA:O | 1:I:448:GLY:N | 2.54 | 0.41 |
| 1:J:214:ARG:HG3 | 1:J:214:ARG:HH11 | 1.86 | 0.41 |
| 1:K:11:ILE:O | 1:M:273:LYS:HE3 | 2.21 | 0.41 |
| 1:Q:189:VAL:HG13 | 1:Q:193:ASP:HB2 | 2.02 | 0.41 |
| 1:Q:374:MET:HB2 | 1:Q:375:SER:H | 1.78 | 0.41 |
| 1:S:212:PHE:CD2 | 1:S:214:ARG:NE | 2.88 | 0.41 |
| 1:S:214:ARG:HG3 | 1:S:214:ARG:HH11 | 1.86 | 0.41 |
| 1:T:189:VAL:HG13 | 1:T:193:ASP:HB2 | 2.02 | 0.41 |
| 1:U:101:MET:CE | 1:U:124:PHE:CE1 | 3.04 | 0.41 |
| 1:W:377:ASP:OD2 | 1:W:377:ASP:N | 2.52 | 0.41 |
| 1:W:424:ARG:NH1 | 1:W:424:ARG:CG | 2.41 | 0.41 |
| 1:B:101:MET:CE | 1:B:124:PHE:CE1 | 3.04 | 0.41 |
| 1:C:189:VAL:HG13 | 1:C:193:ASP:HB2 | 2.02 | 0.41 |
| 1:D:444:ALA:O | 1:D:448:GLY:N | 2.54 | 0.41 |
| 1:E:242:HIS:CE1 | 1:G:12:PHE:HZ | 2.34 | 0.41 |
| 1:H:352:GLU:CG | 1:J:272:GLU:CG | 2.99 | 0.41 |
| 1:M:101:MET:CE | 1:M:124:PHE:CE1 | 3.04 | 0.41 |
| 1:M:444:ALA:O | 1:M:448:GLY:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:297:GLN:HB2 | 1:P:310:ARG:CG | 2.44 | 0.41 |
| 1:O:312:GLU:CA | 1:P:311:ALA:HB1 | 2.33 | 0.41 |
| 1:Q:284:LYS:HG3 | 1:S:7:LEU:HD21 | 2.00 | 0.41 |
| 1:Q:310:ARG:CG | 1:S:297:GLN:HB2 | 2.51 | 0.41 |
| 1:V:101:MET:CE | 1:V:124:PHE:CE1 | 3.04 | 0.41 |
| 1:C:389:TYR:O | 1:P:372:ILE:HG21 | 2.21 | 0.41 |
| 1:D:212:PHE:CD2 | 1:D:214:ARG:NE | 2.88 | 0.41 |
| 1:E:372:ILE:HA | 1:E:372:ILE:HD12 | 1.73 | 0.41 |
| 1:H:444:ALA:O | 1:H:448:GLY:N | 2.54 | 0.41 |
| 1:O:189:VAL:HG13 | 1:O:193:ASP:HB2 | 2.02 | 0.41 |
| 1:P:101:MET:CE | 1:P:124:PHE:CE1 | 3.04 | 0.41 |
| 1:P:372:ILE:HA | 1:P:372:ILE:HD12 | 1.80 | 0.41 |
| 1:S:223:ARG:HG2 | 1:S:223:ARG:NH1 | 2.26 | 0.41 |
| 1:S:472:THR:CG2 | 1:S:498:GLU:CA | 2.84 | 0.41 |
| 1:L:195:VAL:HG11 | 1:T:498:GLU:HG2 | 2.02 | 0.41 |
| 1:U:277:ALA:HB2 | 1:W:11:ILE:HG21 | 2.03 | 0.41 |
| 1:A:212:PHE:CD2 | 1:A:214:ARG:NE | 2.88 | 0.40 |
| 1:A:444:ALA:O | 1:A:448:GLY:N | 2.54 | 0.40 |
| 1:A:53:SER:HA | 1:A:85:LYS:CG | 2.50 | 0.40 |
| 1:B:110:THR:O | 1:B:125:TYR:HA | 2.22 | 0.40 |
| 1:B:189:VAL:HG13 | 1:B:193:ASP:HB2 | 2.02 | 0.40 |
| 1:B:270:PRO:CG | 1:B:273:LYS:CD | 2.94 | 0.40 |
| 1:H:101:MET:CE | 1:H:124:PHE:CE1 | 3.04 | 0.40 |
| 1:I:101:MET:CE | 1:I:124:PHE:CE1 | 3.04 | 0.40 |
| 1:K:188:ALA:CB | 1:K:218:GLN:HG2 | 2.21 | 0.40 |
| 1:K:53:SER:HA | 1:K:85:LYS:CG | 2.50 | 0.40 |
| 1:L:214:ARG:HH11 | 1:L:214:ARG:HG3 | 1.86 | 0.40 |
| 1:L:451:GLU:H | 1:L:451:GLU:HG2 | 1.59 | 0.40 |
| 1:N:101:MET:CE | 1:N:124:PHE:CE1 | 3.04 | 0.40 |
| 1:O:444:ALA:O | 1:O:448:GLY:N | 2.54 | 0.40 |
| 1:Q:110:THR:O | 1:Q:125:TYR:HA | 2.22 | 0.40 |
| 1:Q:138:GLY:HA2 | 1:Q:151:GLN:HE21 | 1.85 | 0.40 |
| 1:Q:273:LYS:HG2 | 1:S:11:ILE:O | 2.21 | 0.40 |
| 1:R:53:SER:HA | 1:R:85:LYS:CG | 2.50 | 0.40 |
| 1:L:229:LYS:CG | 1:S:487:GLY:CA | 2.84 | 0.40 |
| 1:U:53:SER:HA | 1:U:85:LYS:CG | 2.50 | 0.40 |
| 1:W:214:ARG:HG3 | 1:W:214:ARG:HH11 | 1.86 | 0.40 |
| 1:A:101:MET:CE | 1:A:124:PHE:CE1 | 3.04 | 0.40 |
| 1:A:110:THR:O | 1:A:125:TYR:HA | 2.22 | 0.40 |
| 1:A:12:PHE:CE2 | 1:I:242:HIS:HE1 | 2.38 | 0.40 |
| 1:B:451:GLU:O | 1:B:453:LYS:HE2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:451:GLU:O | 1:C:453:LYS:HE2 | 2.22 | 0.40 |
| 1:E:110:THR:O | 1:E:125:TYR:HA | 2.22 | 0.40 |
| 1:F:101:MET:HE1 | 1:F:124:PHE:CE1 | 2.56 | 0.40 |
| 1:F:188:ALA:CB | 1:F:218:GLN:HG2 | 2.21 | 0.40 |
| 1:G:110:THR:O | 1:G:125:TYR:HA | 2.21 | 0.40 |
| 1:H:101:MET:HE1 | 1:H:124:PHE:CE1 | 2.56 | 0.40 |
| 1:I:110:THR:O | 1:I:125:TYR:HA | 2.21 | 0.40 |
| 1:H:494:ILE:HD12 | 1:I:376:ALA:HB1 | 2.03 | 0.40 |
| 1:J:110:THR:O | 1:J:125:TYR:HA | 2.22 | 0.40 |
| 1:M:110:THR:O | 1:M:125:TYR:HA | 2.22 | 0.40 |
| 1:N:424:ARG:NH1 | 1:N:424:ARG:CG | 2.41 | 0.40 |
| 1:O:310:ARG:CG | 1:P:297:GLN:OE1 | 2.60 | 0.40 |
| 1:Q:101:MET:HE1 | 1:Q:124:PHE:CE1 | 2.56 | 0.40 |
| 1:Q:53:SER:HA | 1:Q:85:LYS:CG | 2.50 | 0.40 |
| 1:R:189:VAL:HG13 | 1:R:193:ASP:HB2 | 2.02 | 0.40 |
| 1:R:444:ALA:O | 1:R:448:GLY:N | 2.54 | 0.40 |
| 1:Q:276:VAL:HG13 | 1:S:9:LEU:HD13 | 2.04 | 0.40 |
| 1:T:214:ARG:HH11 | 1:T:214:ARG:HG3 | 1.86 | 0.40 |
| 1:U:310:ARG:CG | 1:W:297:GLN:OE1 | 2.59 | 0.40 |
| 1:X:110:THR:O | 1:X:125:TYR:HA | 2.22 | 0.40 |
| 1:A:451:GLU:O | 1:A:453:LYS:HE2 | 2.22 | 0.40 |
| 1:B:371:HIS:O | 1:B:374:MET:CG | 2.57 | 0.40 |
| 1:C:110:THR:O | 1:C:125:TYR:HA | 2.21 | 0.40 |
| 1:C:451:GLU:HG2 | 1:C:451:GLU:H | 1.59 | 0.40 |
| 1:D:189:VAL:HG13 | 1:D:193:ASP:HB2 | 2.02 | 0.40 |
| 1:E:214:ARG:HH11 | 1:E:214:ARG:HG3 | 1.86 | 0.40 |
| 1:H:110:THR:O | 1:H:125:TYR:HA | 2.22 | 0.40 |
| 1:I:451:GLU:O | 1:I:453:LYS:HE2 | 2.22 | 0.40 |
| 1:J:372:ILE:HD12 | 1:J:372:ILE:HA | 1.73 | 0.40 |
| 1:K:110:THR:O | 1:K:125:TYR:HA | 2.22 | 0.40 |
| 1:L:312:GLU:HG3 | 1:N:311:ALA:HB3 | 2.03 | 0.40 |
| 1:K:273:LYS:HG2 | 1:M:11:ILE:O | 2.22 | 0.40 |
| 1:O:270:PRO:CG | 1:O:273:LYS:CD | 2.94 | 0.40 |
| 1:O:467:LYS:HE2 | 1:O:467:LYS:HB3 | 1.86 | 0.40 |
| 1:Q:101:MET:CE | 1:Q:124:PHE:CE1 | 3.04 | 0.40 |
| 1:Q:214:ARG:HG3 | 1:Q:214:ARG:HH11 | 1.86 | 0.40 |
| 1:R:110:THR:O | 1:R:125:TYR:HA | 2.22 | 0.40 |
| 1:T:401:ASN:N | 2:T:700:FDP:O5P | 2.50 | 0.40 |
| 1:V:371:HIS:O | 1:V:374:MET:CG | 2.57 | 0.40 |
| 1:A:467:LYS:HB3 | 1:A:467:LYS:HE2 | 1.86 | 0.40 |
| 1:A:472:THR:CG2 | 1:A:498:GLU:CA | 2.84 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:372:ILE:HA | 1:C:372:ILE:HD12 | 1.73 | 0.40 |
| 1:F:101:MET:CE | 1:F:124:PHE:CE1 | 3.04 | 0.40 |
| 1:H:318:ASN:CG | 1:J:318:ASN:ND2 | 2.75 | 0.40 |
| 1:K:310:ARG:NH2 | 1:M:297:GLN:OE1 | 2.54 | 0.40 |
| 1:M:451:GLU:O | 1:M:453:LYS:HE2 | 2.22 | 0.40 |
| 1:M:53:SER:HA | 1:M:85:LYS:CG | 2.50 | 0.40 |
| 1:R:101:MET:HE1 | 1:R:124:PHE:CE1 | 2.57 | 0.40 |
| 1:R:451:GLU:O | 1:R:453:LYS:HE2 | 2.22 | 0.40 |
| 1:R:401:ASN:N | 2:R:700:FDP:O5P | 2.54 | 0.40 |
| 1:S:110:THR:O | 1:S:125:TYR:HA | 2.22 | 0.40 |
| 1:U:110:THR:O | 1:U:125:TYR:HA | 2.22 | 0.40 |
| 1:U:372:ILE:HD11 | 1:U:374:MET:CE | 2.51 | 0.40 |
| 1:B:482:ASP:HB3 | 1:B:491:GLN:HE21 | 1.87 | 0.40 |
| 1:H:451:GLU:O | 1:H:453:LYS:HE2 | 2.22 | 0.40 |
| 1:K:297:GLN:HB2 | 1:M:310:ARG:CB | 2.51 | 0.40 |
| 1:M:372:ILE:HD12 | 1:M:374:MET:HG3 | 2.04 | 0.40 |
| 1:O:101:MET:CE | 1:O:124:PHE:CE1 | 3.04 | 0.40 |
| 1:Q:451:GLU:O | 1:Q:453:LYS:HE2 | 2.22 | 0.40 |
| 1:R:101:MET:CE | 1:R:124:PHE:CE1 | 3.04 | 0.40 |
| 1:S:482:ASP:HB3 | 1:S:491:GLN:HE21 | 1.87 | 0.40 |
| 1:U:270:PRO:CB | 1:U:273:LYS:HD2 | 2.50 | 0.40 |
| 1:V:214:ARG:HG3 | 1:V:214:ARG:HH11 | 1.86 | 0.40 |
| 1:W:101:MET:HE1 | 1:W:124:PHE:CE1 | 2.57 | 0.40 |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:J:103:ARG:CD | 1:T:58:GLU:OE1[5_545] | 1.91 | 0.29 |
| 1:F:229:LYS:CE | 1:W:487:GLY:CA[5_545] | 2.08 | 0.12 |
| 1:F:229:LYS:CD | 1:W:487:GLY:CA[5_545] | 2.15 | 0.05 |
| 1:F:229:LYS:CG | 1:W:487:GLY:CA[5_545] | 2.16 | 0.04 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------------|-------------|----------|----------|-------------|----|
| 1 | A | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | B | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | C | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | D | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | E | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | F | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | G | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | H | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | I | 496 / 499 (99%) | 485 (98%) | 10 (2%) | 1 (0%) | 47 | 81 |
| 1 | J | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | K | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | L | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | M | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | N | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | O | 496 / 499 (99%) | 485 (98%) | 10 (2%) | 1 (0%) | 47 | 81 |
| 1 | P | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | Q | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | R | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | S | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | T | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | U | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | V | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | W | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| 1 | X | 496 / 499 (99%) | 486 (98%) | 9 (2%) | 1 (0%) | 47 | 81 |
| All | All | 11904 / 11976 (99%) | 11662 (98%) | 218 (2%) | 24 (0%) | 47 | 81 |

All (24) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 296 | THR |
| 1 | B | 296 | THR |
| 1 | C | 296 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 296 | THR |
| 1 | E | 296 | THR |
| 1 | F | 296 | THR |
| 1 | G | 296 | THR |
| 1 | H | 296 | THR |
| 1 | I | 296 | THR |
| 1 | J | 296 | THR |
| 1 | K | 296 | THR |
| 1 | L | 296 | THR |
| 1 | M | 296 | THR |
| 1 | N | 296 | THR |
| 1 | O | 296 | THR |
| 1 | P | 296 | THR |
| 1 | Q | 296 | THR |
| 1 | R | 296 | THR |
| 1 | S | 296 | THR |
| 1 | T | 296 | THR |
| 1 | U | 296 | THR |
| 1 | V | 296 | THR |
| 1 | W | 296 | THR |
| 1 | X | 296 | THR |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 416/417 (100%) | 376 (90%) | 40 (10%) | 8 | 29 |
| 1 | B | 416/417 (100%) | 375 (90%) | 41 (10%) | 8 | 28 |
| 1 | C | 416/417 (100%) | 374 (90%) | 42 (10%) | 7 | 27 |
| 1 | D | 416/417 (100%) | 375 (90%) | 41 (10%) | 8 | 28 |
| 1 | E | 416/417 (100%) | 376 (90%) | 40 (10%) | 8 | 29 |
| 1 | F | 416/417 (100%) | 375 (90%) | 41 (10%) | 8 | 28 |
| 1 | G | 416/417 (100%) | 375 (90%) | 41 (10%) | 8 | 28 |
| 1 | H | 416/417 (100%) | 375 (90%) | 41 (10%) | 8 | 28 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|------------|-----------|-------------|----|
| 1 | I | 416/417 (100%) | 375 (90%) | 41 (10%) | 8 | 28 |
| 1 | J | 416/417 (100%) | 375 (90%) | 41 (10%) | 8 | 28 |
| 1 | K | 416/417 (100%) | 376 (90%) | 40 (10%) | 8 | 29 |
| 1 | L | 416/417 (100%) | 376 (90%) | 40 (10%) | 8 | 29 |
| 1 | M | 416/417 (100%) | 376 (90%) | 40 (10%) | 8 | 29 |
| 1 | N | 416/417 (100%) | 376 (90%) | 40 (10%) | 8 | 29 |
| 1 | O | 416/417 (100%) | 375 (90%) | 41 (10%) | 8 | 28 |
| 1 | P | 416/417 (100%) | 376 (90%) | 40 (10%) | 8 | 29 |
| 1 | Q | 416/417 (100%) | 375 (90%) | 41 (10%) | 8 | 28 |
| 1 | R | 416/417 (100%) | 376 (90%) | 40 (10%) | 8 | 29 |
| 1 | S | 416/417 (100%) | 376 (90%) | 40 (10%) | 8 | 29 |
| 1 | T | 416/417 (100%) | 376 (90%) | 40 (10%) | 8 | 29 |
| 1 | U | 416/417 (100%) | 376 (90%) | 40 (10%) | 8 | 29 |
| 1 | V | 416/417 (100%) | 376 (90%) | 40 (10%) | 8 | 29 |
| 1 | W | 416/417 (100%) | 374 (90%) | 42 (10%) | 7 | 27 |
| 1 | X | 416/417 (100%) | 377 (91%) | 39 (9%) | 8 | 30 |
| All | All | 9984/10008 (100%) | 9012 (90%) | 972 (10%) | 8 | 29 |

All (972) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 3 | LEU |
| 1 | A | 17 | ASN |
| 1 | A | 31 | THR |
| 1 | A | 38 | LYS |
| 1 | A | 40 | LEU |
| 1 | A | 118 | LYS |
| 1 | A | 175 | ARG |
| 1 | A | 177 | VAL |
| 1 | A | 179 | LEU |
| 1 | A | 194 | ARG |
| 1 | A | 214 | ARG |
| 1 | A | 223 | ARG |
| 1 | A | 265 | LEU |
| 1 | A | 267 | VAL |
| 1 | A | 269 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 304 | TYR |
| 1 | A | 335 | LYS |
| 1 | A | 345 | TYR |
| 1 | A | 362 | PHE |
| 1 | A | 372 | ILE |
| 1 | A | 374 | MET |
| 1 | A | 382 | SER |
| 1 | A | 383 | SER |
| 1 | A | 394 | LYS |
| 1 | A | 396 | MET |
| 1 | A | 398 | VAL |
| 1 | A | 424 | ARG |
| 1 | A | 435 | GLN |
| 1 | A | 446 | LYS |
| 1 | A | 451 | GLU |
| 1 | A | 453 | LYS |
| 1 | A | 454 | GLU |
| 1 | A | 466 | SER |
| 1 | A | 467 | LYS |
| 1 | A | 471 | GLN |
| 1 | A | 472 | THR |
| 1 | A | 490 | ASN |
| 1 | A | 495 | LEU |
| 1 | A | 497 | VAL |
| 1 | A | 498 | GLU |
| 1 | B | 3 | LEU |
| 1 | B | 17 | ASN |
| 1 | B | 31 | THR |
| 1 | B | 38 | LYS |
| 1 | B | 40 | LEU |
| 1 | B | 103 | ARG |
| 1 | B | 118 | LYS |
| 1 | B | 175 | ARG |
| 1 | B | 177 | VAL |
| 1 | B | 179 | LEU |
| 1 | B | 194 | ARG |
| 1 | B | 214 | ARG |
| 1 | B | 223 | ARG |
| 1 | B | 265 | LEU |
| 1 | B | 267 | VAL |
| 1 | B | 269 | ILE |
| 1 | B | 304 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 335 | LYS |
| 1 | B | 345 | TYR |
| 1 | B | 362 | PHE |
| 1 | B | 372 | ILE |
| 1 | B | 374 | MET |
| 1 | B | 382 | SER |
| 1 | B | 383 | SER |
| 1 | B | 394 | LYS |
| 1 | B | 396 | MET |
| 1 | B | 398 | VAL |
| 1 | B | 424 | ARG |
| 1 | B | 435 | GLN |
| 1 | B | 446 | LYS |
| 1 | B | 451 | GLU |
| 1 | B | 453 | LYS |
| 1 | B | 454 | GLU |
| 1 | B | 466 | SER |
| 1 | B | 467 | LYS |
| 1 | B | 471 | GLN |
| 1 | B | 472 | THR |
| 1 | B | 490 | ASN |
| 1 | B | 495 | LEU |
| 1 | B | 497 | VAL |
| 1 | B | 498 | GLU |
| 1 | C | 3 | LEU |
| 1 | C | 12 | PHE |
| 1 | C | 17 | ASN |
| 1 | C | 31 | THR |
| 1 | C | 38 | LYS |
| 1 | C | 40 | LEU |
| 1 | C | 58 | GLU |
| 1 | C | 118 | LYS |
| 1 | C | 175 | ARG |
| 1 | C | 177 | VAL |
| 1 | C | 179 | LEU |
| 1 | C | 194 | ARG |
| 1 | C | 214 | ARG |
| 1 | C | 223 | ARG |
| 1 | C | 265 | LEU |
| 1 | C | 267 | VAL |
| 1 | C | 269 | ILE |
| 1 | C | 304 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 335 | LYS |
| 1 | C | 345 | TYR |
| 1 | C | 362 | PHE |
| 1 | C | 372 | ILE |
| 1 | C | 374 | MET |
| 1 | C | 382 | SER |
| 1 | C | 383 | SER |
| 1 | C | 394 | LYS |
| 1 | C | 396 | MET |
| 1 | C | 398 | VAL |
| 1 | C | 424 | ARG |
| 1 | C | 435 | GLN |
| 1 | C | 446 | LYS |
| 1 | C | 451 | GLU |
| 1 | C | 453 | LYS |
| 1 | C | 454 | GLU |
| 1 | C | 466 | SER |
| 1 | C | 467 | LYS |
| 1 | C | 471 | GLN |
| 1 | C | 472 | THR |
| 1 | C | 490 | ASN |
| 1 | C | 495 | LEU |
| 1 | C | 497 | VAL |
| 1 | C | 498 | GLU |
| 1 | D | 3 | LEU |
| 1 | D | 17 | ASN |
| 1 | D | 31 | THR |
| 1 | D | 38 | LYS |
| 1 | D | 40 | LEU |
| 1 | D | 118 | LYS |
| 1 | D | 175 | ARG |
| 1 | D | 177 | VAL |
| 1 | D | 179 | LEU |
| 1 | D | 194 | ARG |
| 1 | D | 214 | ARG |
| 1 | D | 223 | ARG |
| 1 | D | 265 | LEU |
| 1 | D | 267 | VAL |
| 1 | D | 269 | ILE |
| 1 | D | 304 | TYR |
| 1 | D | 335 | LYS |
| 1 | D | 345 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 362 | PHE |
| 1 | D | 372 | ILE |
| 1 | D | 374 | MET |
| 1 | D | 382 | SER |
| 1 | D | 383 | SER |
| 1 | D | 394 | LYS |
| 1 | D | 396 | MET |
| 1 | D | 398 | VAL |
| 1 | D | 404 | ARG |
| 1 | D | 424 | ARG |
| 1 | D | 435 | GLN |
| 1 | D | 446 | LYS |
| 1 | D | 451 | GLU |
| 1 | D | 453 | LYS |
| 1 | D | 454 | GLU |
| 1 | D | 466 | SER |
| 1 | D | 467 | LYS |
| 1 | D | 471 | GLN |
| 1 | D | 472 | THR |
| 1 | D | 490 | ASN |
| 1 | D | 495 | LEU |
| 1 | D | 497 | VAL |
| 1 | D | 498 | GLU |
| 1 | E | 3 | LEU |
| 1 | E | 17 | ASN |
| 1 | E | 31 | THR |
| 1 | E | 38 | LYS |
| 1 | E | 40 | LEU |
| 1 | E | 118 | LYS |
| 1 | E | 175 | ARG |
| 1 | E | 177 | VAL |
| 1 | E | 179 | LEU |
| 1 | E | 194 | ARG |
| 1 | E | 214 | ARG |
| 1 | E | 223 | ARG |
| 1 | E | 265 | LEU |
| 1 | E | 267 | VAL |
| 1 | E | 269 | ILE |
| 1 | E | 304 | TYR |
| 1 | E | 335 | LYS |
| 1 | E | 345 | TYR |
| 1 | E | 362 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 372 | ILE |
| 1 | E | 374 | MET |
| 1 | E | 382 | SER |
| 1 | E | 383 | SER |
| 1 | E | 394 | LYS |
| 1 | E | 396 | MET |
| 1 | E | 398 | VAL |
| 1 | E | 424 | ARG |
| 1 | E | 435 | GLN |
| 1 | E | 446 | LYS |
| 1 | E | 451 | GLU |
| 1 | E | 453 | LYS |
| 1 | E | 454 | GLU |
| 1 | E | 466 | SER |
| 1 | E | 467 | LYS |
| 1 | E | 471 | GLN |
| 1 | E | 472 | THR |
| 1 | E | 490 | ASN |
| 1 | E | 495 | LEU |
| 1 | E | 497 | VAL |
| 1 | E | 498 | GLU |
| 1 | F | 3 | LEU |
| 1 | F | 12 | PHE |
| 1 | F | 17 | ASN |
| 1 | F | 31 | THR |
| 1 | F | 38 | LYS |
| 1 | F | 40 | LEU |
| 1 | F | 118 | LYS |
| 1 | F | 175 | ARG |
| 1 | F | 177 | VAL |
| 1 | F | 179 | LEU |
| 1 | F | 194 | ARG |
| 1 | F | 214 | ARG |
| 1 | F | 223 | ARG |
| 1 | F | 265 | LEU |
| 1 | F | 267 | VAL |
| 1 | F | 269 | ILE |
| 1 | F | 304 | TYR |
| 1 | F | 335 | LYS |
| 1 | F | 345 | TYR |
| 1 | F | 362 | PHE |
| 1 | F | 372 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 374 | MET |
| 1 | F | 382 | SER |
| 1 | F | 383 | SER |
| 1 | F | 394 | LYS |
| 1 | F | 396 | MET |
| 1 | F | 398 | VAL |
| 1 | F | 424 | ARG |
| 1 | F | 435 | GLN |
| 1 | F | 446 | LYS |
| 1 | F | 451 | GLU |
| 1 | F | 453 | LYS |
| 1 | F | 454 | GLU |
| 1 | F | 466 | SER |
| 1 | F | 467 | LYS |
| 1 | F | 471 | GLN |
| 1 | F | 472 | THR |
| 1 | F | 490 | ASN |
| 1 | F | 495 | LEU |
| 1 | F | 497 | VAL |
| 1 | F | 498 | GLU |
| 1 | G | 3 | LEU |
| 1 | G | 17 | ASN |
| 1 | G | 31 | THR |
| 1 | G | 38 | LYS |
| 1 | G | 40 | LEU |
| 1 | G | 118 | LYS |
| 1 | G | 175 | ARG |
| 1 | G | 177 | VAL |
| 1 | G | 179 | LEU |
| 1 | G | 194 | ARG |
| 1 | G | 214 | ARG |
| 1 | G | 223 | ARG |
| 1 | G | 265 | LEU |
| 1 | G | 267 | VAL |
| 1 | G | 269 | ILE |
| 1 | G | 304 | TYR |
| 1 | G | 335 | LYS |
| 1 | G | 345 | TYR |
| 1 | G | 362 | PHE |
| 1 | G | 372 | ILE |
| 1 | G | 374 | MET |
| 1 | G | 382 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 383 | SER |
| 1 | G | 394 | LYS |
| 1 | G | 396 | MET |
| 1 | G | 398 | VAL |
| 1 | G | 404 | ARG |
| 1 | G | 424 | ARG |
| 1 | G | 435 | GLN |
| 1 | G | 446 | LYS |
| 1 | G | 451 | GLU |
| 1 | G | 453 | LYS |
| 1 | G | 454 | GLU |
| 1 | G | 466 | SER |
| 1 | G | 467 | LYS |
| 1 | G | 471 | GLN |
| 1 | G | 472 | THR |
| 1 | G | 490 | ASN |
| 1 | G | 495 | LEU |
| 1 | G | 497 | VAL |
| 1 | G | 498 | GLU |
| 1 | H | 3 | LEU |
| 1 | H | 17 | ASN |
| 1 | H | 31 | THR |
| 1 | H | 38 | LYS |
| 1 | H | 40 | LEU |
| 1 | H | 118 | LYS |
| 1 | H | 175 | ARG |
| 1 | H | 177 | VAL |
| 1 | H | 179 | LEU |
| 1 | H | 194 | ARG |
| 1 | H | 214 | ARG |
| 1 | H | 223 | ARG |
| 1 | H | 265 | LEU |
| 1 | H | 267 | VAL |
| 1 | H | 269 | ILE |
| 1 | H | 297 | GLN |
| 1 | H | 304 | TYR |
| 1 | H | 335 | LYS |
| 1 | H | 345 | TYR |
| 1 | H | 362 | PHE |
| 1 | H | 371 | HIS |
| 1 | H | 372 | ILE |
| 1 | H | 382 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 383 | SER |
| 1 | H | 394 | LYS |
| 1 | H | 396 | MET |
| 1 | H | 398 | VAL |
| 1 | H | 424 | ARG |
| 1 | H | 435 | GLN |
| 1 | H | 446 | LYS |
| 1 | H | 451 | GLU |
| 1 | H | 453 | LYS |
| 1 | H | 454 | GLU |
| 1 | H | 466 | SER |
| 1 | H | 467 | LYS |
| 1 | H | 471 | GLN |
| 1 | H | 472 | THR |
| 1 | H | 490 | ASN |
| 1 | H | 495 | LEU |
| 1 | H | 497 | VAL |
| 1 | H | 498 | GLU |
| 1 | I | 3 | LEU |
| 1 | I | 17 | ASN |
| 1 | I | 31 | THR |
| 1 | I | 38 | LYS |
| 1 | I | 40 | LEU |
| 1 | I | 118 | LYS |
| 1 | I | 175 | ARG |
| 1 | I | 177 | VAL |
| 1 | I | 179 | LEU |
| 1 | I | 194 | ARG |
| 1 | I | 214 | ARG |
| 1 | I | 223 | ARG |
| 1 | I | 265 | LEU |
| 1 | I | 267 | VAL |
| 1 | I | 269 | ILE |
| 1 | I | 304 | TYR |
| 1 | I | 335 | LYS |
| 1 | I | 345 | TYR |
| 1 | I | 362 | PHE |
| 1 | I | 371 | HIS |
| 1 | I | 372 | ILE |
| 1 | I | 382 | SER |
| 1 | I | 383 | SER |
| 1 | I | 394 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 396 | MET |
| 1 | I | 398 | VAL |
| 1 | I | 404 | ARG |
| 1 | I | 424 | ARG |
| 1 | I | 435 | GLN |
| 1 | I | 446 | LYS |
| 1 | I | 451 | GLU |
| 1 | I | 453 | LYS |
| 1 | I | 454 | GLU |
| 1 | I | 466 | SER |
| 1 | I | 467 | LYS |
| 1 | I | 471 | GLN |
| 1 | I | 472 | THR |
| 1 | I | 490 | ASN |
| 1 | I | 495 | LEU |
| 1 | I | 497 | VAL |
| 1 | I | 498 | GLU |
| 1 | J | 3 | LEU |
| 1 | J | 12 | PHE |
| 1 | J | 17 | ASN |
| 1 | J | 31 | THR |
| 1 | J | 38 | LYS |
| 1 | J | 40 | LEU |
| 1 | J | 118 | LYS |
| 1 | J | 175 | ARG |
| 1 | J | 177 | VAL |
| 1 | J | 179 | LEU |
| 1 | J | 194 | ARG |
| 1 | J | 214 | ARG |
| 1 | J | 223 | ARG |
| 1 | J | 265 | LEU |
| 1 | J | 267 | VAL |
| 1 | J | 269 | ILE |
| 1 | J | 304 | TYR |
| 1 | J | 335 | LYS |
| 1 | J | 345 | TYR |
| 1 | J | 362 | PHE |
| 1 | J | 372 | ILE |
| 1 | J | 374 | MET |
| 1 | J | 382 | SER |
| 1 | J | 383 | SER |
| 1 | J | 394 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 396 | MET |
| 1 | J | 398 | VAL |
| 1 | J | 424 | ARG |
| 1 | J | 435 | GLN |
| 1 | J | 446 | LYS |
| 1 | J | 451 | GLU |
| 1 | J | 453 | LYS |
| 1 | J | 454 | GLU |
| 1 | J | 466 | SER |
| 1 | J | 467 | LYS |
| 1 | J | 471 | GLN |
| 1 | J | 472 | THR |
| 1 | J | 490 | ASN |
| 1 | J | 495 | LEU |
| 1 | J | 497 | VAL |
| 1 | J | 498 | GLU |
| 1 | K | 3 | LEU |
| 1 | K | 17 | ASN |
| 1 | K | 31 | THR |
| 1 | K | 38 | LYS |
| 1 | K | 40 | LEU |
| 1 | K | 118 | LYS |
| 1 | K | 175 | ARG |
| 1 | K | 177 | VAL |
| 1 | K | 179 | LEU |
| 1 | K | 194 | ARG |
| 1 | K | 214 | ARG |
| 1 | K | 223 | ARG |
| 1 | K | 265 | LEU |
| 1 | K | 267 | VAL |
| 1 | K | 269 | ILE |
| 1 | K | 304 | TYR |
| 1 | K | 335 | LYS |
| 1 | K | 345 | TYR |
| 1 | K | 362 | PHE |
| 1 | K | 372 | ILE |
| 1 | K | 374 | MET |
| 1 | K | 382 | SER |
| 1 | K | 383 | SER |
| 1 | K | 394 | LYS |
| 1 | K | 396 | MET |
| 1 | K | 398 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 424 | ARG |
| 1 | K | 435 | GLN |
| 1 | K | 446 | LYS |
| 1 | K | 451 | GLU |
| 1 | K | 453 | LYS |
| 1 | K | 454 | GLU |
| 1 | K | 466 | SER |
| 1 | K | 467 | LYS |
| 1 | K | 471 | GLN |
| 1 | K | 472 | THR |
| 1 | K | 490 | ASN |
| 1 | K | 495 | LEU |
| 1 | K | 497 | VAL |
| 1 | K | 498 | GLU |
| 1 | L | 3 | LEU |
| 1 | L | 17 | ASN |
| 1 | L | 31 | THR |
| 1 | L | 38 | LYS |
| 1 | L | 40 | LEU |
| 1 | L | 118 | LYS |
| 1 | L | 175 | ARG |
| 1 | L | 177 | VAL |
| 1 | L | 179 | LEU |
| 1 | L | 194 | ARG |
| 1 | L | 214 | ARG |
| 1 | L | 223 | ARG |
| 1 | L | 265 | LEU |
| 1 | L | 267 | VAL |
| 1 | L | 269 | ILE |
| 1 | L | 304 | TYR |
| 1 | L | 335 | LYS |
| 1 | L | 337 | LYS |
| 1 | L | 345 | TYR |
| 1 | L | 362 | PHE |
| 1 | L | 372 | ILE |
| 1 | L | 382 | SER |
| 1 | L | 383 | SER |
| 1 | L | 394 | LYS |
| 1 | L | 396 | MET |
| 1 | L | 398 | VAL |
| 1 | L | 424 | ARG |
| 1 | L | 435 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 446 | LYS |
| 1 | L | 451 | GLU |
| 1 | L | 453 | LYS |
| 1 | L | 454 | GLU |
| 1 | L | 466 | SER |
| 1 | L | 467 | LYS |
| 1 | L | 471 | GLN |
| 1 | L | 472 | THR |
| 1 | L | 490 | ASN |
| 1 | L | 495 | LEU |
| 1 | L | 497 | VAL |
| 1 | L | 498 | GLU |
| 1 | M | 3 | LEU |
| 1 | M | 12 | PHE |
| 1 | M | 17 | ASN |
| 1 | M | 31 | THR |
| 1 | M | 38 | LYS |
| 1 | M | 40 | LEU |
| 1 | M | 118 | LYS |
| 1 | M | 175 | ARG |
| 1 | M | 177 | VAL |
| 1 | M | 179 | LEU |
| 1 | M | 194 | ARG |
| 1 | M | 214 | ARG |
| 1 | M | 223 | ARG |
| 1 | M | 265 | LEU |
| 1 | M | 267 | VAL |
| 1 | M | 269 | ILE |
| 1 | M | 304 | TYR |
| 1 | M | 335 | LYS |
| 1 | M | 345 | TYR |
| 1 | M | 362 | PHE |
| 1 | M | 372 | ILE |
| 1 | M | 382 | SER |
| 1 | M | 383 | SER |
| 1 | M | 394 | LYS |
| 1 | M | 396 | MET |
| 1 | M | 398 | VAL |
| 1 | M | 424 | ARG |
| 1 | M | 435 | GLN |
| 1 | M | 446 | LYS |
| 1 | M | 451 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 453 | LYS |
| 1 | M | 454 | GLU |
| 1 | M | 466 | SER |
| 1 | M | 467 | LYS |
| 1 | M | 471 | GLN |
| 1 | M | 472 | THR |
| 1 | M | 490 | ASN |
| 1 | M | 495 | LEU |
| 1 | M | 497 | VAL |
| 1 | M | 498 | GLU |
| 1 | N | 3 | LEU |
| 1 | N | 17 | ASN |
| 1 | N | 31 | THR |
| 1 | N | 38 | LYS |
| 1 | N | 40 | LEU |
| 1 | N | 118 | LYS |
| 1 | N | 175 | ARG |
| 1 | N | 177 | VAL |
| 1 | N | 179 | LEU |
| 1 | N | 194 | ARG |
| 1 | N | 214 | ARG |
| 1 | N | 223 | ARG |
| 1 | N | 265 | LEU |
| 1 | N | 267 | VAL |
| 1 | N | 269 | ILE |
| 1 | N | 304 | TYR |
| 1 | N | 335 | LYS |
| 1 | N | 345 | TYR |
| 1 | N | 362 | PHE |
| 1 | N | 372 | ILE |
| 1 | N | 374 | MET |
| 1 | N | 382 | SER |
| 1 | N | 383 | SER |
| 1 | N | 394 | LYS |
| 1 | N | 396 | MET |
| 1 | N | 398 | VAL |
| 1 | N | 424 | ARG |
| 1 | N | 435 | GLN |
| 1 | N | 446 | LYS |
| 1 | N | 451 | GLU |
| 1 | N | 453 | LYS |
| 1 | N | 454 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 466 | SER |
| 1 | N | 467 | LYS |
| 1 | N | 471 | GLN |
| 1 | N | 472 | THR |
| 1 | N | 490 | ASN |
| 1 | N | 495 | LEU |
| 1 | N | 497 | VAL |
| 1 | N | 498 | GLU |
| 1 | O | 3 | LEU |
| 1 | O | 17 | ASN |
| 1 | O | 31 | THR |
| 1 | O | 38 | LYS |
| 1 | O | 40 | LEU |
| 1 | O | 118 | LYS |
| 1 | O | 175 | ARG |
| 1 | O | 177 | VAL |
| 1 | O | 179 | LEU |
| 1 | O | 194 | ARG |
| 1 | O | 214 | ARG |
| 1 | O | 223 | ARG |
| 1 | O | 265 | LEU |
| 1 | O | 267 | VAL |
| 1 | O | 269 | ILE |
| 1 | O | 304 | TYR |
| 1 | O | 335 | LYS |
| 1 | O | 345 | TYR |
| 1 | O | 362 | PHE |
| 1 | O | 372 | ILE |
| 1 | O | 374 | MET |
| 1 | O | 382 | SER |
| 1 | O | 383 | SER |
| 1 | O | 394 | LYS |
| 1 | O | 396 | MET |
| 1 | O | 398 | VAL |
| 1 | O | 404 | ARG |
| 1 | O | 424 | ARG |
| 1 | O | 435 | GLN |
| 1 | O | 446 | LYS |
| 1 | O | 451 | GLU |
| 1 | O | 453 | LYS |
| 1 | O | 454 | GLU |
| 1 | O | 466 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 467 | LYS |
| 1 | O | 471 | GLN |
| 1 | O | 472 | THR |
| 1 | O | 490 | ASN |
| 1 | O | 495 | LEU |
| 1 | O | 497 | VAL |
| 1 | O | 498 | GLU |
| 1 | P | 3 | LEU |
| 1 | P | 12 | PHE |
| 1 | P | 17 | ASN |
| 1 | P | 31 | THR |
| 1 | P | 38 | LYS |
| 1 | P | 40 | LEU |
| 1 | P | 118 | LYS |
| 1 | P | 175 | ARG |
| 1 | P | 177 | VAL |
| 1 | P | 179 | LEU |
| 1 | P | 194 | ARG |
| 1 | P | 214 | ARG |
| 1 | P | 223 | ARG |
| 1 | P | 265 | LEU |
| 1 | P | 267 | VAL |
| 1 | P | 269 | ILE |
| 1 | P | 304 | TYR |
| 1 | P | 335 | LYS |
| 1 | P | 345 | TYR |
| 1 | P | 362 | PHE |
| 1 | P | 372 | ILE |
| 1 | P | 382 | SER |
| 1 | P | 383 | SER |
| 1 | P | 394 | LYS |
| 1 | P | 396 | MET |
| 1 | P | 398 | VAL |
| 1 | P | 424 | ARG |
| 1 | P | 435 | GLN |
| 1 | P | 446 | LYS |
| 1 | P | 451 | GLU |
| 1 | P | 453 | LYS |
| 1 | P | 454 | GLU |
| 1 | P | 466 | SER |
| 1 | P | 467 | LYS |
| 1 | P | 471 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 472 | THR |
| 1 | P | 490 | ASN |
| 1 | P | 495 | LEU |
| 1 | P | 497 | VAL |
| 1 | P | 498 | GLU |
| 1 | Q | 3 | LEU |
| 1 | Q | 12 | PHE |
| 1 | Q | 17 | ASN |
| 1 | Q | 31 | THR |
| 1 | Q | 38 | LYS |
| 1 | Q | 40 | LEU |
| 1 | Q | 118 | LYS |
| 1 | Q | 175 | ARG |
| 1 | Q | 177 | VAL |
| 1 | Q | 179 | LEU |
| 1 | Q | 194 | ARG |
| 1 | Q | 214 | ARG |
| 1 | Q | 223 | ARG |
| 1 | Q | 265 | LEU |
| 1 | Q | 267 | VAL |
| 1 | Q | 269 | ILE |
| 1 | Q | 304 | TYR |
| 1 | Q | 335 | LYS |
| 1 | Q | 345 | TYR |
| 1 | Q | 362 | PHE |
| 1 | Q | 372 | ILE |
| 1 | Q | 374 | MET |
| 1 | Q | 382 | SER |
| 1 | Q | 383 | SER |
| 1 | Q | 394 | LYS |
| 1 | Q | 396 | MET |
| 1 | Q | 398 | VAL |
| 1 | Q | 424 | ARG |
| 1 | Q | 435 | GLN |
| 1 | Q | 446 | LYS |
| 1 | Q | 451 | GLU |
| 1 | Q | 453 | LYS |
| 1 | Q | 454 | GLU |
| 1 | Q | 466 | SER |
| 1 | Q | 467 | LYS |
| 1 | Q | 471 | GLN |
| 1 | Q | 472 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Q | 490 | ASN |
| 1 | Q | 495 | LEU |
| 1 | Q | 497 | VAL |
| 1 | Q | 498 | GLU |
| 1 | R | 3 | LEU |
| 1 | R | 17 | ASN |
| 1 | R | 31 | THR |
| 1 | R | 38 | LYS |
| 1 | R | 40 | LEU |
| 1 | R | 118 | LYS |
| 1 | R | 175 | ARG |
| 1 | R | 177 | VAL |
| 1 | R | 179 | LEU |
| 1 | R | 194 | ARG |
| 1 | R | 214 | ARG |
| 1 | R | 223 | ARG |
| 1 | R | 265 | LEU |
| 1 | R | 267 | VAL |
| 1 | R | 269 | ILE |
| 1 | R | 297 | GLN |
| 1 | R | 304 | TYR |
| 1 | R | 335 | LYS |
| 1 | R | 345 | TYR |
| 1 | R | 362 | PHE |
| 1 | R | 372 | ILE |
| 1 | R | 382 | SER |
| 1 | R | 383 | SER |
| 1 | R | 394 | LYS |
| 1 | R | 396 | MET |
| 1 | R | 398 | VAL |
| 1 | R | 424 | ARG |
| 1 | R | 435 | GLN |
| 1 | R | 446 | LYS |
| 1 | R | 451 | GLU |
| 1 | R | 453 | LYS |
| 1 | R | 454 | GLU |
| 1 | R | 466 | SER |
| 1 | R | 467 | LYS |
| 1 | R | 471 | GLN |
| 1 | R | 472 | THR |
| 1 | R | 490 | ASN |
| 1 | R | 495 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | R | 497 | VAL |
| 1 | R | 498 | GLU |
| 1 | S | 3 | LEU |
| 1 | S | 12 | PHE |
| 1 | S | 17 | ASN |
| 1 | S | 31 | THR |
| 1 | S | 38 | LYS |
| 1 | S | 40 | LEU |
| 1 | S | 118 | LYS |
| 1 | S | 175 | ARG |
| 1 | S | 177 | VAL |
| 1 | S | 179 | LEU |
| 1 | S | 194 | ARG |
| 1 | S | 214 | ARG |
| 1 | S | 223 | ARG |
| 1 | S | 265 | LEU |
| 1 | S | 267 | VAL |
| 1 | S | 269 | ILE |
| 1 | S | 304 | TYR |
| 1 | S | 335 | LYS |
| 1 | S | 345 | TYR |
| 1 | S | 362 | PHE |
| 1 | S | 374 | MET |
| 1 | S | 382 | SER |
| 1 | S | 383 | SER |
| 1 | S | 394 | LYS |
| 1 | S | 396 | MET |
| 1 | S | 398 | VAL |
| 1 | S | 424 | ARG |
| 1 | S | 435 | GLN |
| 1 | S | 446 | LYS |
| 1 | S | 451 | GLU |
| 1 | S | 453 | LYS |
| 1 | S | 454 | GLU |
| 1 | S | 466 | SER |
| 1 | S | 467 | LYS |
| 1 | S | 471 | GLN |
| 1 | S | 472 | THR |
| 1 | S | 490 | ASN |
| 1 | S | 495 | LEU |
| 1 | S | 497 | VAL |
| 1 | S | 498 | GLU |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | T | 3 | LEU |
| 1 | T | 12 | PHE |
| 1 | T | 17 | ASN |
| 1 | T | 31 | THR |
| 1 | T | 38 | LYS |
| 1 | T | 40 | LEU |
| 1 | T | 118 | LYS |
| 1 | T | 175 | ARG |
| 1 | T | 177 | VAL |
| 1 | T | 179 | LEU |
| 1 | T | 194 | ARG |
| 1 | T | 214 | ARG |
| 1 | T | 223 | ARG |
| 1 | T | 265 | LEU |
| 1 | T | 267 | VAL |
| 1 | T | 269 | ILE |
| 1 | T | 304 | TYR |
| 1 | T | 335 | LYS |
| 1 | T | 345 | TYR |
| 1 | T | 362 | PHE |
| 1 | T | 372 | ILE |
| 1 | T | 382 | SER |
| 1 | T | 383 | SER |
| 1 | T | 394 | LYS |
| 1 | T | 396 | MET |
| 1 | T | 398 | VAL |
| 1 | T | 424 | ARG |
| 1 | T | 435 | GLN |
| 1 | T | 446 | LYS |
| 1 | T | 451 | GLU |
| 1 | T | 453 | LYS |
| 1 | T | 454 | GLU |
| 1 | T | 466 | SER |
| 1 | T | 467 | LYS |
| 1 | T | 471 | GLN |
| 1 | T | 472 | THR |
| 1 | T | 490 | ASN |
| 1 | T | 495 | LEU |
| 1 | T | 497 | VAL |
| 1 | T | 498 | GLU |
| 1 | U | 3 | LEU |
| 1 | U | 17 | ASN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | U | 31 | THR |
| 1 | U | 38 | LYS |
| 1 | U | 40 | LEU |
| 1 | U | 118 | LYS |
| 1 | U | 175 | ARG |
| 1 | U | 177 | VAL |
| 1 | U | 179 | LEU |
| 1 | U | 194 | ARG |
| 1 | U | 214 | ARG |
| 1 | U | 223 | ARG |
| 1 | U | 265 | LEU |
| 1 | U | 267 | VAL |
| 1 | U | 269 | ILE |
| 1 | U | 304 | TYR |
| 1 | U | 335 | LYS |
| 1 | U | 345 | TYR |
| 1 | U | 362 | PHE |
| 1 | U | 372 | ILE |
| 1 | U | 382 | SER |
| 1 | U | 383 | SER |
| 1 | U | 394 | LYS |
| 1 | U | 396 | MET |
| 1 | U | 398 | VAL |
| 1 | U | 404 | ARG |
| 1 | U | 424 | ARG |
| 1 | U | 435 | GLN |
| 1 | U | 446 | LYS |
| 1 | U | 451 | GLU |
| 1 | U | 453 | LYS |
| 1 | U | 454 | GLU |
| 1 | U | 466 | SER |
| 1 | U | 467 | LYS |
| 1 | U | 471 | GLN |
| 1 | U | 472 | THR |
| 1 | U | 490 | ASN |
| 1 | U | 495 | LEU |
| 1 | U | 497 | VAL |
| 1 | U | 498 | GLU |
| 1 | V | 3 | LEU |
| 1 | V | 17 | ASN |
| 1 | V | 31 | THR |
| 1 | V | 38 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | V | 40 | LEU |
| 1 | V | 118 | LYS |
| 1 | V | 175 | ARG |
| 1 | V | 177 | VAL |
| 1 | V | 179 | LEU |
| 1 | V | 194 | ARG |
| 1 | V | 214 | ARG |
| 1 | V | 223 | ARG |
| 1 | V | 265 | LEU |
| 1 | V | 267 | VAL |
| 1 | V | 269 | ILE |
| 1 | V | 304 | TYR |
| 1 | V | 335 | LYS |
| 1 | V | 345 | TYR |
| 1 | V | 362 | PHE |
| 1 | V | 372 | ILE |
| 1 | V | 374 | MET |
| 1 | V | 382 | SER |
| 1 | V | 383 | SER |
| 1 | V | 394 | LYS |
| 1 | V | 396 | MET |
| 1 | V | 398 | VAL |
| 1 | V | 424 | ARG |
| 1 | V | 435 | GLN |
| 1 | V | 446 | LYS |
| 1 | V | 451 | GLU |
| 1 | V | 453 | LYS |
| 1 | V | 454 | GLU |
| 1 | V | 466 | SER |
| 1 | V | 467 | LYS |
| 1 | V | 471 | GLN |
| 1 | V | 472 | THR |
| 1 | V | 490 | ASN |
| 1 | V | 495 | LEU |
| 1 | V | 497 | VAL |
| 1 | V | 498 | GLU |
| 1 | W | 3 | LEU |
| 1 | W | 12 | PHE |
| 1 | W | 17 | ASN |
| 1 | W | 31 | THR |
| 1 | W | 38 | LYS |
| 1 | W | 40 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | W | 118 | LYS |
| 1 | W | 175 | ARG |
| 1 | W | 177 | VAL |
| 1 | W | 179 | LEU |
| 1 | W | 194 | ARG |
| 1 | W | 214 | ARG |
| 1 | W | 223 | ARG |
| 1 | W | 265 | LEU |
| 1 | W | 267 | VAL |
| 1 | W | 269 | ILE |
| 1 | W | 304 | TYR |
| 1 | W | 335 | LYS |
| 1 | W | 345 | TYR |
| 1 | W | 362 | PHE |
| 1 | W | 372 | ILE |
| 1 | W | 374 | MET |
| 1 | W | 382 | SER |
| 1 | W | 383 | SER |
| 1 | W | 394 | LYS |
| 1 | W | 396 | MET |
| 1 | W | 398 | VAL |
| 1 | W | 404 | ARG |
| 1 | W | 424 | ARG |
| 1 | W | 435 | GLN |
| 1 | W | 446 | LYS |
| 1 | W | 451 | GLU |
| 1 | W | 453 | LYS |
| 1 | W | 454 | GLU |
| 1 | W | 466 | SER |
| 1 | W | 467 | LYS |
| 1 | W | 471 | GLN |
| 1 | W | 472 | THR |
| 1 | W | 490 | ASN |
| 1 | W | 495 | LEU |
| 1 | W | 497 | VAL |
| 1 | W | 498 | GLU |
| 1 | X | 17 | ASN |
| 1 | X | 31 | THR |
| 1 | X | 38 | LYS |
| 1 | X | 40 | LEU |
| 1 | X | 118 | LYS |
| 1 | X | 175 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | X | 177 | VAL |
| 1 | X | 179 | LEU |
| 1 | X | 194 | ARG |
| 1 | X | 214 | ARG |
| 1 | X | 223 | ARG |
| 1 | X | 265 | LEU |
| 1 | X | 267 | VAL |
| 1 | X | 269 | ILE |
| 1 | X | 304 | TYR |
| 1 | X | 335 | LYS |
| 1 | X | 345 | TYR |
| 1 | X | 362 | PHE |
| 1 | X | 372 | ILE |
| 1 | X | 374 | MET |
| 1 | X | 382 | SER |
| 1 | X | 383 | SER |
| 1 | X | 394 | LYS |
| 1 | X | 396 | MET |
| 1 | X | 398 | VAL |
| 1 | X | 424 | ARG |
| 1 | X | 435 | GLN |
| 1 | X | 446 | LYS |
| 1 | X | 451 | GLU |
| 1 | X | 453 | LYS |
| 1 | X | 454 | GLU |
| 1 | X | 466 | SER |
| 1 | X | 467 | LYS |
| 1 | X | 471 | GLN |
| 1 | X | 472 | THR |
| 1 | X | 490 | ASN |
| 1 | X | 495 | LEU |
| 1 | X | 497 | VAL |
| 1 | X | 498 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (267) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 17 | ASN |
| 1 | A | 139 | ASN |
| 1 | A | 151 | GLN |
| 1 | A | 178 | ASN |
| 1 | A | 218 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 286 | ASN |
| 1 | A | 305 | ASN |
| 1 | A | 371 | HIS |
| 1 | A | 490 | ASN |
| 1 | B | 17 | ASN |
| 1 | B | 139 | ASN |
| 1 | B | 151 | GLN |
| 1 | B | 178 | ASN |
| 1 | B | 218 | GLN |
| 1 | B | 242 | HIS |
| 1 | B | 286 | ASN |
| 1 | B | 305 | ASN |
| 1 | B | 371 | HIS |
| 1 | B | 490 | ASN |
| 1 | C | 17 | ASN |
| 1 | C | 139 | ASN |
| 1 | C | 151 | GLN |
| 1 | C | 178 | ASN |
| 1 | C | 218 | GLN |
| 1 | C | 242 | HIS |
| 1 | C | 286 | ASN |
| 1 | C | 305 | ASN |
| 1 | C | 371 | HIS |
| 1 | C | 483 | HIS |
| 1 | C | 490 | ASN |
| 1 | D | 17 | ASN |
| 1 | D | 139 | ASN |
| 1 | D | 151 | GLN |
| 1 | D | 178 | ASN |
| 1 | D | 218 | GLN |
| 1 | D | 242 | HIS |
| 1 | D | 286 | ASN |
| 1 | D | 305 | ASN |
| 1 | D | 371 | HIS |
| 1 | D | 483 | HIS |
| 1 | D | 490 | ASN |
| 1 | E | 17 | ASN |
| 1 | E | 139 | ASN |
| 1 | E | 151 | GLN |
| 1 | E | 178 | ASN |
| 1 | E | 218 | GLN |
| 1 | E | 242 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 286 | ASN |
| 1 | E | 305 | ASN |
| 1 | E | 371 | HIS |
| 1 | E | 483 | HIS |
| 1 | E | 490 | ASN |
| 1 | F | 17 | ASN |
| 1 | F | 139 | ASN |
| 1 | F | 151 | GLN |
| 1 | F | 178 | ASN |
| 1 | F | 218 | GLN |
| 1 | F | 242 | HIS |
| 1 | F | 286 | ASN |
| 1 | F | 305 | ASN |
| 1 | F | 371 | HIS |
| 1 | F | 483 | HIS |
| 1 | F | 490 | ASN |
| 1 | G | 17 | ASN |
| 1 | G | 139 | ASN |
| 1 | G | 151 | GLN |
| 1 | G | 178 | ASN |
| 1 | G | 218 | GLN |
| 1 | G | 286 | ASN |
| 1 | G | 305 | ASN |
| 1 | G | 371 | HIS |
| 1 | G | 483 | HIS |
| 1 | G | 490 | ASN |
| 1 | H | 17 | ASN |
| 1 | H | 139 | ASN |
| 1 | H | 151 | GLN |
| 1 | H | 178 | ASN |
| 1 | H | 218 | GLN |
| 1 | H | 242 | HIS |
| 1 | H | 286 | ASN |
| 1 | H | 305 | ASN |
| 1 | H | 318 | ASN |
| 1 | H | 371 | HIS |
| 1 | H | 483 | HIS |
| 1 | H | 490 | ASN |
| 1 | I | 17 | ASN |
| 1 | I | 139 | ASN |
| 1 | I | 151 | GLN |
| 1 | I | 178 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 218 | GLN |
| 1 | I | 242 | HIS |
| 1 | I | 286 | ASN |
| 1 | I | 305 | ASN |
| 1 | I | 371 | HIS |
| 1 | I | 483 | HIS |
| 1 | I | 490 | ASN |
| 1 | J | 17 | ASN |
| 1 | J | 139 | ASN |
| 1 | J | 151 | GLN |
| 1 | J | 178 | ASN |
| 1 | J | 218 | GLN |
| 1 | J | 242 | HIS |
| 1 | J | 286 | ASN |
| 1 | J | 305 | ASN |
| 1 | J | 318 | ASN |
| 1 | J | 371 | HIS |
| 1 | J | 490 | ASN |
| 1 | K | 17 | ASN |
| 1 | K | 139 | ASN |
| 1 | K | 151 | GLN |
| 1 | K | 178 | ASN |
| 1 | K | 218 | GLN |
| 1 | K | 242 | HIS |
| 1 | K | 286 | ASN |
| 1 | K | 305 | ASN |
| 1 | K | 318 | ASN |
| 1 | K | 371 | HIS |
| 1 | K | 483 | HIS |
| 1 | K | 490 | ASN |
| 1 | L | 17 | ASN |
| 1 | L | 139 | ASN |
| 1 | L | 151 | GLN |
| 1 | L | 178 | ASN |
| 1 | L | 218 | GLN |
| 1 | L | 242 | HIS |
| 1 | L | 286 | ASN |
| 1 | L | 305 | ASN |
| 1 | L | 371 | HIS |
| 1 | L | 483 | HIS |
| 1 | L | 490 | ASN |
| 1 | M | 17 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 139 | ASN |
| 1 | M | 151 | GLN |
| 1 | M | 178 | ASN |
| 1 | M | 218 | GLN |
| 1 | M | 242 | HIS |
| 1 | M | 286 | ASN |
| 1 | M | 305 | ASN |
| 1 | M | 318 | ASN |
| 1 | M | 371 | HIS |
| 1 | M | 483 | HIS |
| 1 | M | 490 | ASN |
| 1 | N | 17 | ASN |
| 1 | N | 139 | ASN |
| 1 | N | 151 | GLN |
| 1 | N | 178 | ASN |
| 1 | N | 218 | GLN |
| 1 | N | 242 | HIS |
| 1 | N | 286 | ASN |
| 1 | N | 305 | ASN |
| 1 | N | 371 | HIS |
| 1 | N | 483 | HIS |
| 1 | N | 490 | ASN |
| 1 | O | 17 | ASN |
| 1 | O | 139 | ASN |
| 1 | O | 151 | GLN |
| 1 | O | 178 | ASN |
| 1 | O | 218 | GLN |
| 1 | O | 242 | HIS |
| 1 | O | 286 | ASN |
| 1 | O | 305 | ASN |
| 1 | O | 318 | ASN |
| 1 | O | 371 | HIS |
| 1 | O | 490 | ASN |
| 1 | P | 17 | ASN |
| 1 | P | 139 | ASN |
| 1 | P | 151 | GLN |
| 1 | P | 178 | ASN |
| 1 | P | 218 | GLN |
| 1 | P | 242 | HIS |
| 1 | P | 286 | ASN |
| 1 | P | 305 | ASN |
| 1 | P | 318 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 371 | HIS |
| 1 | P | 483 | HIS |
| 1 | P | 490 | ASN |
| 1 | Q | 17 | ASN |
| 1 | Q | 139 | ASN |
| 1 | Q | 151 | GLN |
| 1 | Q | 178 | ASN |
| 1 | Q | 218 | GLN |
| 1 | Q | 242 | HIS |
| 1 | Q | 286 | ASN |
| 1 | Q | 305 | ASN |
| 1 | Q | 371 | HIS |
| 1 | Q | 483 | HIS |
| 1 | Q | 490 | ASN |
| 1 | R | 17 | ASN |
| 1 | R | 139 | ASN |
| 1 | R | 151 | GLN |
| 1 | R | 178 | ASN |
| 1 | R | 218 | GLN |
| 1 | R | 242 | HIS |
| 1 | R | 286 | ASN |
| 1 | R | 297 | GLN |
| 1 | R | 305 | ASN |
| 1 | R | 371 | HIS |
| 1 | R | 483 | HIS |
| 1 | R | 490 | ASN |
| 1 | S | 17 | ASN |
| 1 | S | 139 | ASN |
| 1 | S | 151 | GLN |
| 1 | S | 178 | ASN |
| 1 | S | 218 | GLN |
| 1 | S | 242 | HIS |
| 1 | S | 286 | ASN |
| 1 | S | 305 | ASN |
| 1 | S | 371 | HIS |
| 1 | S | 490 | ASN |
| 1 | T | 17 | ASN |
| 1 | T | 139 | ASN |
| 1 | T | 151 | GLN |
| 1 | T | 178 | ASN |
| 1 | T | 218 | GLN |
| 1 | T | 286 | ASN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | T | 305 | ASN |
| 1 | T | 371 | HIS |
| 1 | T | 483 | HIS |
| 1 | T | 490 | ASN |
| 1 | T | 491 | GLN |
| 1 | U | 17 | ASN |
| 1 | U | 139 | ASN |
| 1 | U | 151 | GLN |
| 1 | U | 178 | ASN |
| 1 | U | 218 | GLN |
| 1 | U | 242 | HIS |
| 1 | U | 286 | ASN |
| 1 | U | 305 | ASN |
| 1 | U | 318 | ASN |
| 1 | U | 371 | HIS |
| 1 | U | 483 | HIS |
| 1 | U | 490 | ASN |
| 1 | V | 17 | ASN |
| 1 | V | 139 | ASN |
| 1 | V | 151 | GLN |
| 1 | V | 178 | ASN |
| 1 | V | 218 | GLN |
| 1 | V | 242 | HIS |
| 1 | V | 286 | ASN |
| 1 | V | 297 | GLN |
| 1 | V | 305 | ASN |
| 1 | V | 371 | HIS |
| 1 | V | 483 | HIS |
| 1 | V | 490 | ASN |
| 1 | W | 17 | ASN |
| 1 | W | 139 | ASN |
| 1 | W | 151 | GLN |
| 1 | W | 178 | ASN |
| 1 | W | 218 | GLN |
| 1 | W | 242 | HIS |
| 1 | W | 286 | ASN |
| 1 | W | 305 | ASN |
| 1 | W | 318 | ASN |
| 1 | W | 371 | HIS |
| 1 | W | 483 | HIS |
| 1 | W | 490 | ASN |
| 1 | X | 17 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | X | 139 | ASN |
| 1 | X | 151 | GLN |
| 1 | X | 178 | ASN |
| 1 | X | 218 | GLN |
| 1 | X | 242 | HIS |
| 1 | X | 286 | ASN |
| 1 | X | 305 | ASN |
| 1 | X | 371 | HIS |
| 1 | X | 483 | HIS |
| 1 | X | 490 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

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 | FDP | Q | 700 | - | 19,20,20 | 1.07 | 2 (10%) | 30,32,32 | 1.36 | 4 (13%) |
| 2 | FDP | T | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.36 | 4 (13%) |
| 2 | FDP | H | 700 | - | 19,20,20 | 1.07 | 2 (10%) | 30,32,32 | 1.36 | 5 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FDP | N | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.35 | 5 (16%) |
| 2 | FDP | S | 700 | - | 19,20,20 | 1.07 | 2 (10%) | 30,32,32 | 1.36 | 5 (16%) |
| 2 | FDP | W | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.35 | 5 (16%) |
| 2 | FDP | U | 700 | - | 19,20,20 | 1.07 | 2 (10%) | 30,32,32 | 1.35 | 4 (13%) |
| 2 | FDP | K | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.36 | 5 (16%) |
| 2 | FDP | M | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.35 | 4 (13%) |
| 2 | FDP | E | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.36 | 5 (16%) |
| 2 | FDP | J | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.36 | 5 (16%) |
| 2 | FDP | L | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.35 | 4 (13%) |
| 2 | FDP | B | 700 | - | 19,20,20 | 1.07 | 2 (10%) | 30,32,32 | 1.36 | 5 (16%) |
| 2 | FDP | F | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.36 | 4 (13%) |
| 2 | FDP | I | 700 | - | 19,20,20 | 1.07 | 2 (10%) | 30,32,32 | 1.36 | 5 (16%) |
| 2 | FDP | O | 700 | - | 19,20,20 | 1.07 | 2 (10%) | 30,32,32 | 1.36 | 5 (16%) |
| 2 | FDP | X | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.35 | 4 (13%) |
| 2 | FDP | A | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.36 | 4 (13%) |
| 2 | FDP | P | 700 | - | 19,20,20 | 1.07 | 2 (10%) | 30,32,32 | 1.35 | 4 (13%) |
| 2 | FDP | D | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.36 | 5 (16%) |
| 2 | FDP | C | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.35 | 4 (13%) |
| 2 | FDP | R | 700 | - | 19,20,20 | 1.07 | 2 (10%) | 30,32,32 | 1.36 | 4 (13%) |
| 2 | FDP | G | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.36 | 5 (16%) |
| 2 | FDP | V | 700 | - | 19,20,20 | 1.08 | 2 (10%) | 30,32,32 | 1.35 | 4 (13%) |

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 | FDP | Q | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | T | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | H | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | N | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | S | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | W | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | U | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | K | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | M | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | E | 700 | - | - | 1/12/34/34 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | FDP | J | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | L | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | B | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | F | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | I | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | O | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | X | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | A | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | P | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | D | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | C | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | R | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | G | 700 | - | - | 1/12/34/34 | 0/1/1/1 |
| 2 | FDP | V | 700 | - | - | 1/12/34/34 | 0/1/1/1 |

All (48) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2 | K | 700 | FDP | O4-C4 | -2.48 | 1.37 | 1.43 |
| 2 | X | 700 | FDP | O4-C4 | -2.47 | 1.37 | 1.43 |
| 2 | A | 700 | FDP | O4-C4 | -2.47 | 1.37 | 1.43 |
| 2 | W | 700 | FDP | O4-C4 | -2.47 | 1.37 | 1.43 |
| 2 | E | 700 | FDP | O4-C4 | -2.47 | 1.37 | 1.43 |
| 2 | C | 700 | FDP | O4-C4 | -2.46 | 1.37 | 1.43 |
| 2 | V | 700 | FDP | O4-C4 | -2.46 | 1.37 | 1.43 |
| 2 | M | 700 | FDP | O4-C4 | -2.45 | 1.37 | 1.43 |
| 2 | N | 700 | FDP | O4-C4 | -2.45 | 1.37 | 1.43 |
| 2 | D | 700 | FDP | O4-C4 | -2.45 | 1.37 | 1.43 |
| 2 | F | 700 | FDP | O4-C4 | -2.45 | 1.37 | 1.43 |
| 2 | L | 700 | FDP | O4-C4 | -2.45 | 1.37 | 1.43 |
| 2 | B | 700 | FDP | O4-C4 | -2.44 | 1.37 | 1.43 |
| 2 | P | 700 | FDP | O4-C4 | -2.44 | 1.37 | 1.43 |
| 2 | J | 700 | FDP | O4-C4 | -2.44 | 1.37 | 1.43 |
| 2 | I | 700 | FDP | O4-C4 | -2.43 | 1.37 | 1.43 |
| 2 | Q | 700 | FDP | O4-C4 | -2.43 | 1.37 | 1.43 |
| 2 | O | 700 | FDP | O4-C4 | -2.43 | 1.37 | 1.43 |
| 2 | G | 700 | FDP | O4-C4 | -2.43 | 1.37 | 1.43 |
| 2 | S | 700 | FDP | O4-C4 | -2.42 | 1.37 | 1.43 |
| 2 | U | 700 | FDP | O4-C4 | -2.42 | 1.37 | 1.43 |
| 2 | T | 700 | FDP | O4-C4 | -2.42 | 1.37 | 1.43 |
| 2 | H | 700 | FDP | O4-C4 | -2.42 | 1.37 | 1.43 |
| 2 | R | 700 | FDP | O4-C4 | -2.41 | 1.37 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | N | 700 | FDP | P2-O5P | -2.23 | 1.46 | 1.54 |
| 2 | E | 700 | FDP | P2-O5P | -2.23 | 1.46 | 1.54 |
| 2 | H | 700 | FDP | P2-O5P | -2.23 | 1.46 | 1.54 |
| 2 | P | 700 | FDP | P2-O5P | -2.23 | 1.46 | 1.54 |
| 2 | Q | 700 | FDP | P2-O5P | -2.22 | 1.46 | 1.54 |
| 2 | T | 700 | FDP | P2-O5P | -2.22 | 1.46 | 1.54 |
| 2 | W | 700 | FDP | P2-O5P | -2.22 | 1.46 | 1.54 |
| 2 | A | 700 | FDP | P2-O5P | -2.22 | 1.46 | 1.54 |
| 2 | U | 700 | FDP | P2-O5P | -2.21 | 1.46 | 1.54 |
| 2 | M | 700 | FDP | P2-O5P | -2.21 | 1.46 | 1.54 |
| 2 | K | 700 | FDP | P2-O5P | -2.21 | 1.46 | 1.54 |
| 2 | X | 700 | FDP | P2-O5P | -2.21 | 1.46 | 1.54 |
| 2 | I | 700 | FDP | P2-O5P | -2.21 | 1.46 | 1.54 |
| 2 | G | 700 | FDP | P2-O5P | -2.21 | 1.46 | 1.54 |
| 2 | V | 700 | FDP | P2-O5P | -2.21 | 1.46 | 1.54 |
| 2 | C | 700 | FDP | P2-O5P | -2.21 | 1.46 | 1.54 |
| 2 | J | 700 | FDP | P2-O5P | -2.21 | 1.46 | 1.54 |
| 2 | S | 700 | FDP | P2-O5P | -2.21 | 1.46 | 1.54 |
| 2 | R | 700 | FDP | P2-O5P | -2.21 | 1.46 | 1.54 |
| 2 | O | 700 | FDP | P2-O5P | -2.21 | 1.46 | 1.54 |
| 2 | D | 700 | FDP | P2-O5P | -2.21 | 1.46 | 1.54 |
| 2 | L | 700 | FDP | P2-O5P | -2.20 | 1.46 | 1.54 |
| 2 | B | 700 | FDP | P2-O5P | -2.20 | 1.46 | 1.54 |
| 2 | F | 700 | FDP | P2-O5P | -2.20 | 1.46 | 1.54 |

All (108) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2 | T | 700 | FDP | O2-C2-C3 | 3.22 | 118.53 | 108.18 |
| 2 | E | 700 | FDP | O2-C2-C3 | 3.22 | 118.52 | 108.18 |
| 2 | R | 700 | FDP | O2-C2-C3 | 3.22 | 118.52 | 108.18 |
| 2 | F | 700 | FDP | O2-C2-C3 | 3.22 | 118.52 | 108.18 |
| 2 | I | 700 | FDP | O2-C2-C3 | 3.22 | 118.51 | 108.18 |
| 2 | J | 700 | FDP | O2-C2-C3 | 3.21 | 118.50 | 108.18 |
| 2 | W | 700 | FDP | O2-C2-C3 | 3.21 | 118.50 | 108.18 |
| 2 | K | 700 | FDP | O2-C2-C3 | 3.21 | 118.50 | 108.18 |
| 2 | V | 700 | FDP | O2-C2-C3 | 3.21 | 118.50 | 108.18 |
| 2 | C | 700 | FDP | O2-C2-C3 | 3.21 | 118.49 | 108.18 |
| 2 | G | 700 | FDP | O2-C2-C3 | 3.21 | 118.49 | 108.18 |
| 2 | Q | 700 | FDP | O2-C2-C3 | 3.21 | 118.49 | 108.18 |
| 2 | B | 700 | FDP | O2-C2-C3 | 3.21 | 118.48 | 108.18 |
| 2 | H | 700 | FDP | O2-C2-C3 | 3.20 | 118.48 | 108.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | O | 700 | FDP | O2-C2-C3 | 3.20 | 118.48 | 108.18 |
| 2 | S | 700 | FDP | O2-C2-C3 | 3.20 | 118.46 | 108.18 |
| 2 | M | 700 | FDP | O2-C2-C3 | 3.20 | 118.46 | 108.18 |
| 2 | A | 700 | FDP | O2-C2-C3 | 3.20 | 118.46 | 108.18 |
| 2 | X | 700 | FDP | O2-C2-C3 | 3.20 | 118.46 | 108.18 |
| 2 | L | 700 | FDP | O2-C2-C3 | 3.20 | 118.45 | 108.18 |
| 2 | U | 700 | FDP | O2-C2-C3 | 3.20 | 118.45 | 108.18 |
| 2 | P | 700 | FDP | O2-C2-C3 | 3.19 | 118.44 | 108.18 |
| 2 | N | 700 | FDP | O2-C2-C3 | 3.19 | 118.43 | 108.18 |
| 2 | D | 700 | FDP | O2-C2-C3 | 3.19 | 118.43 | 108.18 |
| 2 | V | 700 | FDP | O6-P2-O4P | 3.08 | 115.10 | 106.47 |
| 2 | O | 700 | FDP | O6-P2-O4P | 3.07 | 115.09 | 106.47 |
| 2 | M | 700 | FDP | O6-P2-O4P | 3.07 | 115.09 | 106.47 |
| 2 | X | 700 | FDP | O6-P2-O4P | 3.07 | 115.09 | 106.47 |
| 2 | F | 700 | FDP | O6-P2-O4P | 3.07 | 115.08 | 106.47 |
| 2 | I | 700 | FDP | O6-P2-O4P | 3.07 | 115.07 | 106.47 |
| 2 | S | 700 | FDP | O6-P2-O4P | 3.06 | 115.07 | 106.47 |
| 2 | B | 700 | FDP | O6-P2-O4P | 3.06 | 115.07 | 106.47 |
| 2 | Q | 700 | FDP | O6-P2-O4P | 3.06 | 115.06 | 106.47 |
| 2 | L | 700 | FDP | O6-P2-O4P | 3.06 | 115.06 | 106.47 |
| 2 | G | 700 | FDP | O6-P2-O4P | 3.06 | 115.06 | 106.47 |
| 2 | R | 700 | FDP | O6-P2-O4P | 3.06 | 115.05 | 106.47 |
| 2 | J | 700 | FDP | O6-P2-O4P | 3.05 | 115.04 | 106.47 |
| 2 | T | 700 | FDP | O6-P2-O4P | 3.05 | 115.04 | 106.47 |
| 2 | A | 700 | FDP | O6-P2-O4P | 3.05 | 115.03 | 106.47 |
| 2 | U | 700 | FDP | O6-P2-O4P | 3.05 | 115.03 | 106.47 |
| 2 | K | 700 | FDP | O6-P2-O4P | 3.05 | 115.03 | 106.47 |
| 2 | E | 700 | FDP | O6-P2-O4P | 3.05 | 115.03 | 106.47 |
| 2 | D | 700 | FDP | O6-P2-O4P | 3.05 | 115.03 | 106.47 |
| 2 | P | 700 | FDP | O6-P2-O4P | 3.05 | 115.02 | 106.47 |
| 2 | H | 700 | FDP | O6-P2-O4P | 3.04 | 115.01 | 106.47 |
| 2 | C | 700 | FDP | O6-P2-O4P | 3.04 | 115.01 | 106.47 |
| 2 | N | 700 | FDP | O6-P2-O4P | 3.04 | 115.00 | 106.47 |
| 2 | W | 700 | FDP | O6-P2-O4P | 3.04 | 115.00 | 106.47 |
| 2 | F | 700 | FDP | C6-C5-C4 | -2.64 | 105.28 | 115.18 |
| 2 | X | 700 | FDP | C6-C5-C4 | -2.64 | 105.29 | 115.18 |
| 2 | W | 700 | FDP | C6-C5-C4 | -2.64 | 105.30 | 115.18 |
| 2 | O | 700 | FDP | C6-C5-C4 | -2.64 | 105.30 | 115.18 |
| 2 | Q | 700 | FDP | C6-C5-C4 | -2.63 | 105.31 | 115.18 |
| 2 | R | 700 | FDP | C6-C5-C4 | -2.63 | 105.31 | 115.18 |
| 2 | U | 700 | FDP | C6-C5-C4 | -2.63 | 105.32 | 115.18 |
| 2 | D | 700 | FDP | C6-C5-C4 | -2.63 | 105.32 | 115.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | C | 700 | FDP | C6-C5-C4 | -2.63 | 105.32 | 115.18 |
| 2 | B | 700 | FDP | C6-C5-C4 | -2.63 | 105.32 | 115.18 |
| 2 | T | 700 | FDP | C6-C5-C4 | -2.63 | 105.32 | 115.18 |
| 2 | N | 700 | FDP | C6-C5-C4 | -2.63 | 105.32 | 115.18 |
| 2 | K | 700 | FDP | C6-C5-C4 | -2.63 | 105.33 | 115.18 |
| 2 | J | 700 | FDP | C6-C5-C4 | -2.63 | 105.33 | 115.18 |
| 2 | A | 700 | FDP | C6-C5-C4 | -2.63 | 105.33 | 115.18 |
| 2 | I | 700 | FDP | C6-C5-C4 | -2.63 | 105.33 | 115.18 |
| 2 | P | 700 | FDP | C6-C5-C4 | -2.63 | 105.34 | 115.18 |
| 2 | G | 700 | FDP | C6-C5-C4 | -2.63 | 105.34 | 115.18 |
| 2 | M | 700 | FDP | C6-C5-C4 | -2.63 | 105.34 | 115.18 |
| 2 | E | 700 | FDP | C6-C5-C4 | -2.62 | 105.35 | 115.18 |
| 2 | S | 700 | FDP | C6-C5-C4 | -2.62 | 105.35 | 115.18 |
| 2 | L | 700 | FDP | C6-C5-C4 | -2.62 | 105.36 | 115.18 |
| 2 | H | 700 | FDP | C6-C5-C4 | -2.62 | 105.38 | 115.18 |
| 2 | V | 700 | FDP | C6-C5-C4 | -2.62 | 105.38 | 115.18 |
| 2 | R | 700 | FDP | O5-C2-C3 | -2.24 | 100.88 | 105.49 |
| 2 | A | 700 | FDP | O5-C2-C3 | -2.23 | 100.89 | 105.49 |
| 2 | O | 700 | FDP | O5-C2-C3 | -2.23 | 100.90 | 105.49 |
| 2 | L | 700 | FDP | O5-C2-C3 | -2.23 | 100.90 | 105.49 |
| 2 | P | 700 | FDP | O5-C2-C3 | -2.22 | 100.91 | 105.49 |
| 2 | B | 700 | FDP | O5-C2-C3 | -2.22 | 100.91 | 105.49 |
| 2 | Q | 700 | FDP | O5-C2-C3 | -2.22 | 100.92 | 105.49 |
| 2 | I | 700 | FDP | O5-C2-C3 | -2.21 | 100.92 | 105.49 |
| 2 | K | 700 | FDP | O5-C2-C3 | -2.21 | 100.93 | 105.49 |
| 2 | V | 700 | FDP | O5-C2-C3 | -2.21 | 100.93 | 105.49 |
| 2 | F | 700 | FDP | O5-C2-C3 | -2.21 | 100.93 | 105.49 |
| 2 | U | 700 | FDP | O5-C2-C3 | -2.21 | 100.94 | 105.49 |
| 2 | S | 700 | FDP | O5-C2-C3 | -2.21 | 100.94 | 105.49 |
| 2 | T | 700 | FDP | O5-C2-C3 | -2.20 | 100.94 | 105.49 |
| 2 | M | 700 | FDP | O5-C2-C3 | -2.20 | 100.95 | 105.49 |
| 2 | N | 700 | FDP | O5-C2-C3 | -2.20 | 100.95 | 105.49 |
| 2 | H | 700 | FDP | O5-C2-C3 | -2.20 | 100.95 | 105.49 |
| 2 | E | 700 | FDP | O5-C2-C3 | -2.20 | 100.96 | 105.49 |
| 2 | J | 700 | FDP | O5-C2-C3 | -2.20 | 100.96 | 105.49 |
| 2 | D | 700 | FDP | O5-C2-C3 | -2.19 | 100.96 | 105.49 |
| 2 | C | 700 | FDP | O5-C2-C3 | -2.19 | 100.97 | 105.49 |
| 2 | G | 700 | FDP | O5-C2-C3 | -2.19 | 100.97 | 105.49 |
| 2 | X | 700 | FDP | O5-C2-C3 | -2.19 | 100.97 | 105.49 |
| 2 | W | 700 | FDP | O5-C2-C3 | -2.19 | 100.97 | 105.49 |
| 2 | K | 700 | FDP | C1-C2-C3 | -2.01 | 108.62 | 114.56 |
| 2 | H | 700 | FDP | C1-C2-C3 | -2.01 | 108.62 | 114.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | O | 700 | FDP | C1-C2-C3 | -2.01 | 108.63 | 114.56 |
| 2 | J | 700 | FDP | C1-C2-C3 | -2.01 | 108.63 | 114.56 |
| 2 | G | 700 | FDP | C1-C2-C3 | -2.01 | 108.64 | 114.56 |
| 2 | S | 700 | FDP | C1-C2-C3 | -2.01 | 108.64 | 114.56 |
| 2 | B | 700 | FDP | C1-C2-C3 | -2.01 | 108.64 | 114.56 |
| 2 | W | 700 | FDP | C1-C2-C3 | -2.00 | 108.64 | 114.56 |
| 2 | E | 700 | FDP | C1-C2-C3 | -2.00 | 108.65 | 114.56 |
| 2 | I | 700 | FDP | C1-C2-C3 | -2.00 | 108.65 | 114.56 |
| 2 | N | 700 | FDP | C1-C2-C3 | -2.00 | 108.65 | 114.56 |
| 2 | D | 700 | FDP | C1-C2-C3 | -2.00 | 108.66 | 114.56 |

There are no chirality outliers.

All (24) torsion outliers are listed below:

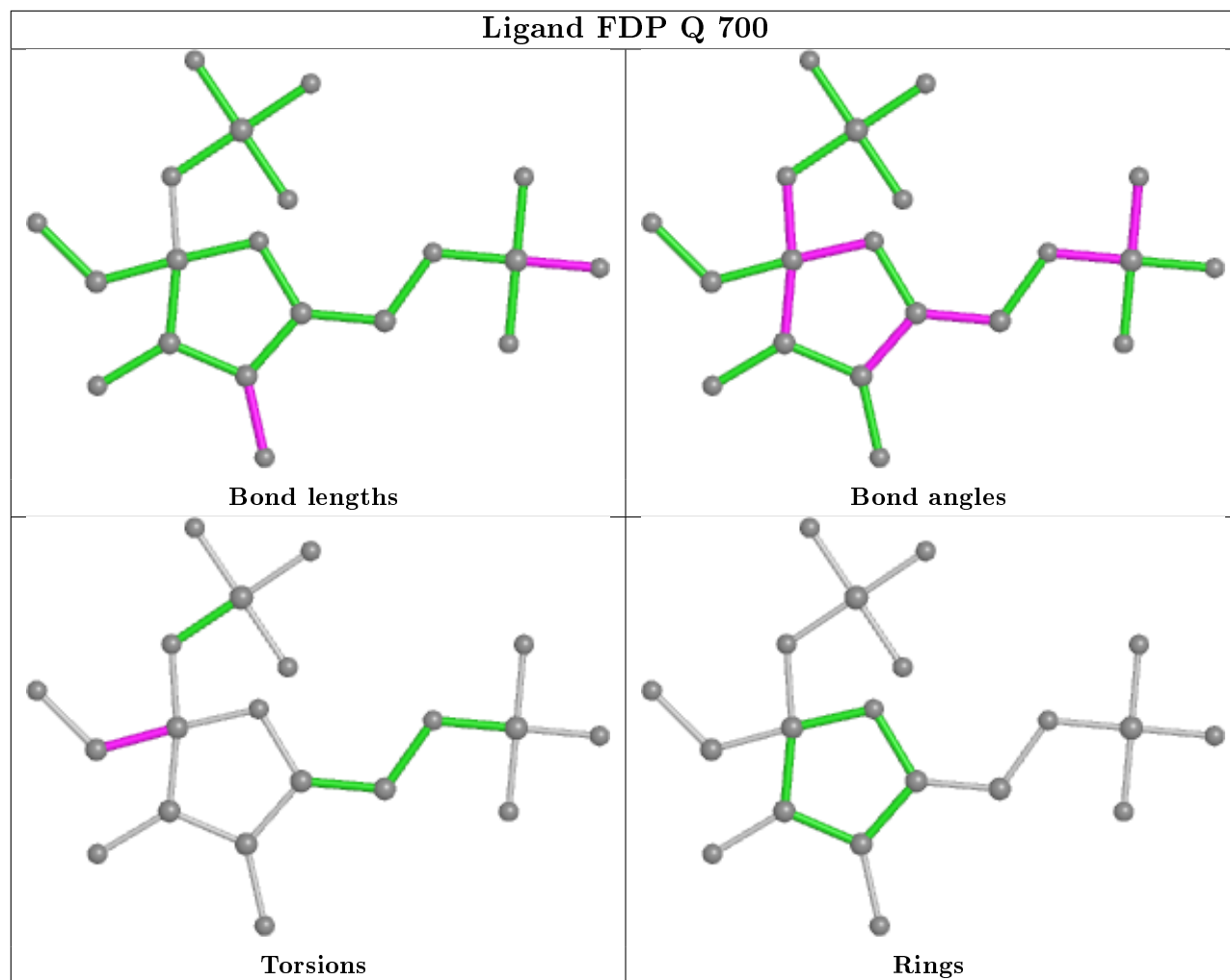
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 2 | Q | 700 | FDP | O1-C1-C2-C3 |
| 2 | T | 700 | FDP | O1-C1-C2-C3 |
| 2 | H | 700 | FDP | O1-C1-C2-C3 |
| 2 | N | 700 | FDP | O1-C1-C2-C3 |
| 2 | S | 700 | FDP | O1-C1-C2-C3 |
| 2 | W | 700 | FDP | O1-C1-C2-C3 |
| 2 | U | 700 | FDP | O1-C1-C2-C3 |
| 2 | K | 700 | FDP | O1-C1-C2-C3 |
| 2 | M | 700 | FDP | O1-C1-C2-C3 |
| 2 | E | 700 | FDP | O1-C1-C2-C3 |
| 2 | J | 700 | FDP | O1-C1-C2-C3 |
| 2 | L | 700 | FDP | O1-C1-C2-C3 |
| 2 | B | 700 | FDP | O1-C1-C2-C3 |
| 2 | F | 700 | FDP | O1-C1-C2-C3 |
| 2 | I | 700 | FDP | O1-C1-C2-C3 |
| 2 | O | 700 | FDP | O1-C1-C2-C3 |
| 2 | X | 700 | FDP | O1-C1-C2-C3 |
| 2 | A | 700 | FDP | O1-C1-C2-C3 |
| 2 | P | 700 | FDP | O1-C1-C2-C3 |
| 2 | D | 700 | FDP | O1-C1-C2-C3 |
| 2 | C | 700 | FDP | O1-C1-C2-C3 |
| 2 | R | 700 | FDP | O1-C1-C2-C3 |
| 2 | G | 700 | FDP | O1-C1-C2-C3 |
| 2 | V | 700 | FDP | O1-C1-C2-C3 |

There are no ring outliers.

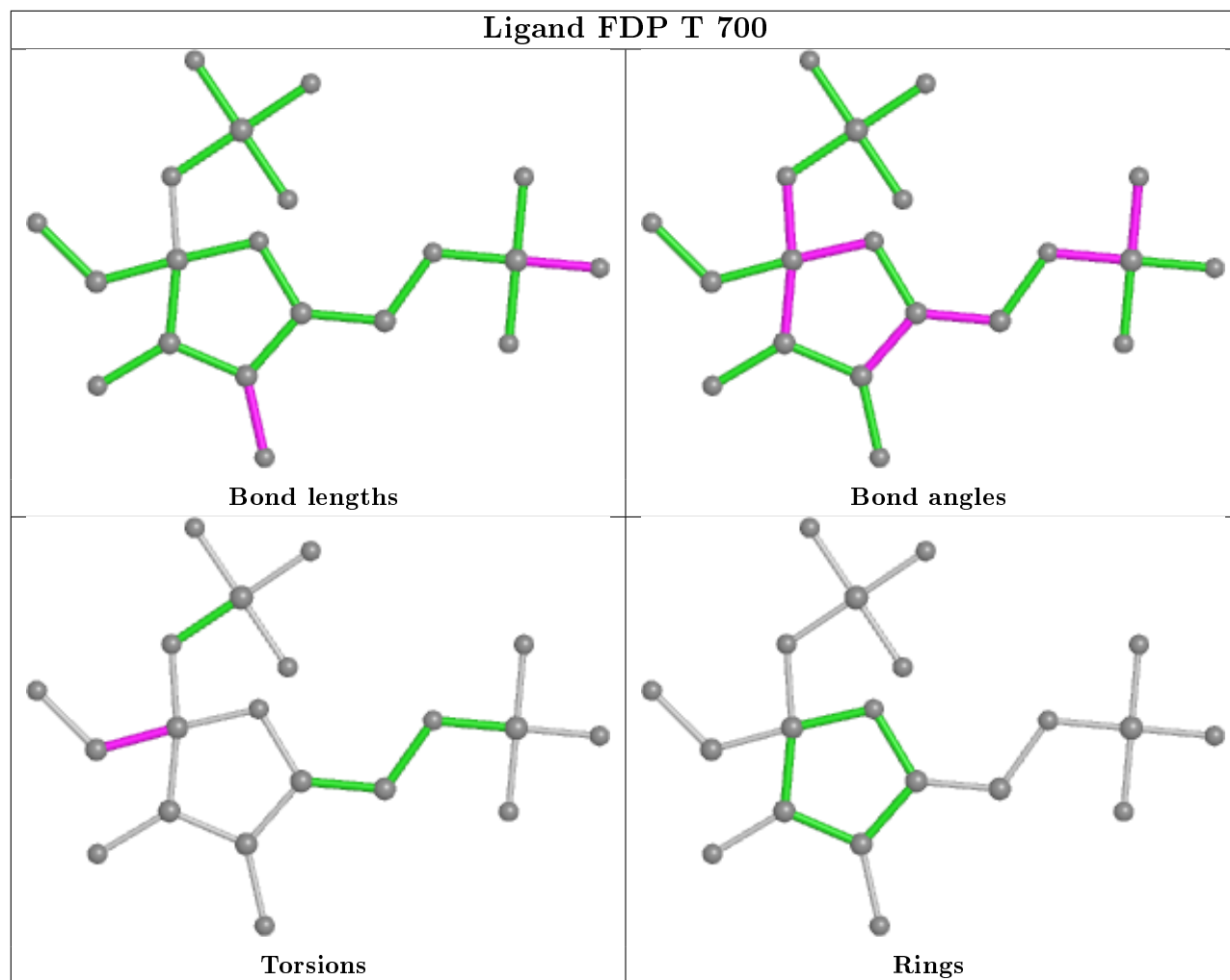
24 monomers are involved in 106 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | Q | 700 | FDP | 4 | 0 |
| 2 | T | 700 | FDP | 5 | 0 |
| 2 | H | 700 | FDP | 5 | 0 |
| 2 | N | 700 | FDP | 4 | 0 |
| 2 | S | 700 | FDP | 4 | 0 |
| 2 | W | 700 | FDP | 5 | 0 |
| 2 | U | 700 | FDP | 4 | 0 |
| 2 | K | 700 | FDP | 5 | 0 |
| 2 | M | 700 | FDP | 4 | 0 |
| 2 | E | 700 | FDP | 4 | 0 |
| 2 | J | 700 | FDP | 4 | 0 |
| 2 | L | 700 | FDP | 5 | 0 |
| 2 | B | 700 | FDP | 4 | 0 |
| 2 | F | 700 | FDP | 4 | 0 |
| 2 | I | 700 | FDP | 4 | 0 |
| 2 | O | 700 | FDP | 5 | 0 |
| 2 | X | 700 | FDP | 5 | 0 |
| 2 | A | 700 | FDP | 4 | 0 |
| 2 | P | 700 | FDP | 5 | 0 |
| 2 | D | 700 | FDP | 4 | 0 |
| 2 | C | 700 | FDP | 4 | 0 |
| 2 | R | 700 | FDP | 5 | 0 |
| 2 | G | 700 | FDP | 4 | 0 |
| 2 | V | 700 | FDP | 5 | 0 |

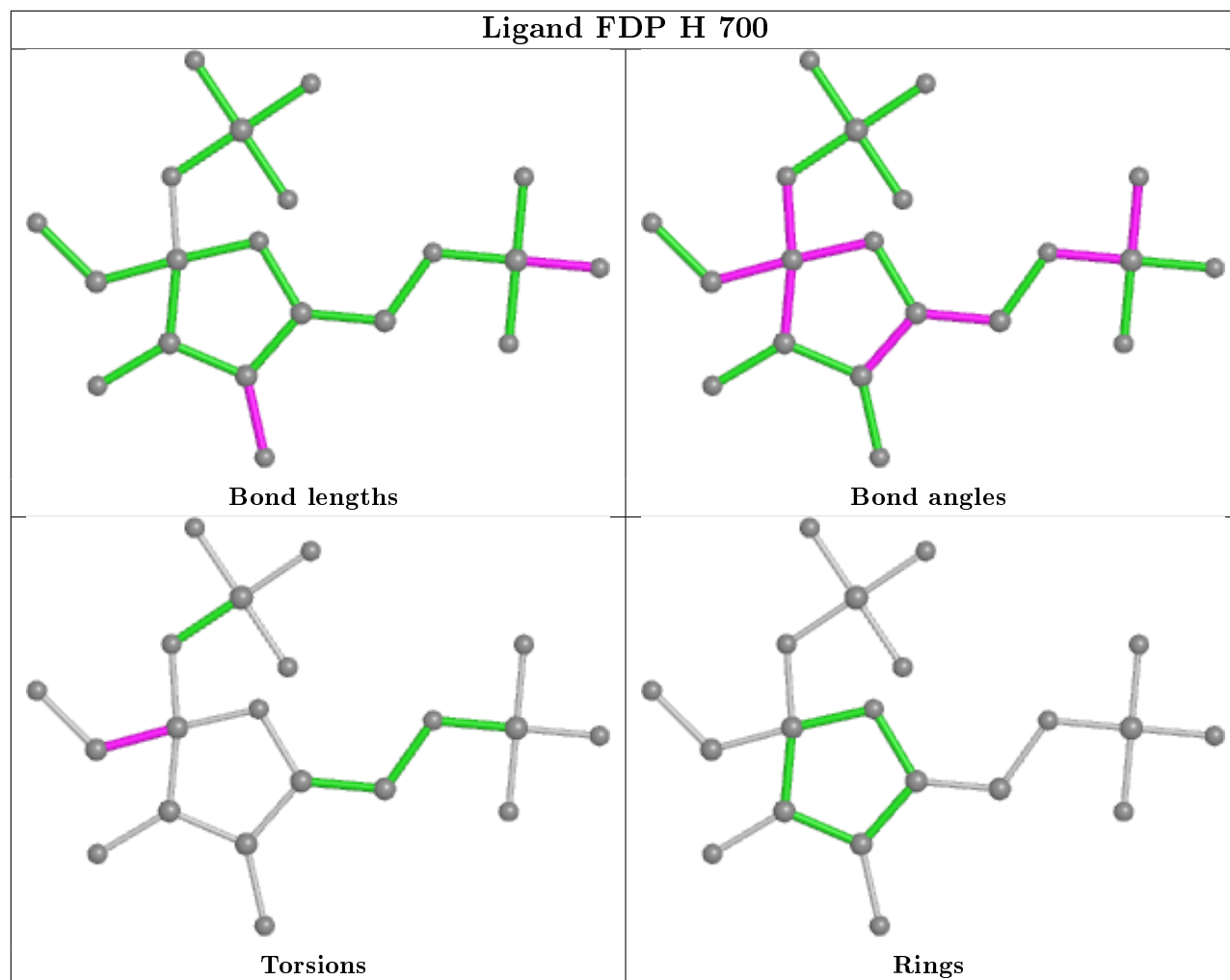
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



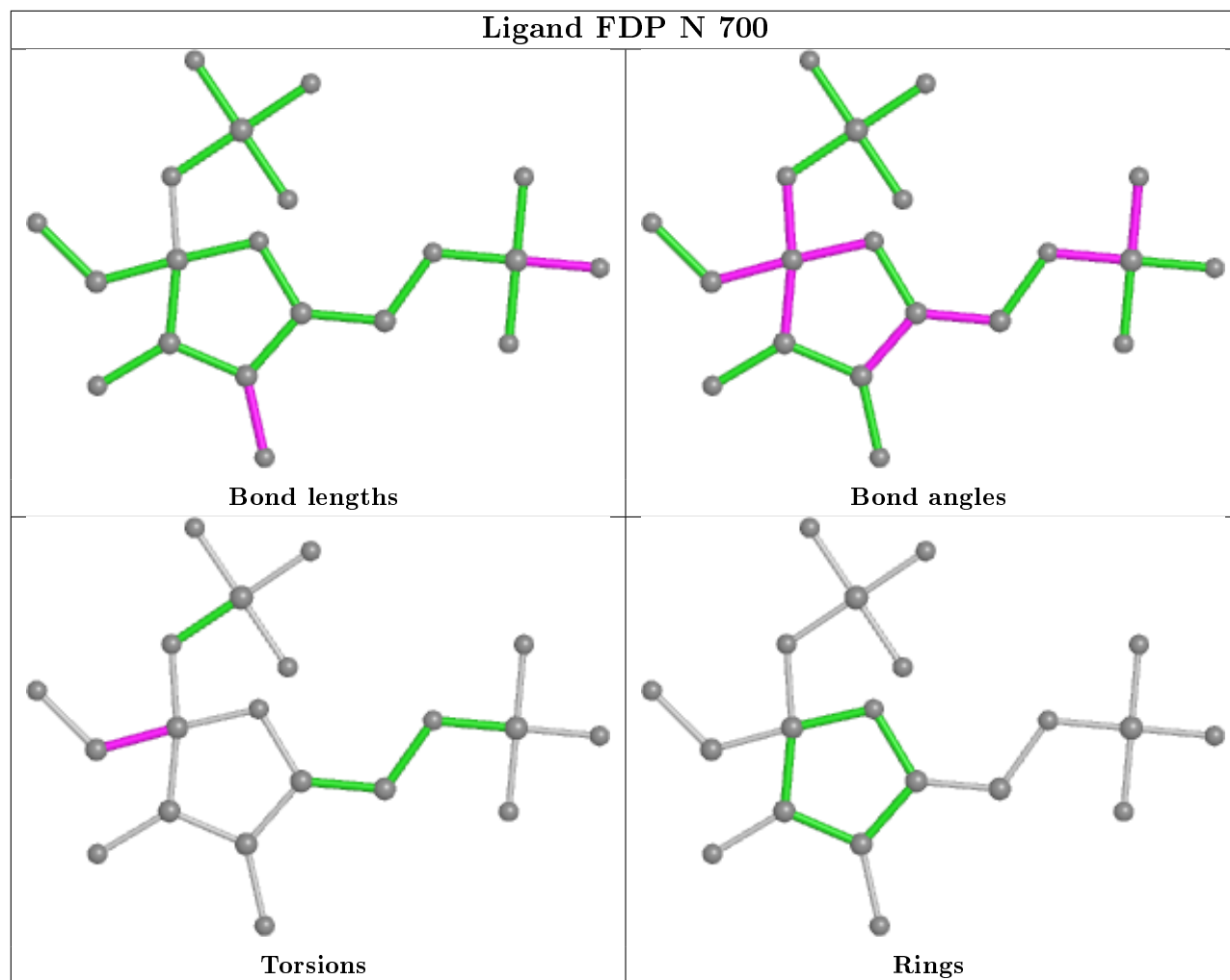
Ligand FDP T 700

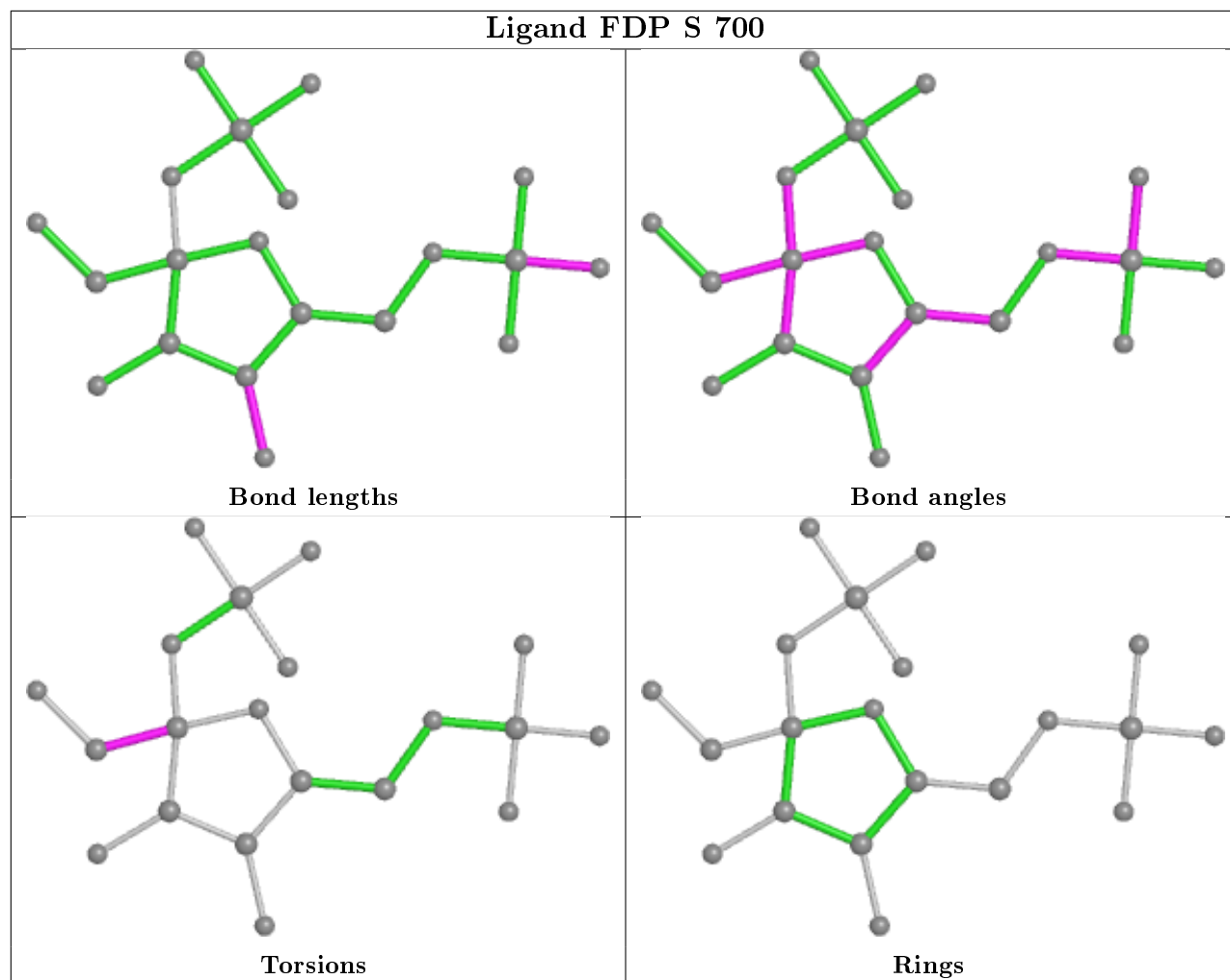


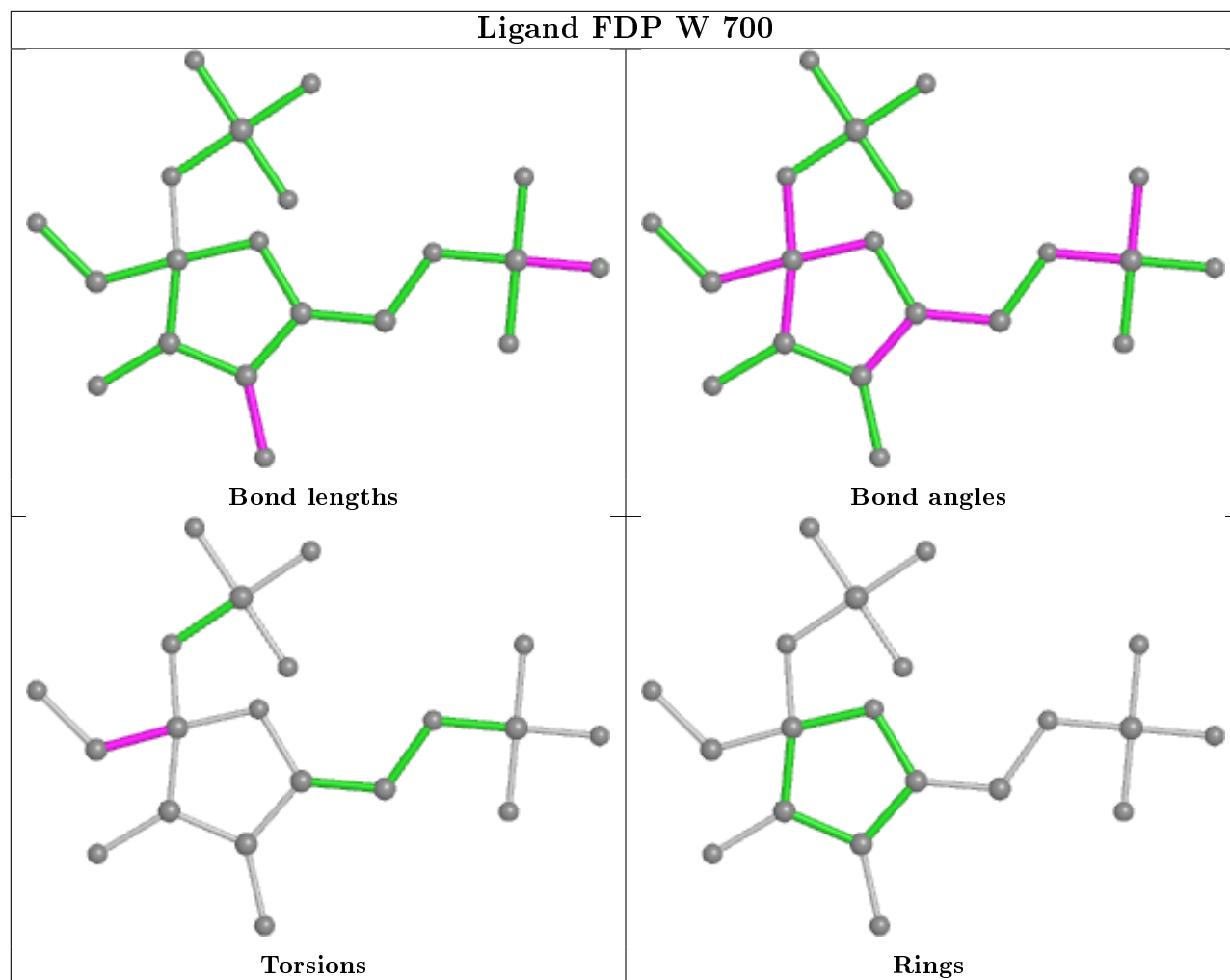
Ligand FDP H 700



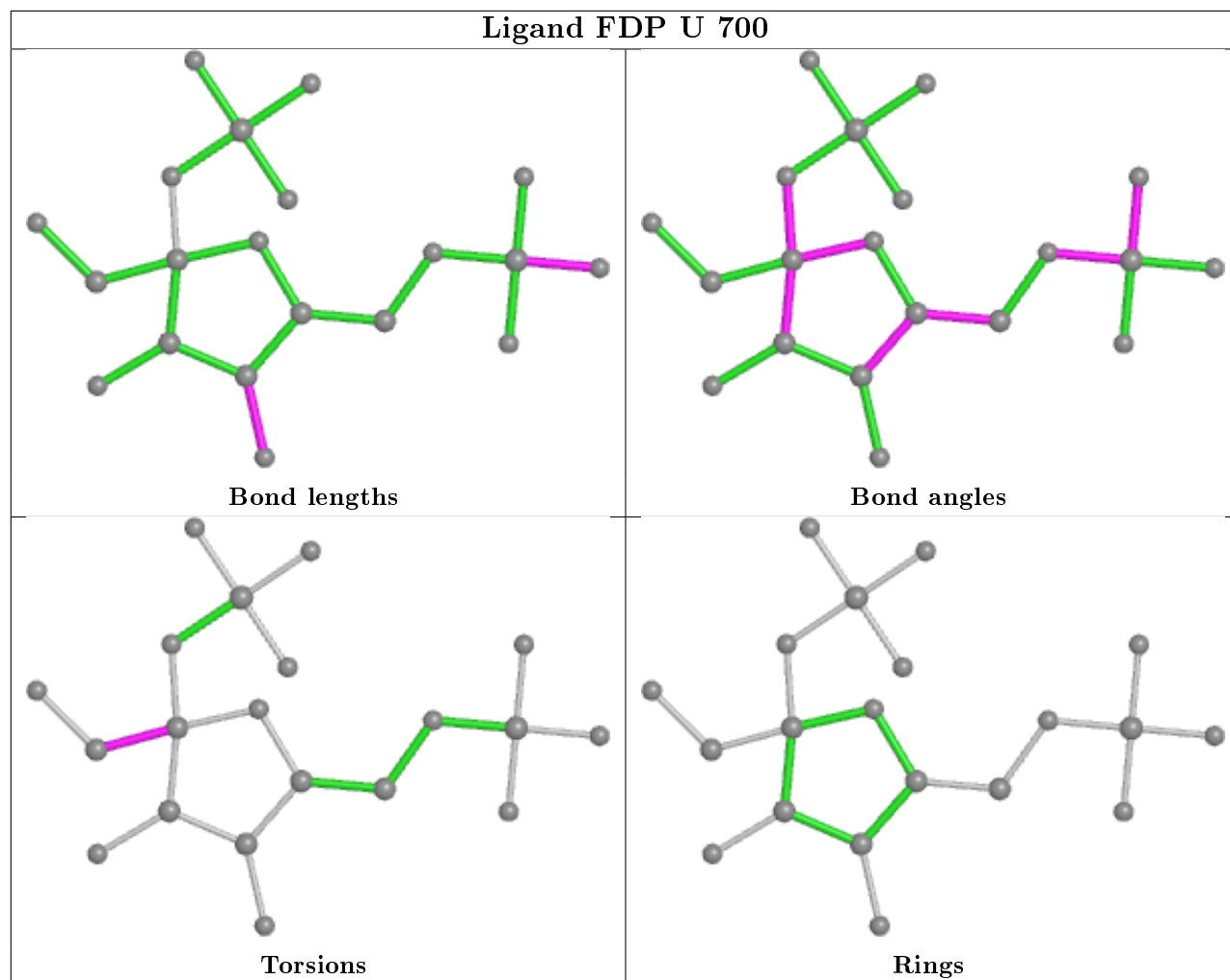
Ligand FDP N 700

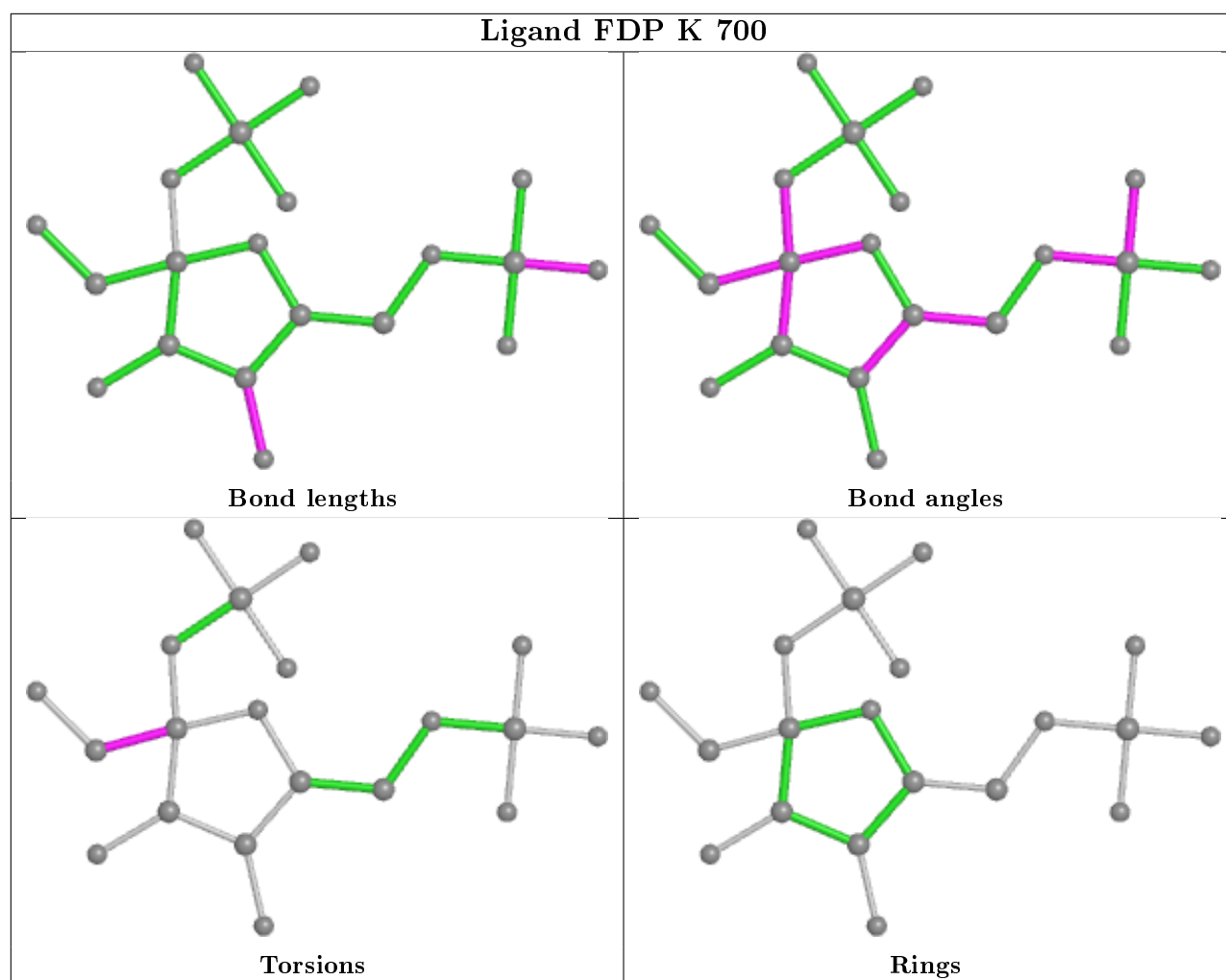


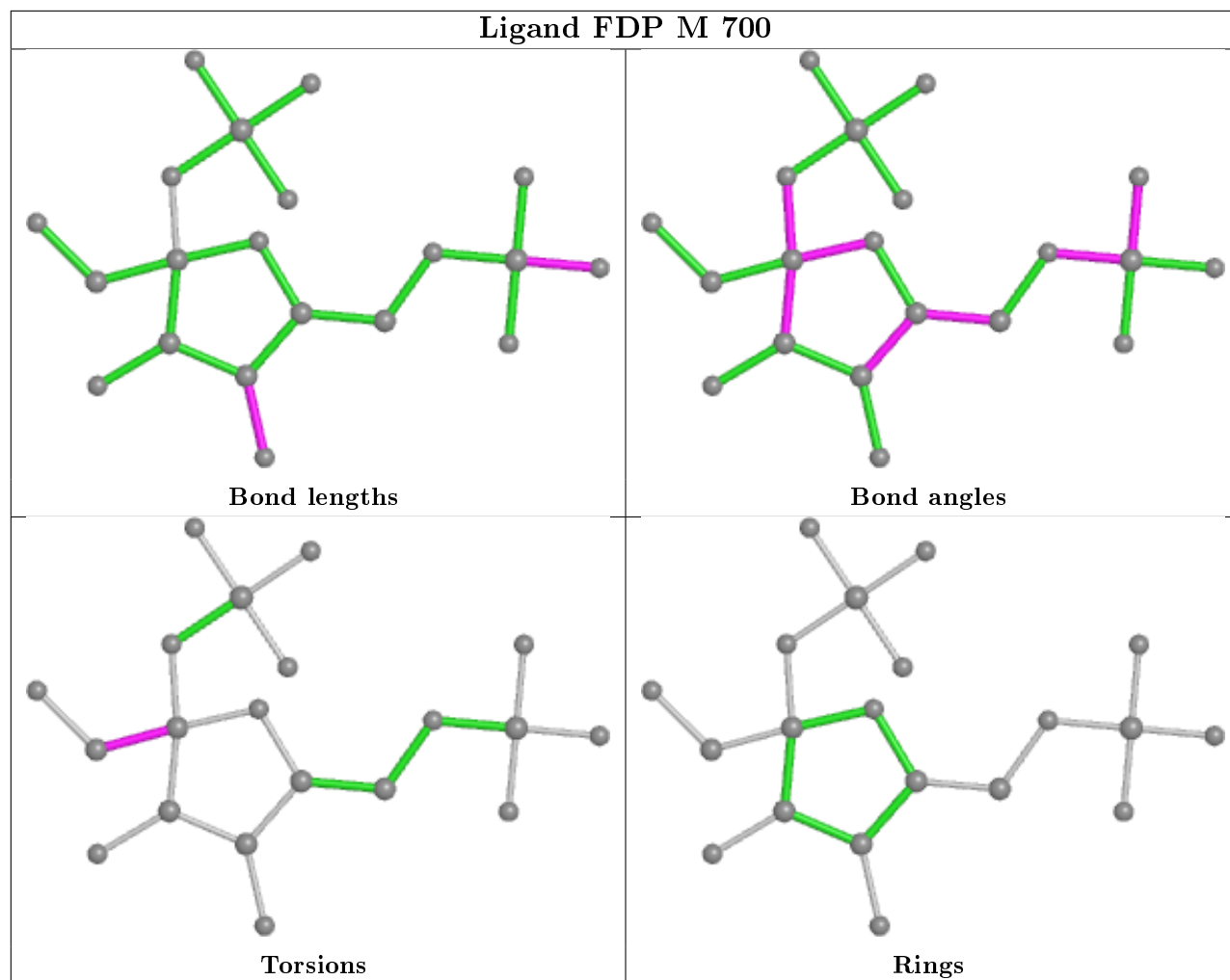




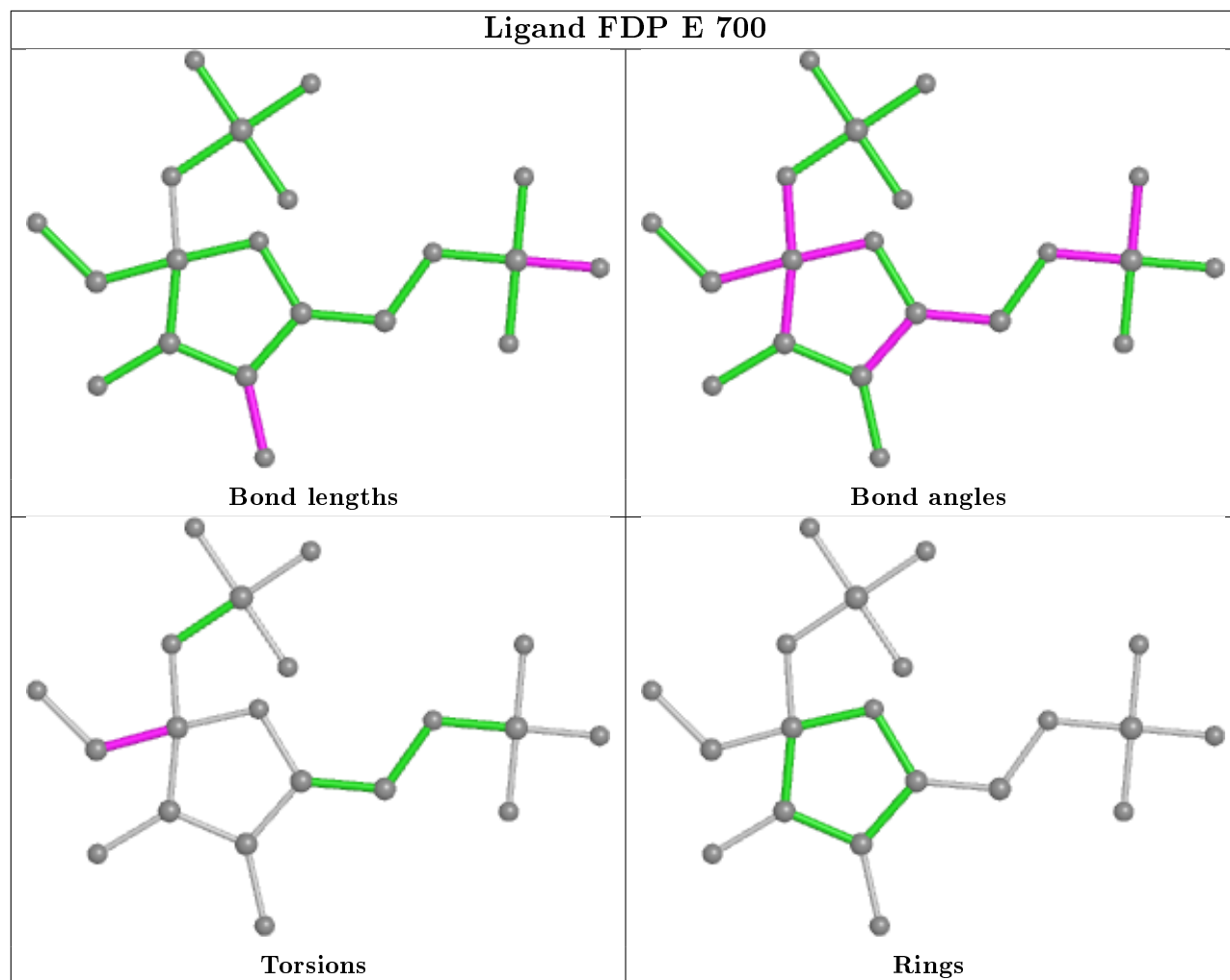
Ligand FDP U 700



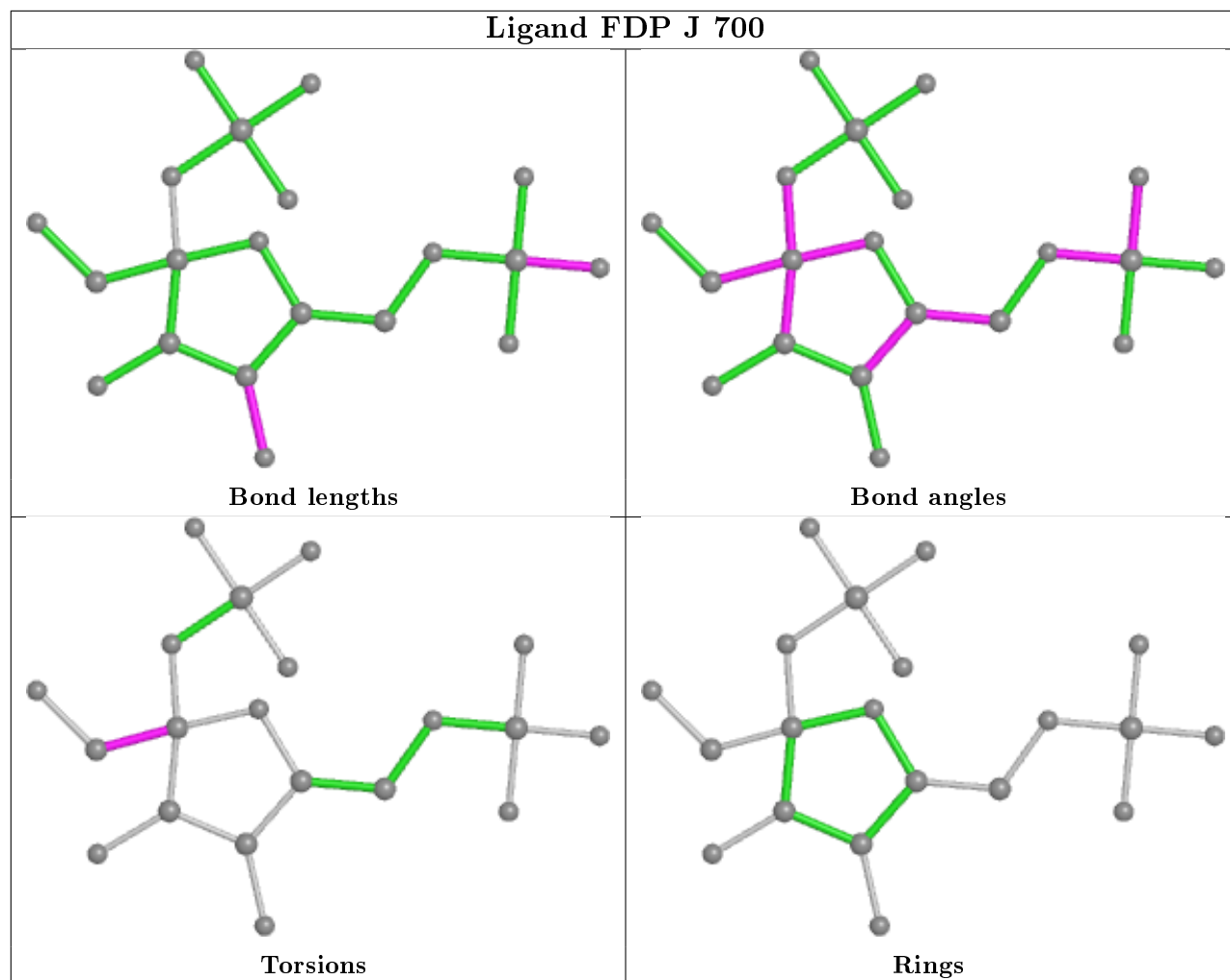




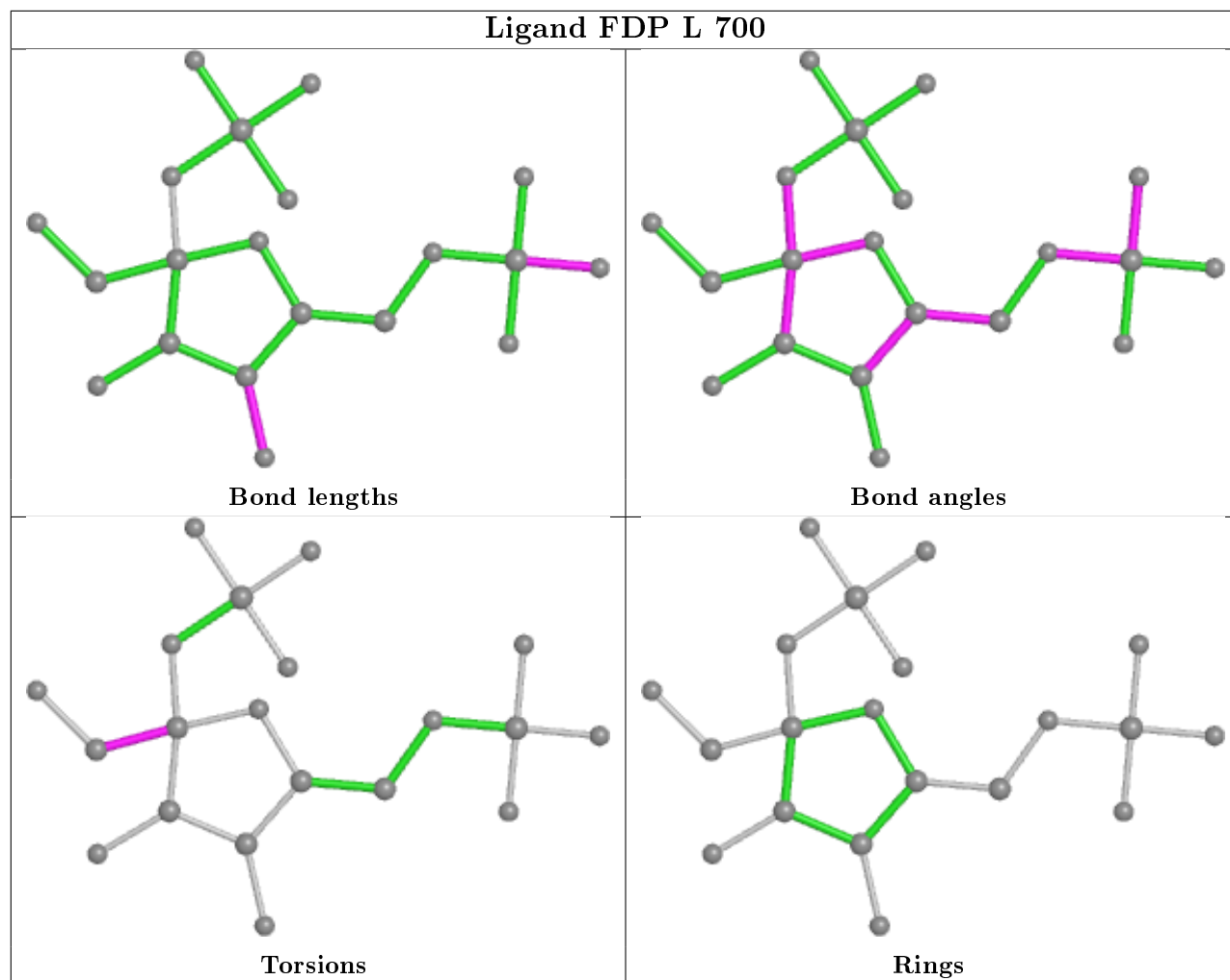
Ligand FDP E 700



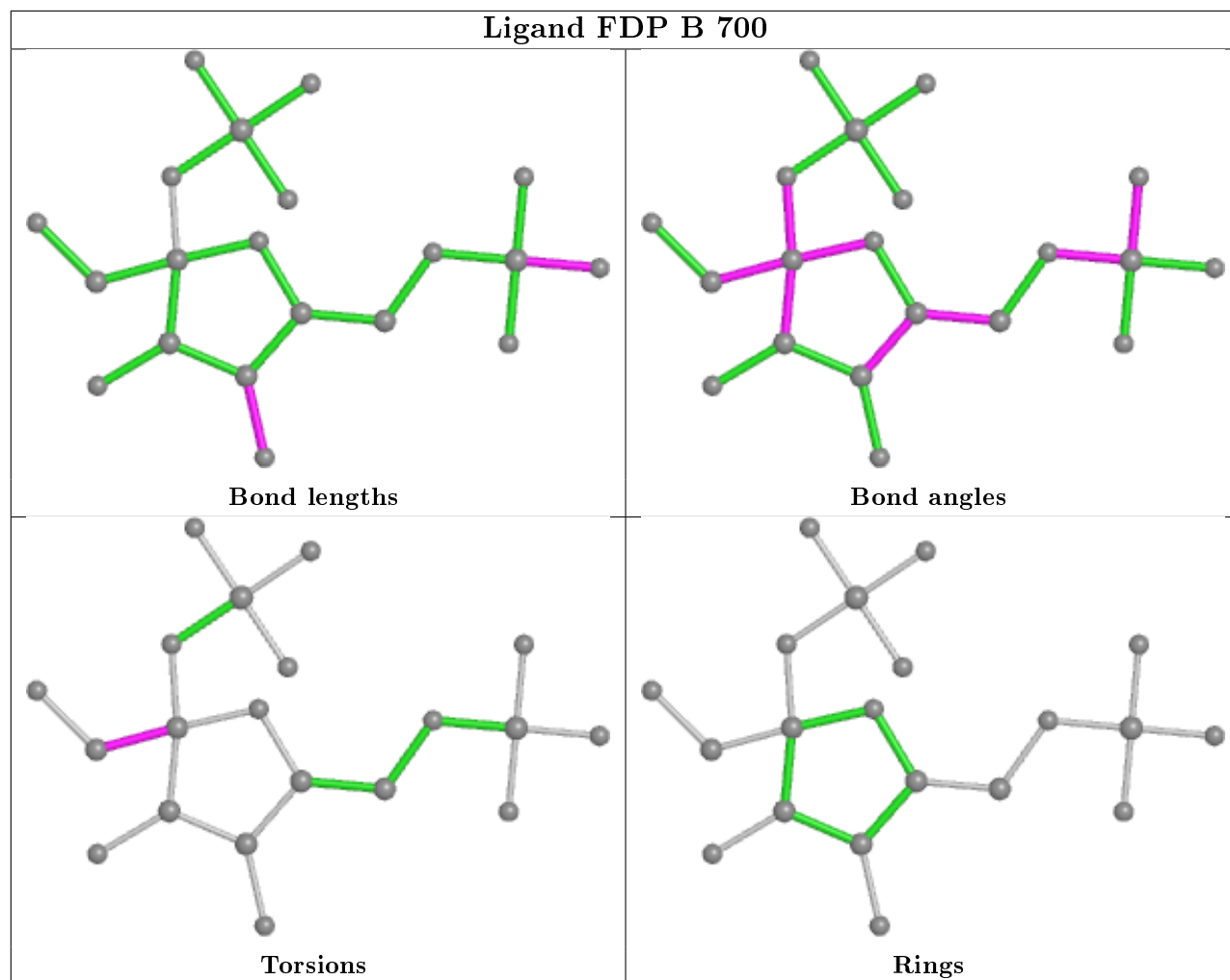
Ligand FDP J 700



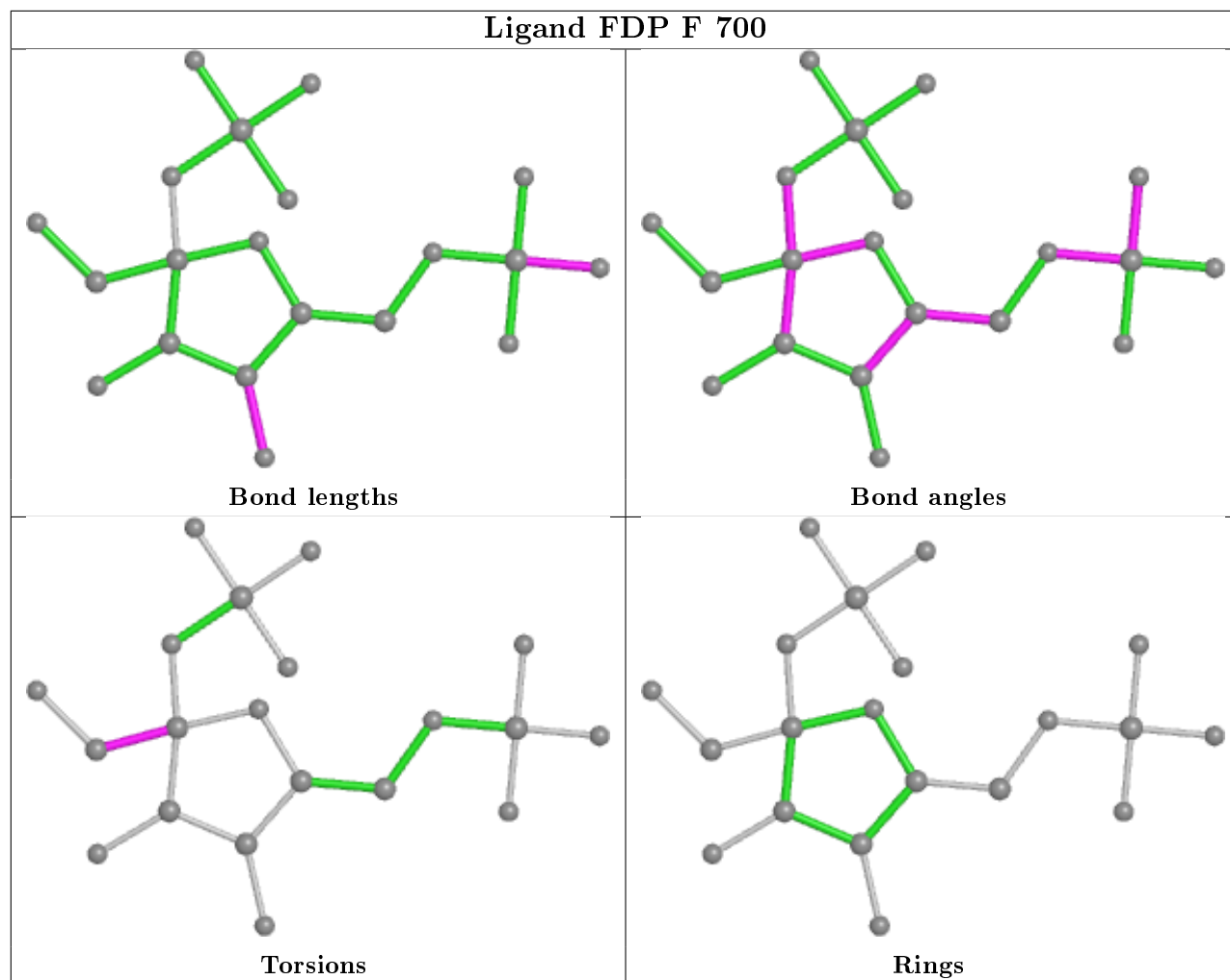
Ligand FDP L 700



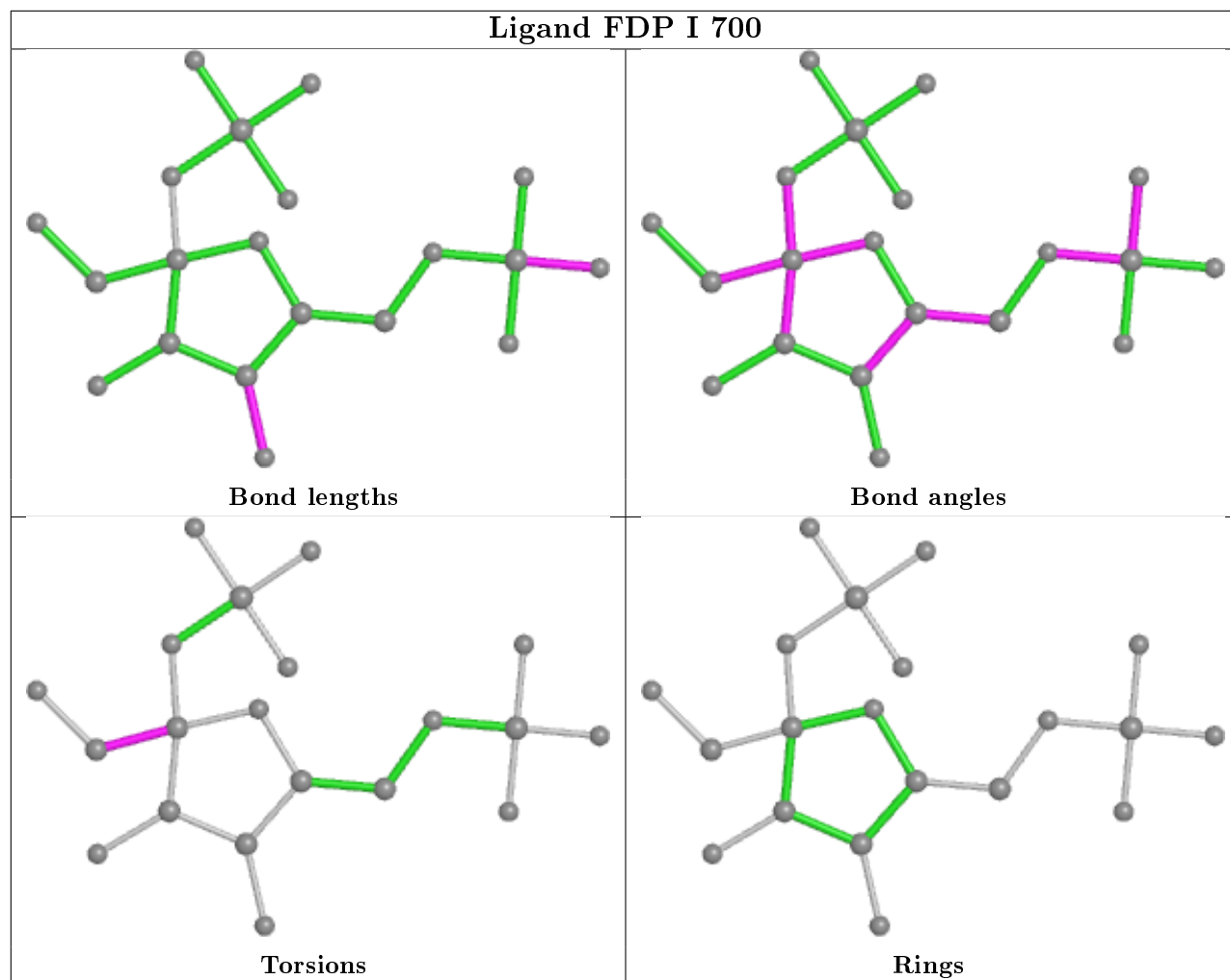
Ligand FDP B 700



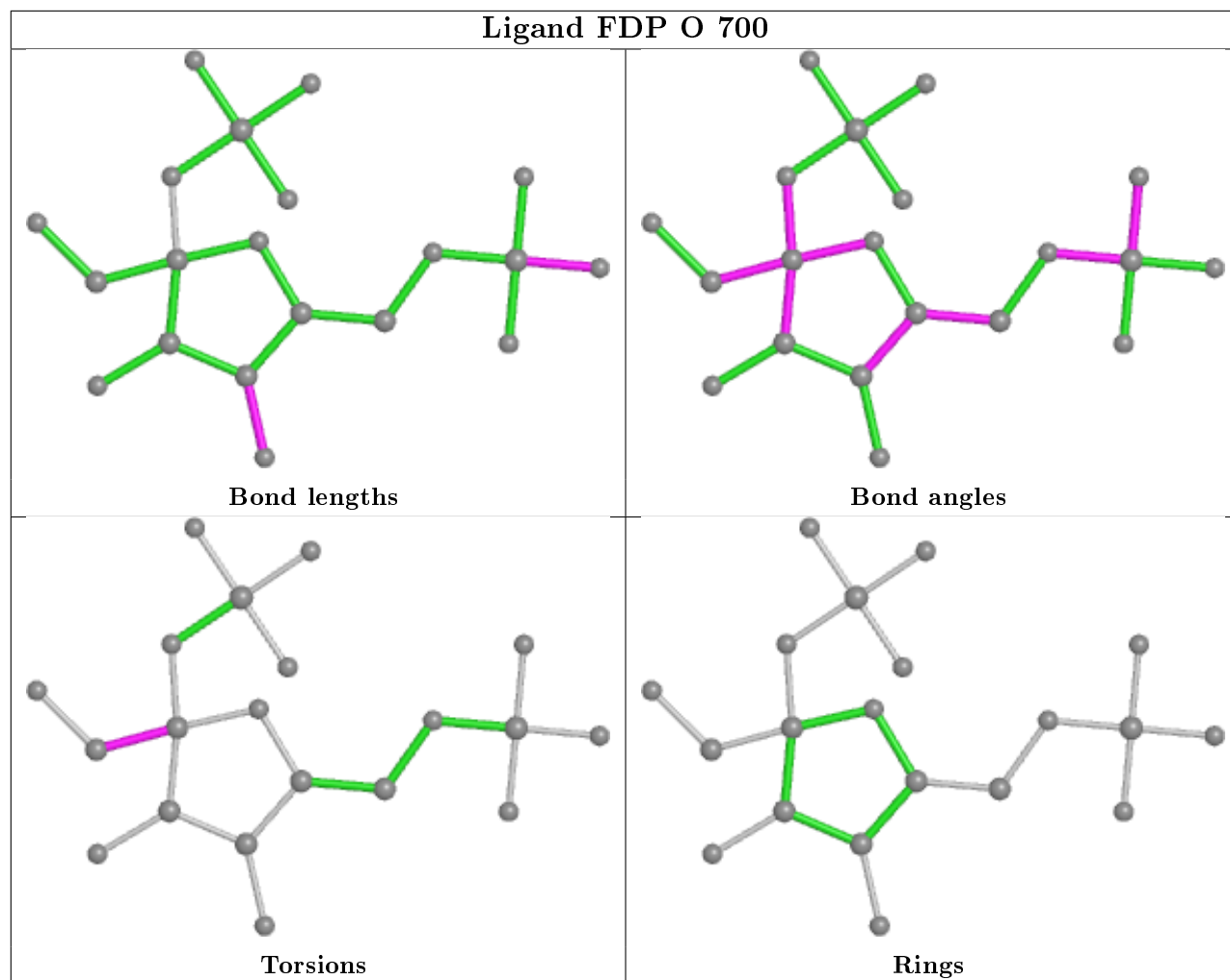
Ligand FDP F 700



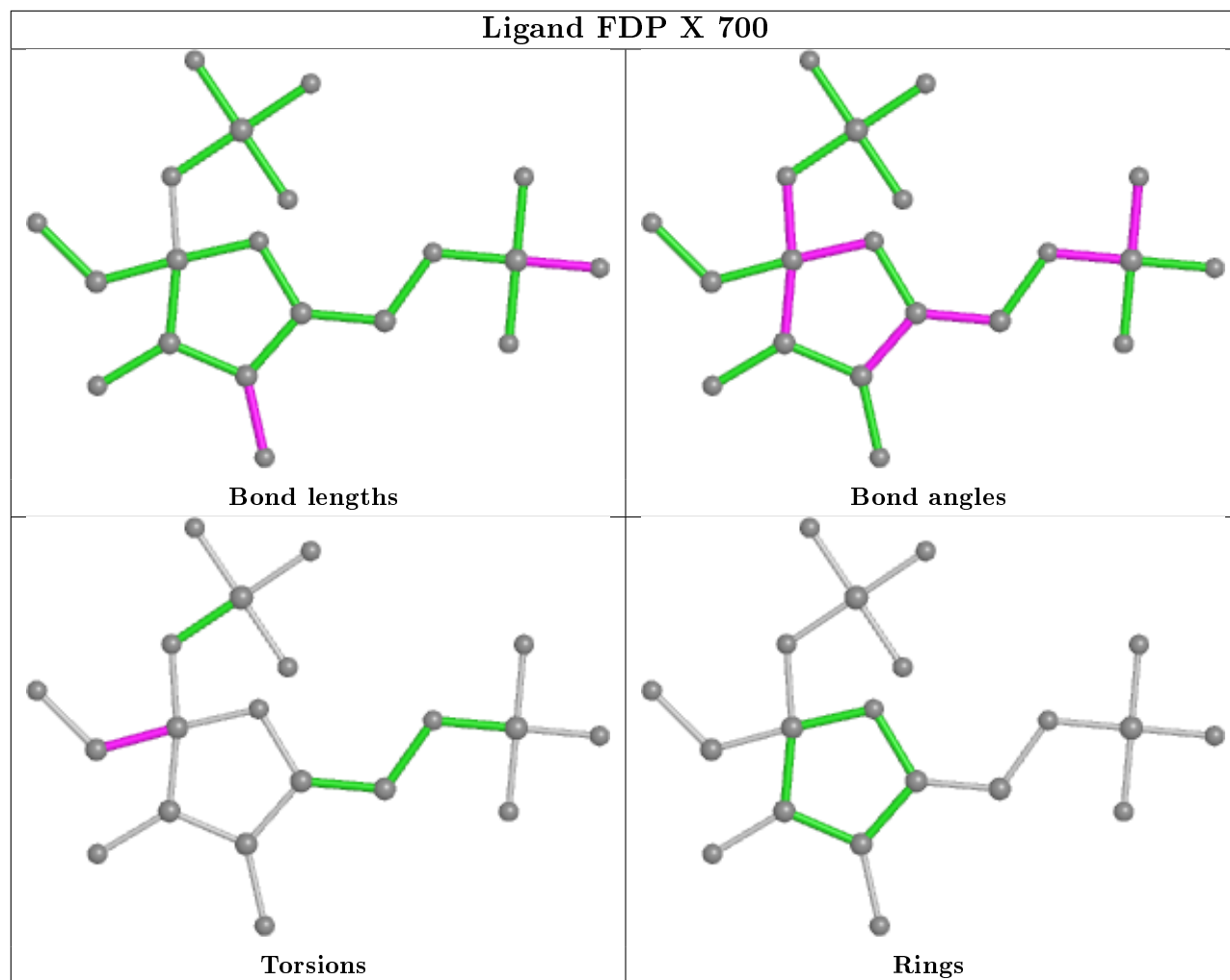
Ligand FDP I 700



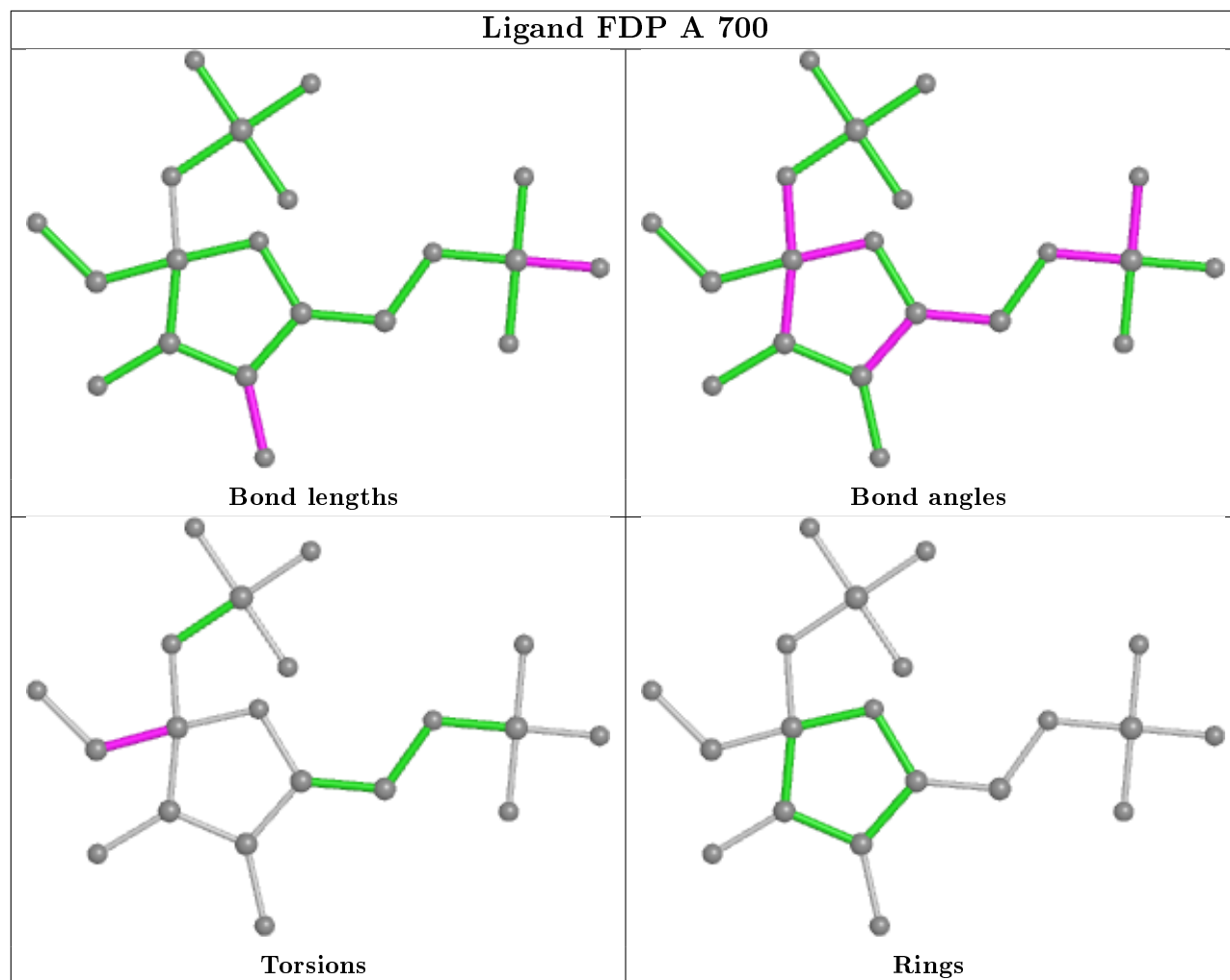
Ligand FDP O 700



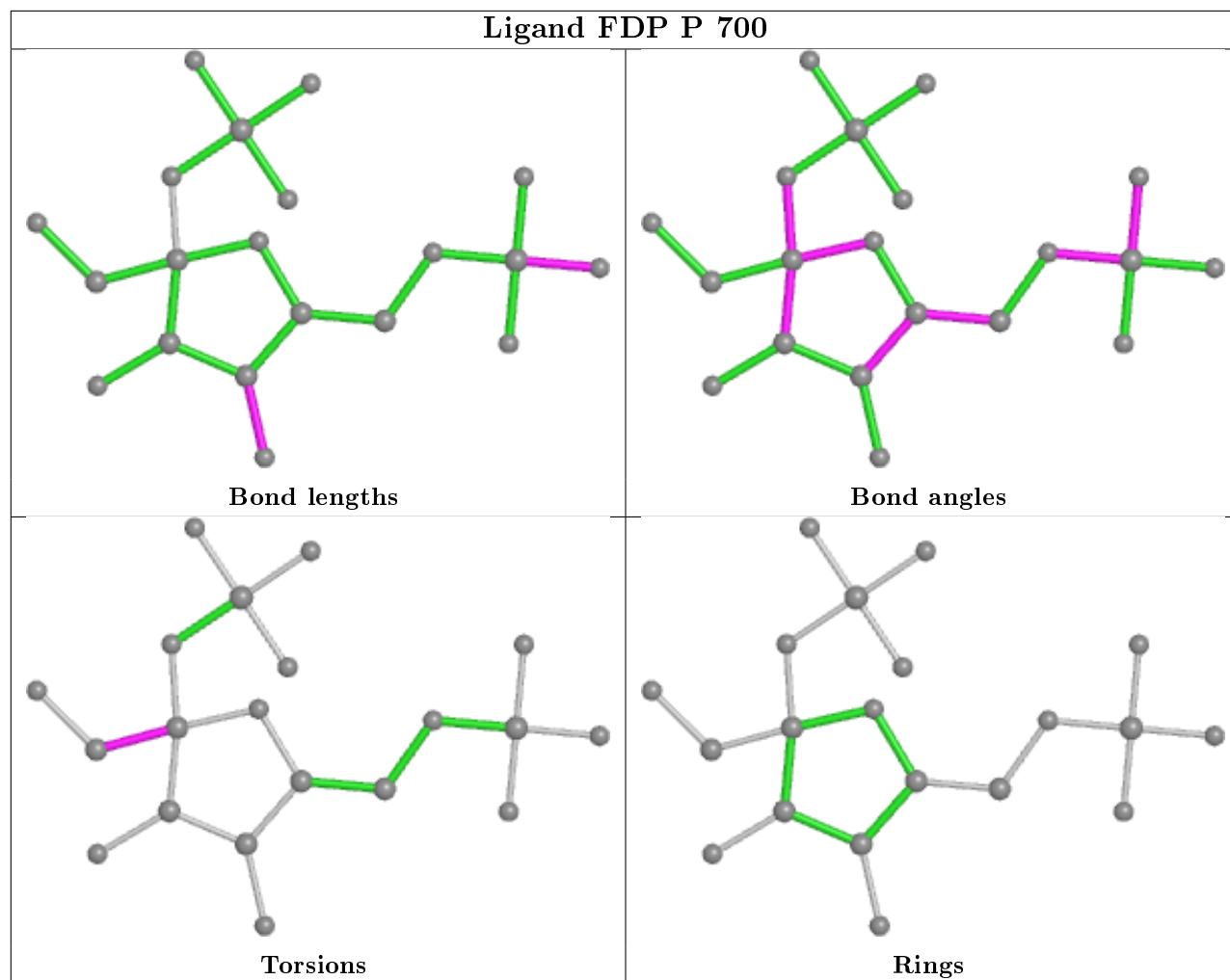
Ligand FDP X 700



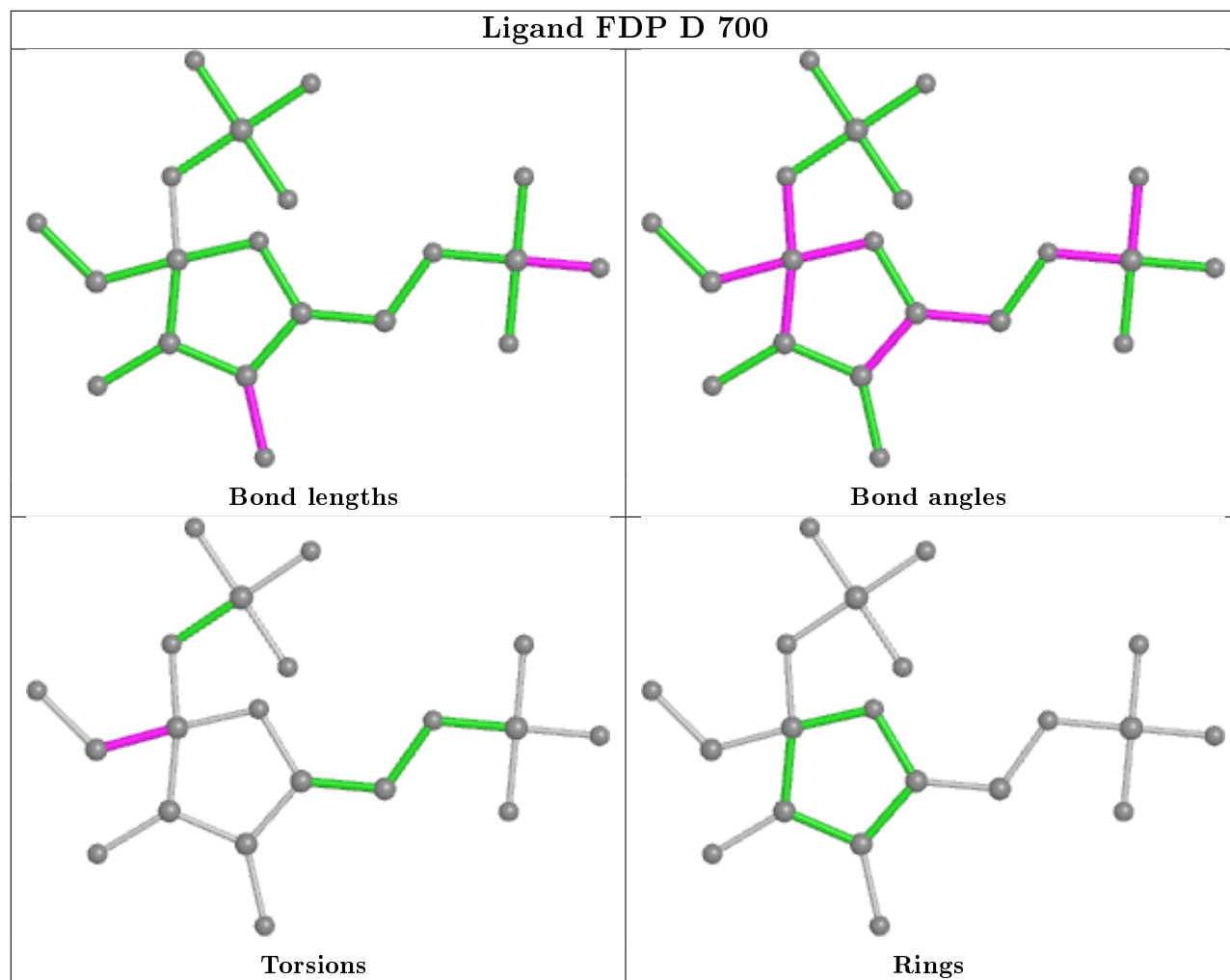
Ligand FDP A 700



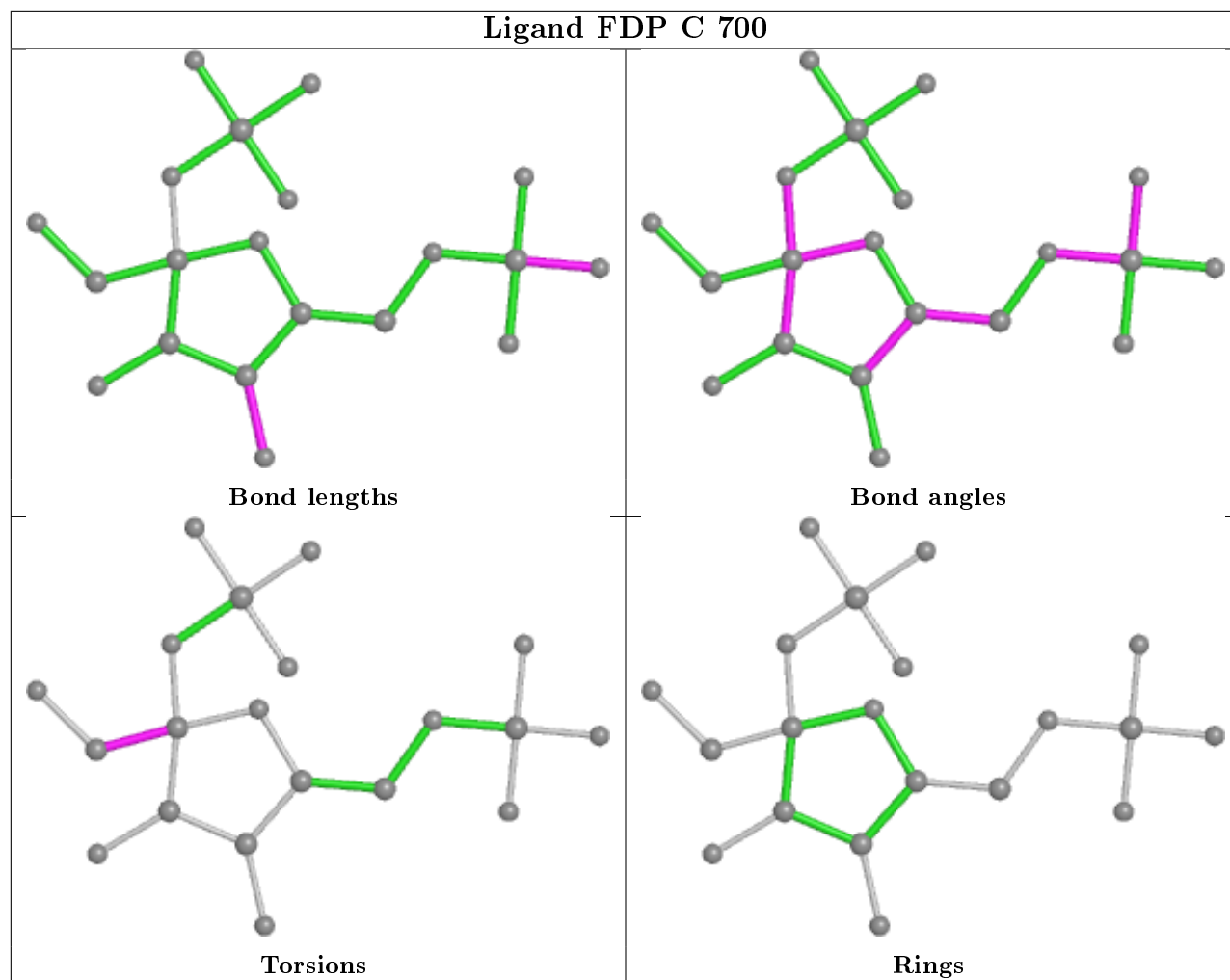
Ligand FDP P 700



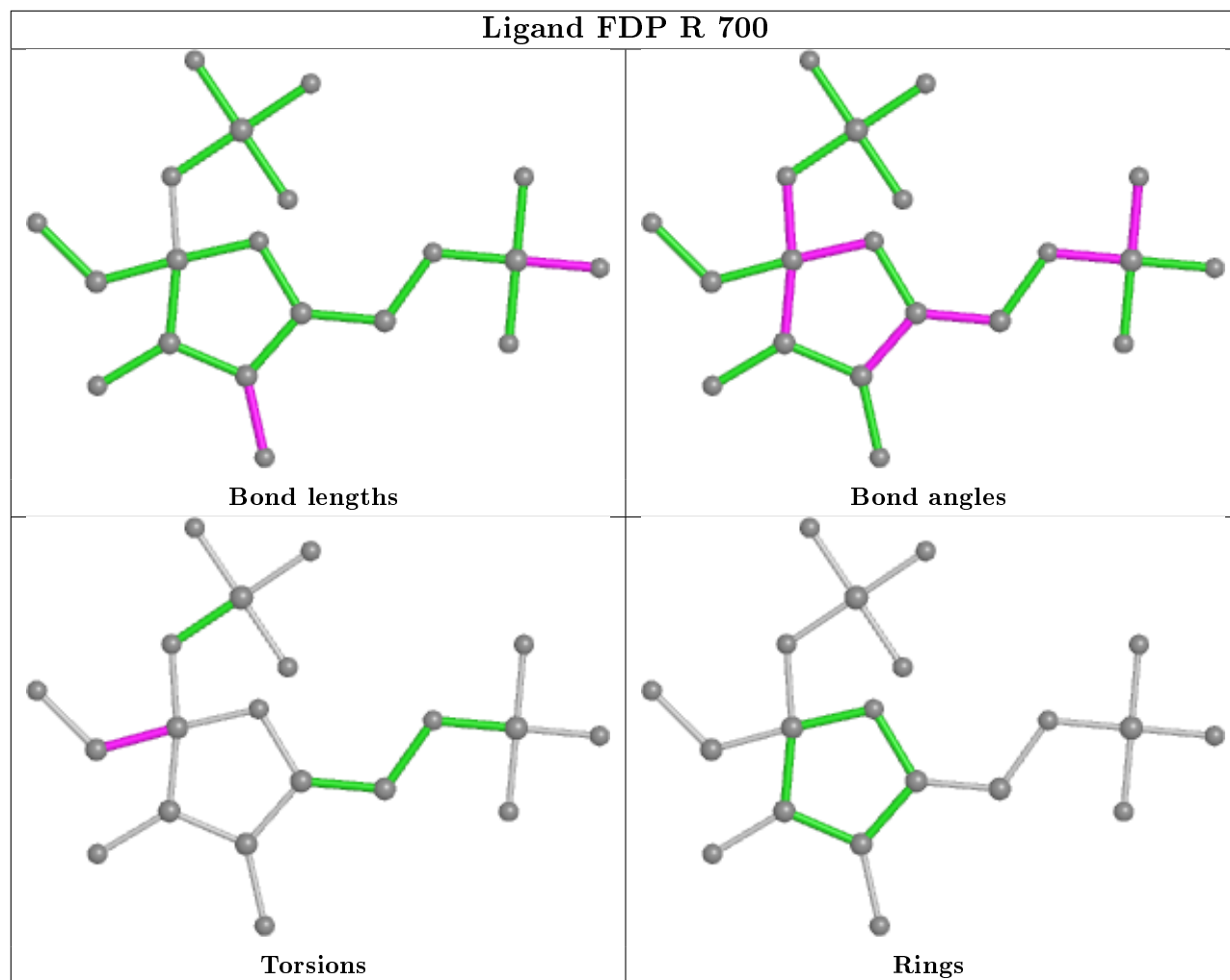
Ligand FDP D 700

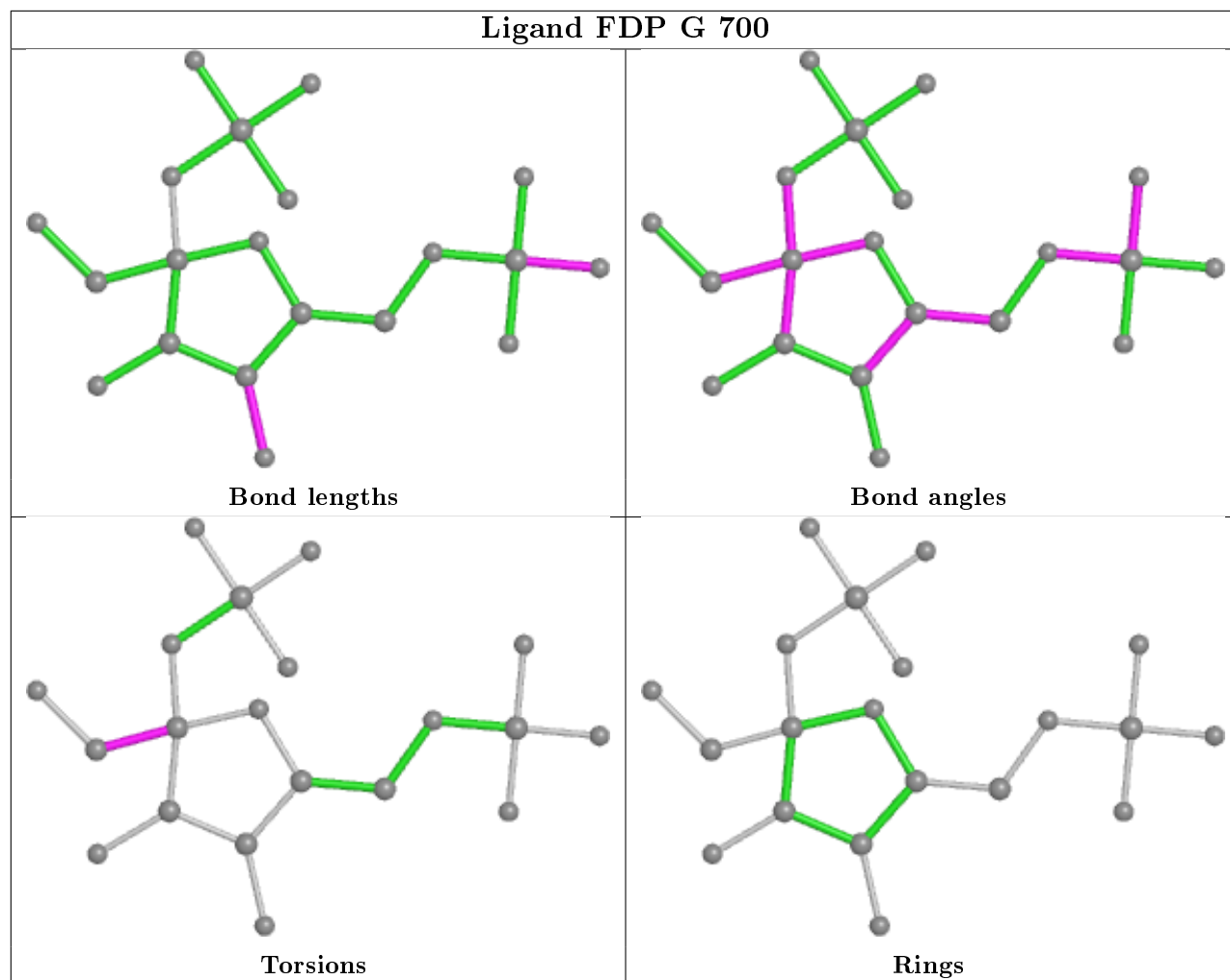


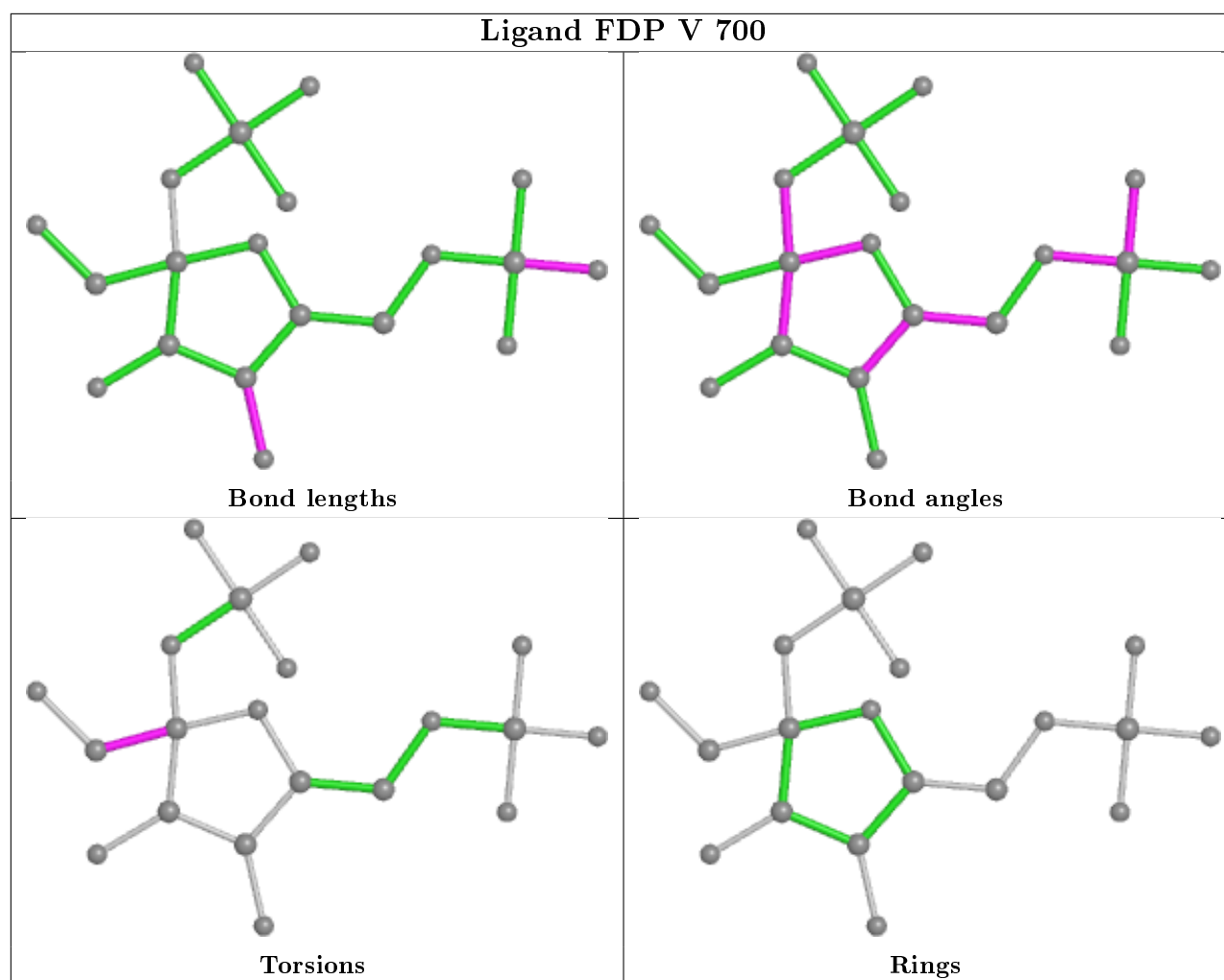
Ligand FDP C 700



Ligand FDP R 700







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1 | A | 498/499 (99%) | 0.52 | 28 (5%) 24 21 | 13, 23, 36, 46 | 0 |
| 1 | B | 498/499 (99%) | 0.35 | 16 (3%) 47 38 | 13, 23, 36, 46 | 0 |
| 1 | C | 498/499 (99%) | 0.38 | 11 (2%) 62 52 | 13, 23, 36, 46 | 0 |
| 1 | D | 498/499 (99%) | 0.42 | 19 (3%) 40 33 | 13, 23, 36, 46 | 0 |
| 1 | E | 498/499 (99%) | 0.39 | 14 (2%) 53 43 | 13, 23, 36, 46 | 0 |
| 1 | F | 498/499 (99%) | 0.40 | 14 (2%) 53 43 | 13, 23, 36, 46 | 0 |
| 1 | G | 498/499 (99%) | 0.37 | 14 (2%) 53 43 | 13, 23, 36, 46 | 0 |
| 1 | H | 498/499 (99%) | 0.34 | 15 (3%) 50 40 | 13, 23, 36, 46 | 0 |
| 1 | I | 498/499 (99%) | 0.36 | 12 (2%) 59 49 | 13, 23, 36, 46 | 0 |
| 1 | J | 498/499 (99%) | 0.42 | 19 (3%) 40 33 | 13, 23, 36, 46 | 0 |
| 1 | K | 498/499 (99%) | 0.38 | 17 (3%) 45 37 | 13, 23, 36, 46 | 0 |
| 1 | L | 498/499 (99%) | 0.41 | 11 (2%) 62 52 | 13, 23, 36, 46 | 0 |
| 1 | M | 498/499 (99%) | 0.32 | 5 (1%) 82 74 | 13, 23, 36, 46 | 0 |
| 1 | N | 498/499 (99%) | 0.40 | 14 (2%) 53 43 | 13, 23, 36, 46 | 0 |
| 1 | O | 498/499 (99%) | 0.47 | 30 (6%) 21 18 | 13, 23, 36, 46 | 0 |
| 1 | P | 498/499 (99%) | 0.37 | 16 (3%) 47 38 | 13, 23, 36, 46 | 0 |
| 1 | Q | 498/499 (99%) | 0.34 | 7 (1%) 75 65 | 13, 23, 36, 46 | 0 |
| 1 | R | 498/499 (99%) | 0.38 | 14 (2%) 53 43 | 13, 23, 36, 46 | 0 |
| 1 | S | 498/499 (99%) | 0.33 | 7 (1%) 75 65 | 13, 23, 36, 46 | 0 |
| 1 | T | 498/499 (99%) | 0.43 | 21 (4%) 36 30 | 13, 23, 36, 46 | 0 |
| 1 | U | 498/499 (99%) | 0.37 | 10 (2%) 65 56 | 13, 23, 36, 46 | 0 |
| 1 | V | 498/499 (99%) | 0.41 | 8 (1%) 72 62 | 13, 23, 36, 46 | 0 |
| 1 | W | 498/499 (99%) | 0.41 | 14 (2%) 53 43 | 13, 23, 36, 46 | 0 |
| 1 | X | 498/499 (99%) | 0.50 | 28 (5%) 24 21 | 13, 23, 36, 46 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|----------|----|----|-----------------------|-------|
| All | All | 11952/11976 (99%) | 0.40 | 364 (3%) | 50 | 40 | 13, 23, 36, 46 | 0 |

All (364) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 135 | VAL | 6.1 |
| 1 | O | 163 | CYS | 5.7 |
| 1 | A | 132 | SER | 5.4 |
| 1 | A | 131 | LEU | 5.2 |
| 1 | T | 116 | ALA | 5.1 |
| 1 | A | 134 | VAL | 5.0 |
| 1 | S | 49 | ARG | 4.9 |
| 1 | A | 100 | VAL | 4.8 |
| 1 | O | 162 | GLU | 4.5 |
| 1 | X | 95 | VAL | 4.3 |
| 1 | I | 124 | PHE | 4.3 |
| 1 | G | 105 | ALA | 4.2 |
| 1 | L | 141 | ILE | 4.2 |
| 1 | Q | 87 | PRO | 4.2 |
| 1 | R | 498 | GLU | 4.2 |
| 1 | U | 498 | GLU | 4.1 |
| 1 | P | 260 | VAL | 4.1 |
| 1 | O | 92 | GLY | 3.9 |
| 1 | B | 493 | ARG | 3.8 |
| 1 | H | 101 | MET | 3.8 |
| 1 | O | 91 | THR | 3.7 |
| 1 | X | 96 | GLY | 3.7 |
| 1 | I | 123 | LYS | 3.7 |
| 1 | G | 171 | ILE | 3.7 |
| 1 | J | 346 | MET | 3.7 |
| 1 | H | 498 | GLU | 3.6 |
| 1 | L | 135 | VAL | 3.5 |
| 1 | A | 332 | GLU | 3.5 |
| 1 | T | 117 | ASP | 3.4 |
| 1 | A | 109 | VAL | 3.4 |
| 1 | O | 99 | ALA | 3.4 |
| 1 | K | 172 | SER | 3.4 |
| 1 | E | 328 | MET | 3.3 |
| 1 | A | 440 | VAL | 3.3 |
| 1 | E | 172 | SER | 3.3 |
| 1 | K | 169 | HIS | 3.3 |
| 1 | G | 102 | GLU | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 188 | ALA | 3.3 |
| 1 | F | 342 | VAL | 3.3 |
| 1 | K | 171 | ILE | 3.3 |
| 1 | W | 184 | VAL | 3.3 |
| 1 | A | 439 | SER | 3.2 |
| 1 | P | 173 | ASP | 3.2 |
| 1 | S | 50 | MET | 3.2 |
| 1 | A | 38 | LYS | 3.2 |
| 1 | O | 184 | VAL | 3.2 |
| 1 | X | 120 | THR | 3.2 |
| 1 | X | 170 | THR | 3.2 |
| 1 | G | 101 | MET | 3.2 |
| 1 | T | 106 | THR | 3.2 |
| 1 | H | 93 | GLN | 3.1 |
| 1 | G | 106 | THR | 3.1 |
| 1 | A | 494 | ILE | 3.1 |
| 1 | I | 106 | THR | 3.1 |
| 1 | Q | 161 | LEU | 3.1 |
| 1 | B | 396 | MET | 3.1 |
| 1 | N | 124 | PHE | 3.1 |
| 1 | J | 106 | THR | 3.1 |
| 1 | K | 155 | HIS | 3.1 |
| 1 | D | 96 | GLY | 3.1 |
| 1 | E | 131 | LEU | 3.0 |
| 1 | Q | 494 | ILE | 3.0 |
| 1 | T | 165 | VAL | 3.0 |
| 1 | E | 100 | VAL | 3.0 |
| 1 | T | 93 | GLN | 3.0 |
| 1 | X | 171 | ILE | 3.0 |
| 1 | O | 101 | MET | 3.0 |
| 1 | K | 141 | ILE | 3.0 |
| 1 | W | 102 | GLU | 3.0 |
| 1 | T | 184 | VAL | 3.0 |
| 1 | U | 494 | ILE | 3.0 |
| 1 | W | 49 | ARG | 3.0 |
| 1 | D | 370 | GLN | 2.9 |
| 1 | D | 88 | GLU | 2.9 |
| 1 | X | 143 | ILE | 2.9 |
| 1 | O | 259 | MET | 2.9 |
| 1 | L | 140 | TYR | 2.9 |
| 1 | R | 320 | VAL | 2.9 |
| 1 | O | 154 | SER | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | L | 150 | LEU | 2.9 |
| 1 | B | 367 | LYS | 2.9 |
| 1 | D | 97 | GLY | 2.9 |
| 1 | D | 101 | MET | 2.9 |
| 1 | P | 381 | CYS | 2.9 |
| 1 | P | 258 | ILE | 2.8 |
| 1 | V | 85 | LYS | 2.8 |
| 1 | R | 106 | THR | 2.8 |
| 1 | Q | 162 | GLU | 2.8 |
| 1 | P | 57 | HIS | 2.8 |
| 1 | B | 240 | GLU | 2.8 |
| 1 | O | 129 | GLN | 2.8 |
| 1 | K | 214 | ARG | 2.8 |
| 1 | R | 99 | ALA | 2.8 |
| 1 | C | 171 | ILE | 2.8 |
| 1 | G | 165 | VAL | 2.8 |
| 1 | V | 396 | MET | 2.8 |
| 1 | G | 27 | ILE | 2.7 |
| 1 | M | 346 | MET | 2.7 |
| 1 | J | 207 | MET | 2.7 |
| 1 | T | 232 | ASP | 2.7 |
| 1 | A | 184 | VAL | 2.7 |
| 1 | C | 188 | ALA | 2.7 |
| 1 | O | 153 | GLN | 2.7 |
| 1 | H | 92 | GLY | 2.7 |
| 1 | D | 259 | MET | 2.7 |
| 1 | G | 197 | LEU | 2.7 |
| 1 | P | 439 | SER | 2.7 |
| 1 | F | 96 | GLY | 2.7 |
| 1 | U | 93 | GLN | 2.7 |
| 1 | H | 166 | THR | 2.7 |
| 1 | X | 316 | VAL | 2.7 |
| 1 | P | 261 | ALA | 2.7 |
| 1 | H | 124 | PHE | 2.7 |
| 1 | C | 390 | GLU | 2.7 |
| 1 | B | 327 | VAL | 2.7 |
| 1 | G | 100 | VAL | 2.7 |
| 1 | H | 165 | VAL | 2.7 |
| 1 | K | 161 | LEU | 2.7 |
| 1 | A | 27 | ILE | 2.7 |
| 1 | B | 478 | VAL | 2.7 |
| 1 | J | 397 | VAL | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 327 | VAL | 2.6 |
| 1 | C | 101 | MET | 2.6 |
| 1 | F | 124 | PHE | 2.6 |
| 1 | O | 398 | VAL | 2.6 |
| 1 | B | 449 | HIS | 2.6 |
| 1 | K | 170 | THR | 2.6 |
| 1 | B | 328 | MET | 2.6 |
| 1 | C | 150 | LEU | 2.6 |
| 1 | C | 396 | MET | 2.6 |
| 1 | X | 135 | VAL | 2.6 |
| 1 | K | 143 | ILE | 2.6 |
| 1 | W | 124 | PHE | 2.6 |
| 1 | A | 407 | ARG | 2.6 |
| 1 | N | 239 | ILE | 2.6 |
| 1 | I | 259 | MET | 2.6 |
| 1 | T | 101 | MET | 2.6 |
| 1 | X | 306 | PRO | 2.6 |
| 1 | O | 126 | ILE | 2.6 |
| 1 | J | 479 | ILE | 2.6 |
| 1 | G | 376 | ALA | 2.6 |
| 1 | J | 476 | CYS | 2.5 |
| 1 | H | 161 | LEU | 2.5 |
| 1 | J | 150 | LEU | 2.5 |
| 1 | O | 182 | CYS | 2.5 |
| 1 | O | 298 | MET | 2.5 |
| 1 | K | 156 | GLU | 2.5 |
| 1 | T | 102 | GLU | 2.5 |
| 1 | W | 412 | TYR | 2.5 |
| 1 | E | 335 | LYS | 2.5 |
| 1 | I | 91 | THR | 2.5 |
| 1 | F | 346 | MET | 2.5 |
| 1 | I | 101 | MET | 2.5 |
| 1 | K | 45 | MET | 2.5 |
| 1 | N | 49 | ARG | 2.5 |
| 1 | O | 479 | ILE | 2.5 |
| 1 | F | 353 | ALA | 2.5 |
| 1 | B | 409 | VAL | 2.5 |
| 1 | I | 150 | LEU | 2.5 |
| 1 | D | 209 | PHE | 2.5 |
| 1 | I | 377 | ASP | 2.5 |
| 1 | F | 476 | CYS | 2.5 |
| 1 | A | 46 | SER | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | J | 381 | CYS | 2.5 |
| 1 | E | 170 | THR | 2.5 |
| 1 | I | 299 | LEU | 2.5 |
| 1 | N | 131 | LEU | 2.5 |
| 1 | S | 48 | ALA | 2.5 |
| 1 | J | 163 | CYS | 2.5 |
| 1 | X | 209 | PHE | 2.5 |
| 1 | A | 412 | TYR | 2.4 |
| 1 | X | 486 | LYS | 2.4 |
| 1 | D | 239 | ILE | 2.4 |
| 1 | P | 434 | THR | 2.4 |
| 1 | L | 352 | GLU | 2.4 |
| 1 | D | 188 | ALA | 2.4 |
| 1 | E | 180 | PRO | 2.4 |
| 1 | Q | 486 | LYS | 2.4 |
| 1 | W | 493 | ARG | 2.4 |
| 1 | D | 412 | TYR | 2.4 |
| 1 | W | 99 | ALA | 2.4 |
| 1 | E | 184 | VAL | 2.4 |
| 1 | B | 294 | CYS | 2.4 |
| 1 | T | 50 | MET | 2.4 |
| 1 | C | 287 | VAL | 2.4 |
| 1 | J | 11 | ILE | 2.4 |
| 1 | O | 128 | TYR | 2.4 |
| 1 | F | 492 | THR | 2.4 |
| 1 | P | 143 | ILE | 2.4 |
| 1 | T | 164 | THR | 2.4 |
| 1 | X | 488 | TYR | 2.4 |
| 1 | K | 367 | LYS | 2.4 |
| 1 | W | 123 | LYS | 2.4 |
| 1 | K | 137 | PRO | 2.4 |
| 1 | E | 135 | VAL | 2.4 |
| 1 | T | 105 | ALA | 2.4 |
| 1 | H | 430 | GLN | 2.4 |
| 1 | D | 122 | ASP | 2.4 |
| 1 | O | 433 | ILE | 2.4 |
| 1 | A | 299 | LEU | 2.4 |
| 1 | X | 214 | ARG | 2.3 |
| 1 | E | 390 | GLU | 2.3 |
| 1 | F | 49 | ARG | 2.3 |
| 1 | L | 439 | SER | 2.3 |
| 1 | W | 183 | ASP | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | V | 184 | VAL | 2.3 |
| 1 | V | 437 | VAL | 2.3 |
| 1 | W | 377 | ASP | 2.3 |
| 1 | B | 492 | THR | 2.3 |
| 1 | A | 479 | ILE | 2.3 |
| 1 | J | 446 | LYS | 2.3 |
| 1 | A | 302 | MET | 2.3 |
| 1 | N | 50 | MET | 2.3 |
| 1 | O | 189 | VAL | 2.3 |
| 1 | M | 96 | GLY | 2.3 |
| 1 | X | 198 | GLN | 2.3 |
| 1 | W | 19 | ARG | 2.3 |
| 1 | D | 261 | ALA | 2.3 |
| 1 | I | 476 | CYS | 2.3 |
| 1 | H | 126 | ILE | 2.3 |
| 1 | H | 494 | ILE | 2.3 |
| 1 | T | 376 | ALA | 2.3 |
| 1 | A | 185 | ASP | 2.3 |
| 1 | O | 87 | PRO | 2.3 |
| 1 | M | 325 | ASP | 2.3 |
| 1 | X | 183 | ASP | 2.3 |
| 1 | J | 107 | CYS | 2.3 |
| 1 | T | 316 | VAL | 2.3 |
| 1 | G | 239 | ILE | 2.3 |
| 1 | O | 345 | TYR | 2.3 |
| 1 | J | 268 | GLU | 2.3 |
| 1 | H | 476 | CYS | 2.3 |
| 1 | V | 84 | THR | 2.3 |
| 1 | X | 119 | GLY | 2.3 |
| 1 | K | 154 | SER | 2.2 |
| 1 | F | 328 | MET | 2.2 |
| 1 | T | 100 | VAL | 2.2 |
| 1 | N | 150 | LEU | 2.2 |
| 1 | L | 346 | MET | 2.2 |
| 1 | T | 492 | THR | 2.2 |
| 1 | P | 171 | ILE | 2.2 |
| 1 | A | 124 | PHE | 2.2 |
| 1 | L | 298 | MET | 2.2 |
| 1 | U | 154 | SER | 2.2 |
| 1 | V | 390 | GLU | 2.2 |
| 1 | O | 18 | TYR | 2.2 |
| 1 | X | 492 | THR | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 98 | ASP | 2.2 |
| 1 | O | 183 | ASP | 2.2 |
| 1 | H | 312 | GLU | 2.2 |
| 1 | D | 258 | ILE | 2.2 |
| 1 | J | 478 | VAL | 2.2 |
| 1 | J | 73 | GLU | 2.2 |
| 1 | A | 152 | VAL | 2.2 |
| 1 | N | 165 | VAL | 2.2 |
| 1 | X | 157 | ASP | 2.2 |
| 1 | P | 406 | ALA | 2.2 |
| 1 | X | 399 | LEU | 2.2 |
| 1 | B | 435 | GLN | 2.2 |
| 1 | N | 162 | GLU | 2.2 |
| 1 | S | 359 | GLU | 2.2 |
| 1 | R | 148 | LEU | 2.2 |
| 1 | X | 494 | ILE | 2.2 |
| 1 | R | 261 | ALA | 2.2 |
| 1 | C | 419 | VAL | 2.2 |
| 1 | F | 480 | HIS | 2.2 |
| 1 | J | 396 | MET | 2.2 |
| 1 | I | 118 | LYS | 2.2 |
| 1 | R | 346 | MET | 2.2 |
| 1 | P | 239 | ILE | 2.2 |
| 1 | M | 150 | LEU | 2.2 |
| 1 | A | 126 | ILE | 2.2 |
| 1 | F | 327 | VAL | 2.2 |
| 1 | F | 350 | CYS | 2.2 |
| 1 | A | 408 | LEU | 2.1 |
| 1 | A | 475 | TYR | 2.1 |
| 1 | U | 73 | GLU | 2.1 |
| 1 | L | 149 | ILE | 2.1 |
| 1 | T | 494 | ILE | 2.1 |
| 1 | N | 91 | THR | 2.1 |
| 1 | T | 173 | ASP | 2.1 |
| 1 | N | 82 | LEU | 2.1 |
| 1 | D | 19 | ARG | 2.1 |
| 1 | Q | 476 | CYS | 2.1 |
| 1 | B | 184 | VAL | 2.1 |
| 1 | H | 102 | GLU | 2.1 |
| 1 | W | 169 | HIS | 2.1 |
| 1 | X | 239 | ILE | 2.1 |
| 1 | R | 49 | ARG | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | J | 124 | PHE | 2.1 |
| 1 | D | 494 | ILE | 2.1 |
| 1 | K | 241 | ASN | 2.1 |
| 1 | O | 434 | THR | 2.1 |
| 1 | T | 49 | ARG | 2.1 |
| 1 | D | 414 | PRO | 2.1 |
| 1 | X | 201 | VAL | 2.1 |
| 1 | L | 294 | CYS | 2.1 |
| 1 | W | 476 | CYS | 2.1 |
| 1 | H | 207 | MET | 2.1 |
| 1 | I | 438 | GLU | 2.1 |
| 1 | K | 244 | GLY | 2.1 |
| 1 | E | 490 | ASN | 2.1 |
| 1 | Q | 134 | VAL | 2.1 |
| 1 | P | 213 | ILE | 2.1 |
| 1 | T | 412 | TYR | 2.1 |
| 1 | X | 409 | VAL | 2.1 |
| 1 | R | 171 | ILE | 2.1 |
| 1 | U | 412 | TYR | 2.1 |
| 1 | G | 135 | VAL | 2.1 |
| 1 | P | 104 | GLY | 2.1 |
| 1 | R | 316 | VAL | 2.1 |
| 1 | S | 399 | LEU | 2.1 |
| 1 | G | 124 | PHE | 2.1 |
| 1 | O | 174 | ARG | 2.1 |
| 1 | X | 237 | CYS | 2.1 |
| 1 | U | 117 | ASP | 2.1 |
| 1 | X | 136 | ARG | 2.1 |
| 1 | O | 176 | GLY | 2.1 |
| 1 | V | 17 | ASN | 2.1 |
| 1 | B | 293 | ILE | 2.1 |
| 1 | C | 50 | MET | 2.1 |
| 1 | B | 421 | VAL | 2.1 |
| 1 | K | 40 | LEU | 2.1 |
| 1 | V | 131 | LEU | 2.1 |
| 1 | C | 149 | ILE | 2.1 |
| 1 | E | 336 | GLY | 2.1 |
| 1 | U | 232 | ASP | 2.0 |
| 1 | N | 85 | LYS | 2.0 |
| 1 | A | 110 | THR | 2.0 |
| 1 | N | 238 | LYS | 2.0 |
| 1 | U | 367 | LYS | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | U | 124 | PHE | 2.0 |
| 1 | W | 203 | GLN | 2.0 |
| 1 | T | 9 | LEU | 2.0 |
| 1 | J | 294 | CYS | 2.0 |
| 1 | B | 93 | GLN | 2.0 |
| 1 | S | 126 | ILE | 2.0 |
| 1 | F | 494 | ILE | 2.0 |
| 1 | X | 456 | ARG | 2.0 |
| 1 | X | 313 | VAL | 2.0 |
| 1 | C | 456 | ARG | 2.0 |
| 1 | D | 128 | TYR | 2.0 |
| 1 | D | 289 | GLY | 2.0 |
| 1 | F | 381 | CYS | 2.0 |
| 1 | N | 52 | PHE | 2.0 |
| 1 | R | 242 | HIS | 2.0 |
| 1 | O | 89 | ILE | 2.0 |
| 1 | O | 359 | GLU | 2.0 |
| 1 | L | 406 | ALA | 2.0 |
| 1 | X | 339 | PRO | 2.0 |
| 1 | A | 367 | LYS | 2.0 |
| 1 | N | 161 | LEU | 2.0 |
| 1 | P | 244 | GLY | 2.0 |
| 1 | M | 152 | VAL | 2.0 |
| 1 | P | 291 | PRO | 2.0 |
| 1 | J | 460 | GLY | 2.0 |
| 1 | R | 105 | ALA | 2.0 |
| 1 | R | 495 | LEU | 2.0 |
| 1 | O | 100 | VAL | 2.0 |
| 1 | S | 57 | HIS | 2.0 |
| 1 | D | 89 | ILE | 2.0 |
| 1 | O | 131 | LEU | 2.0 |
| 1 | R | 184 | VAL | 2.0 |
| 1 | G | 93 | GLN | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

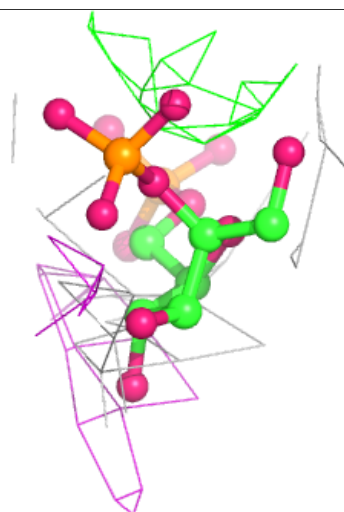
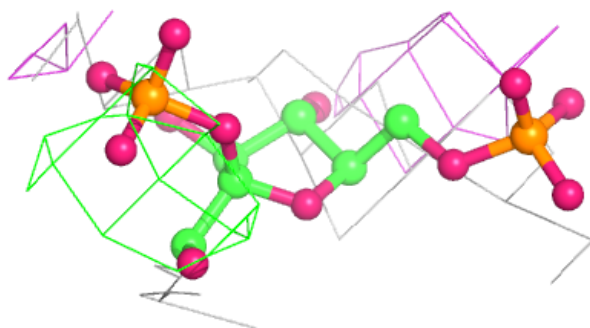
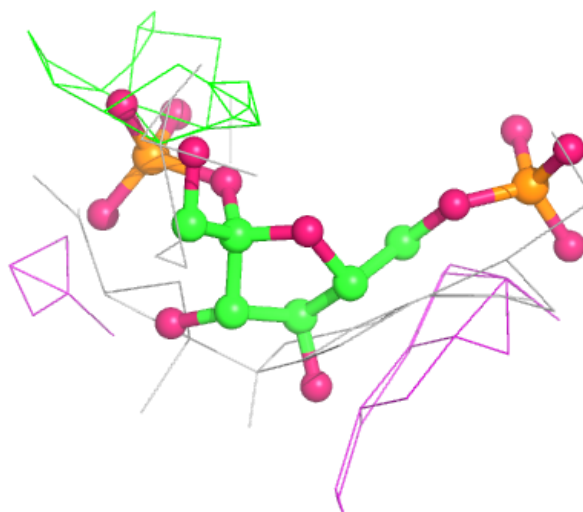
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2 | FDP | X | 700 | 20/20 | 0.63 | 0.34 | 25,32,34,35 | 0 |
| 2 | FDP | L | 700 | 20/20 | 0.64 | 0.30 | 25,32,34,35 | 0 |
| 2 | FDP | J | 700 | 20/20 | 0.64 | 0.37 | 25,32,34,35 | 0 |
| 2 | FDP | C | 700 | 20/20 | 0.64 | 0.32 | 25,32,34,35 | 0 |
| 2 | FDP | P | 700 | 20/20 | 0.66 | 0.29 | 25,32,34,35 | 0 |
| 2 | FDP | T | 700 | 20/20 | 0.67 | 0.25 | 25,32,34,35 | 0 |
| 2 | FDP | S | 700 | 20/20 | 0.70 | 0.33 | 25,32,34,35 | 0 |
| 2 | FDP | H | 700 | 20/20 | 0.71 | 0.31 | 25,32,34,35 | 0 |
| 2 | FDP | K | 700 | 20/20 | 0.73 | 0.27 | 25,32,34,35 | 0 |
| 2 | FDP | U | 700 | 20/20 | 0.73 | 0.32 | 25,32,34,35 | 0 |
| 2 | FDP | E | 700 | 20/20 | 0.74 | 0.24 | 25,32,34,35 | 0 |
| 2 | FDP | Q | 700 | 20/20 | 0.74 | 0.30 | 25,32,34,35 | 0 |
| 2 | FDP | R | 700 | 20/20 | 0.75 | 0.23 | 25,32,34,35 | 0 |
| 2 | FDP | G | 700 | 20/20 | 0.76 | 0.31 | 25,32,34,35 | 0 |
| 2 | FDP | F | 700 | 20/20 | 0.78 | 0.31 | 25,32,34,35 | 0 |
| 2 | FDP | B | 700 | 20/20 | 0.78 | 0.19 | 25,32,34,35 | 0 |
| 2 | FDP | V | 700 | 20/20 | 0.79 | 0.30 | 25,32,34,35 | 0 |
| 2 | FDP | W | 700 | 20/20 | 0.80 | 0.32 | 25,32,34,35 | 0 |
| 2 | FDP | N | 700 | 20/20 | 0.80 | 0.26 | 25,32,34,35 | 0 |
| 2 | FDP | A | 700 | 20/20 | 0.81 | 0.19 | 25,32,34,35 | 0 |
| 2 | FDP | I | 700 | 20/20 | 0.81 | 0.25 | 25,32,34,35 | 0 |
| 2 | FDP | O | 700 | 20/20 | 0.82 | 0.26 | 25,32,34,35 | 0 |
| 2 | FDP | M | 700 | 20/20 | 0.82 | 0.22 | 25,32,34,35 | 0 |
| 2 | FDP | D | 700 | 20/20 | 0.87 | 0.23 | 25,32,34,35 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

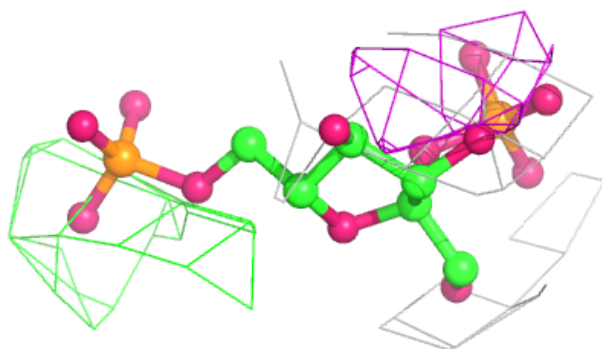
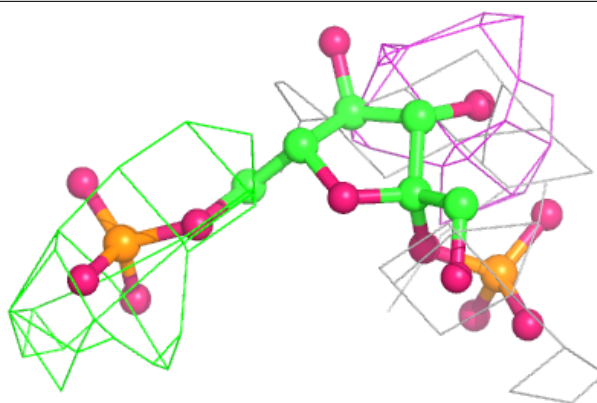
Electron density around FDP X 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

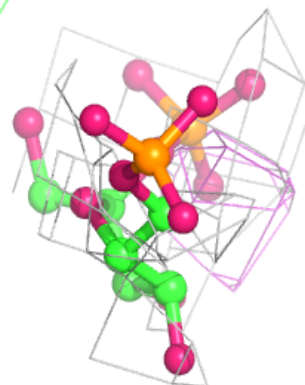
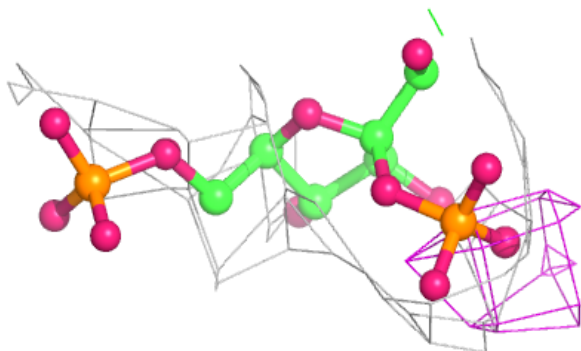
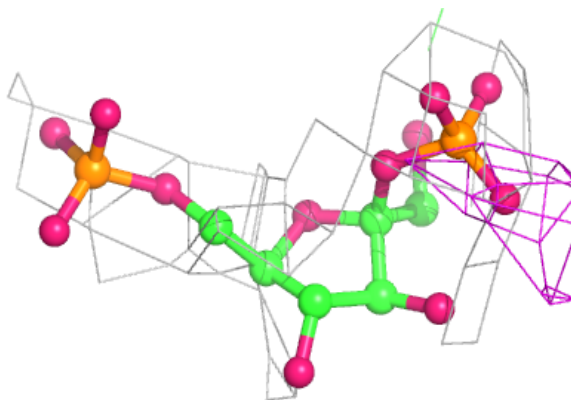


Electron density around FDP L 700:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

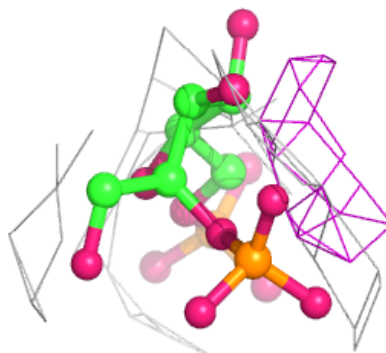
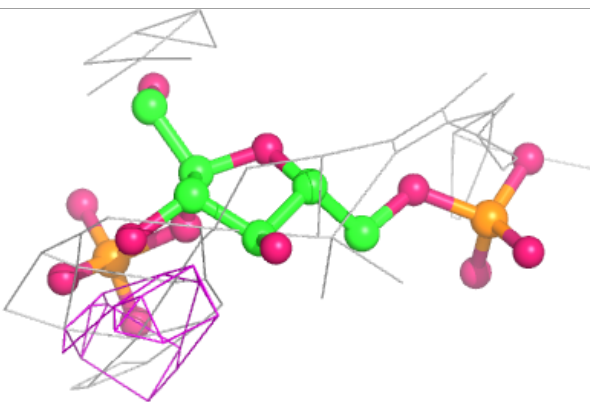
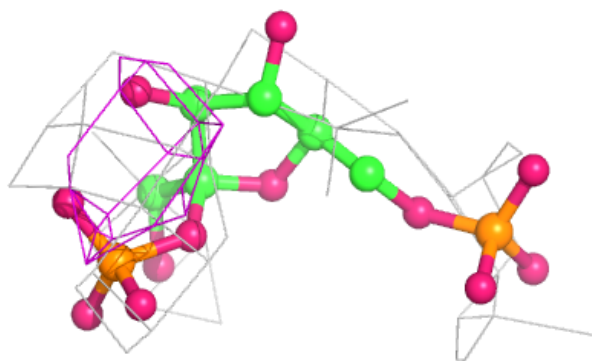
**Electron density around FDP J 700:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

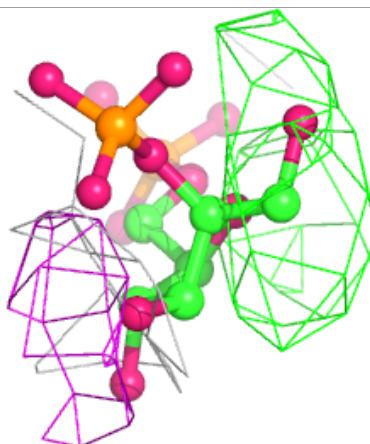
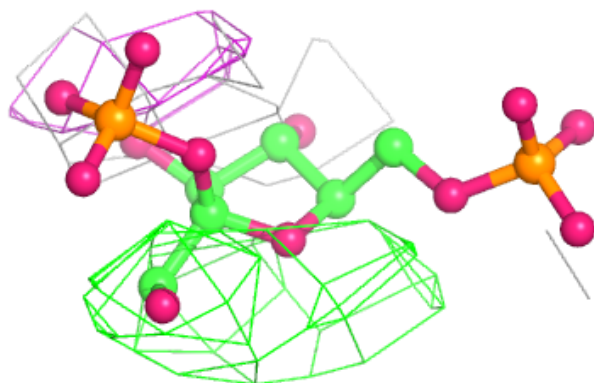
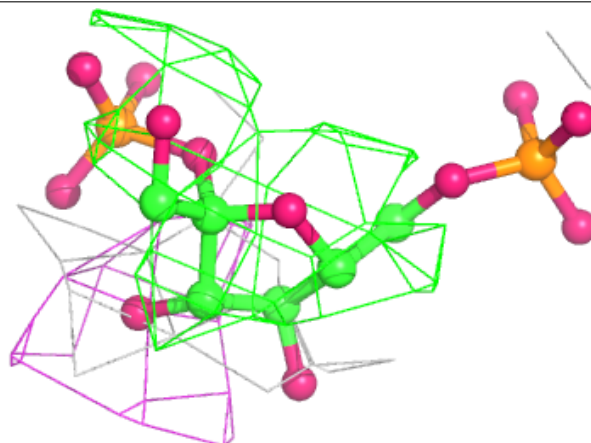


Electron density around FDP C 700:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

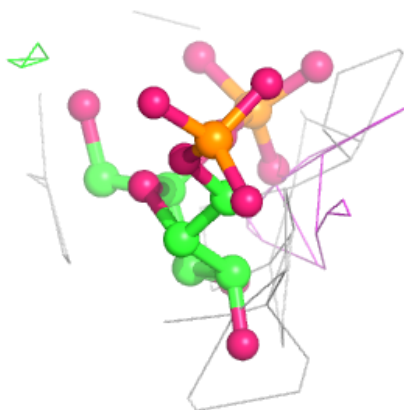
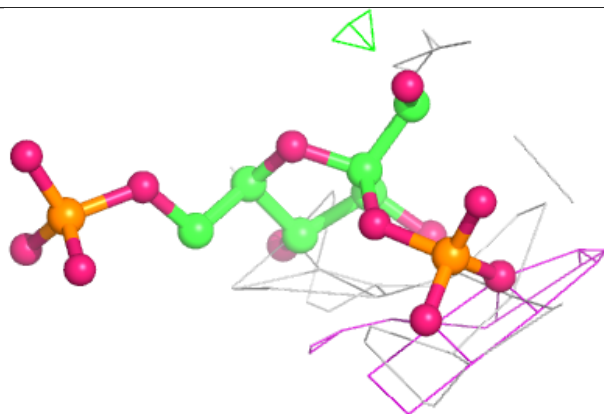
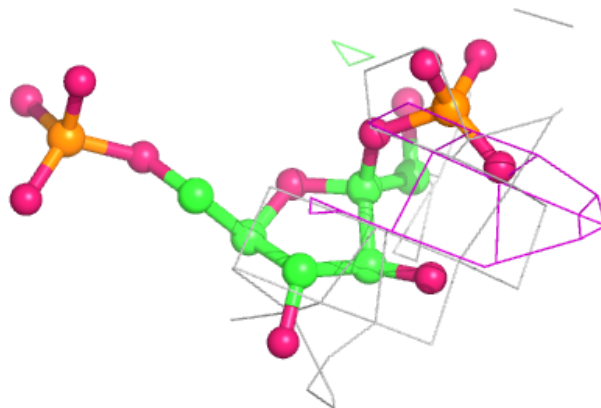
**Electron density around FDP P 700:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



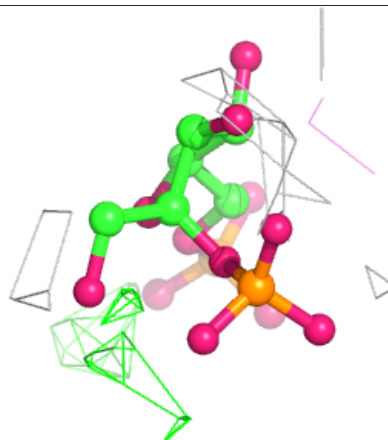
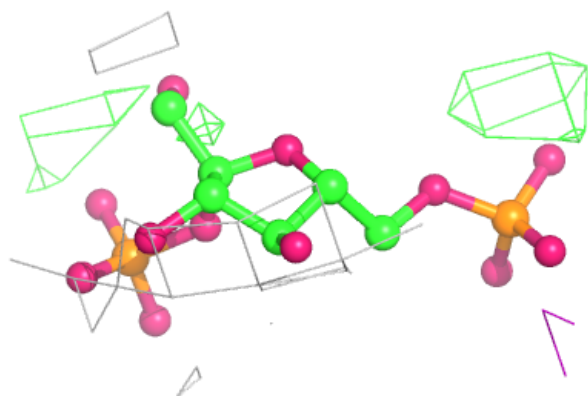
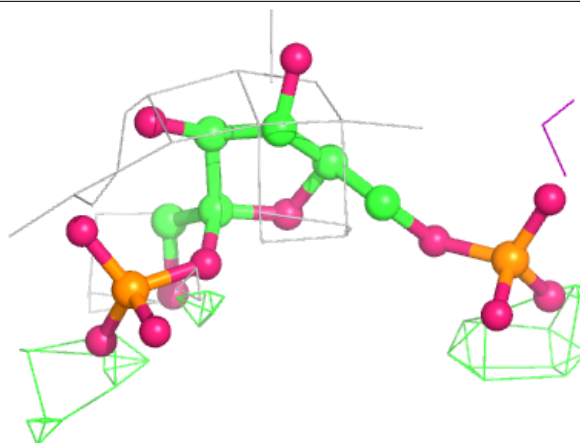
Electron density around FDP T 700:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



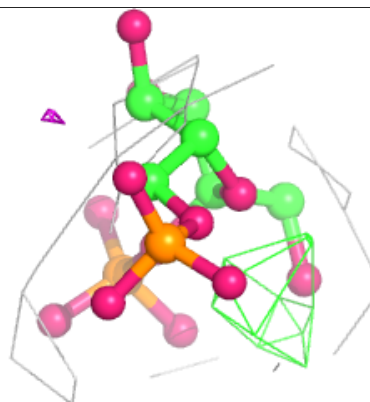
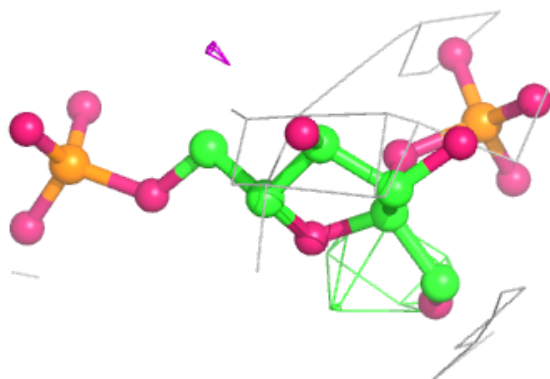
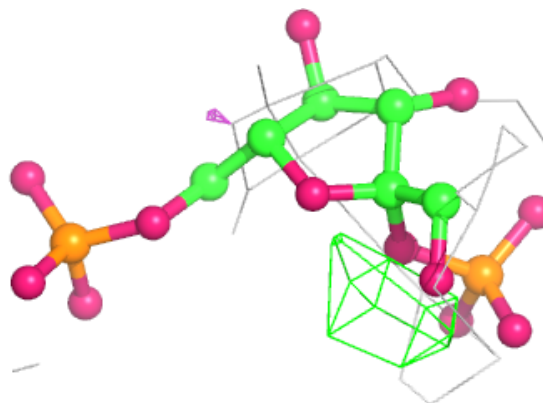
Electron density around FDP S 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



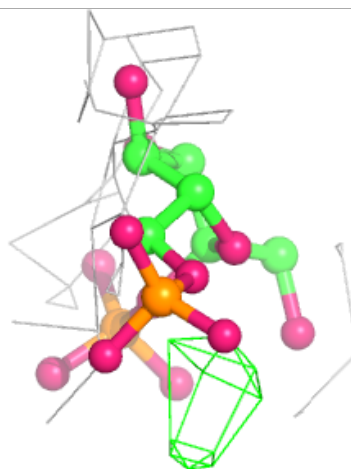
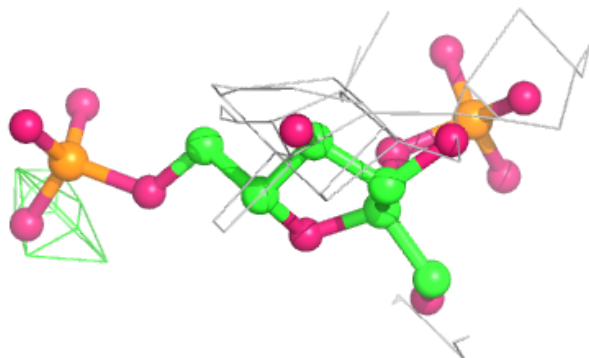
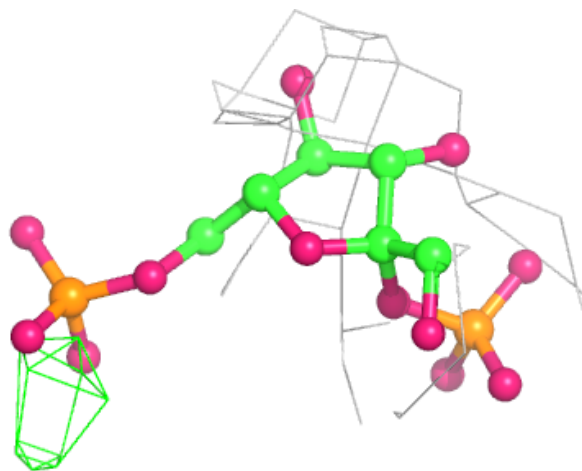
Electron density around FDP H 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



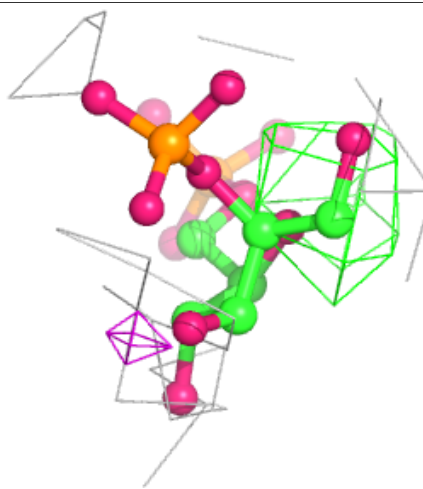
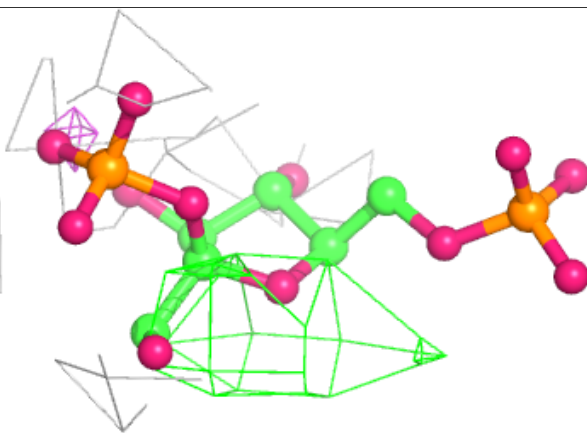
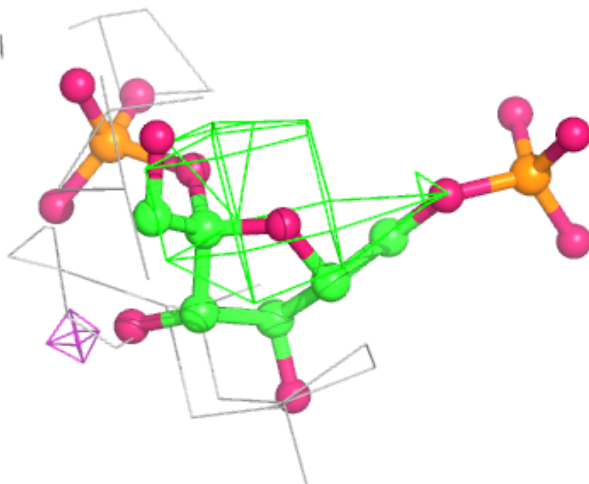
Electron density around FDP K 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



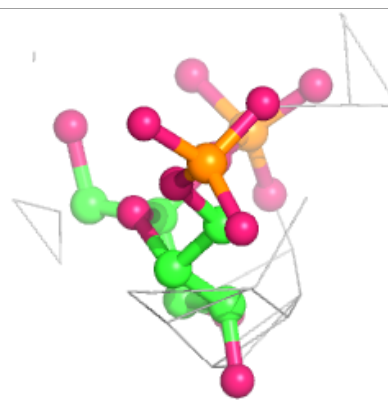
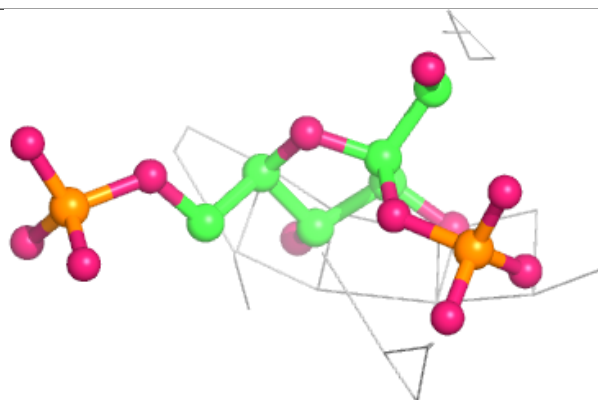
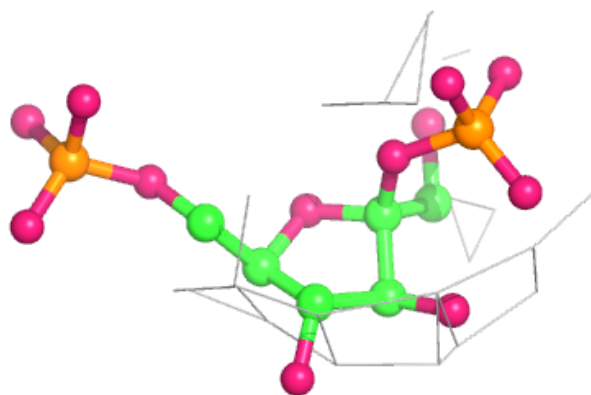
Electron density around FDP U 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)

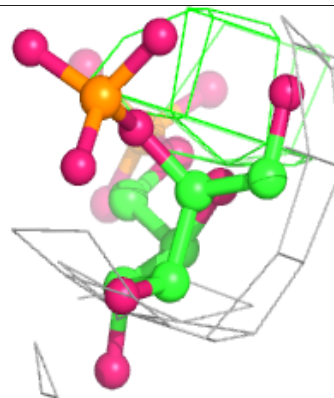
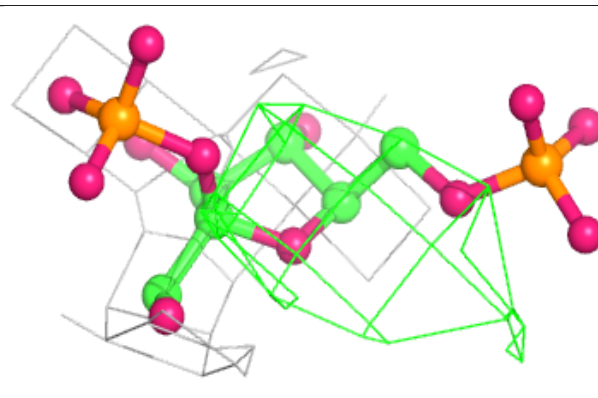
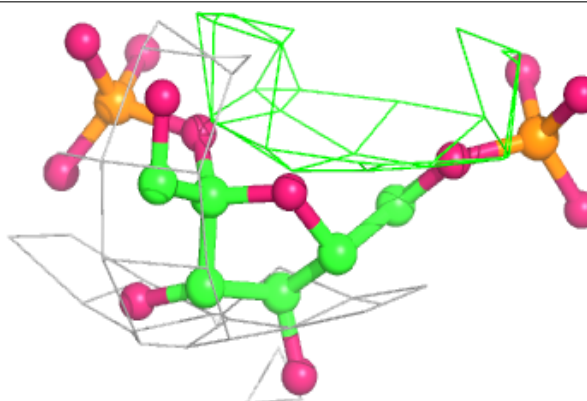


Electron density around FDP E 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

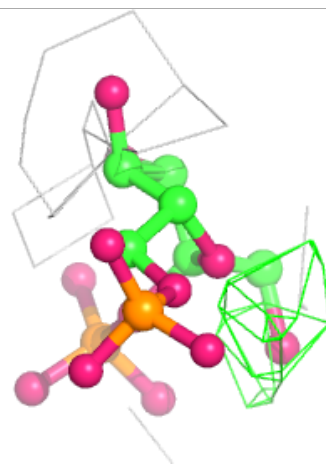
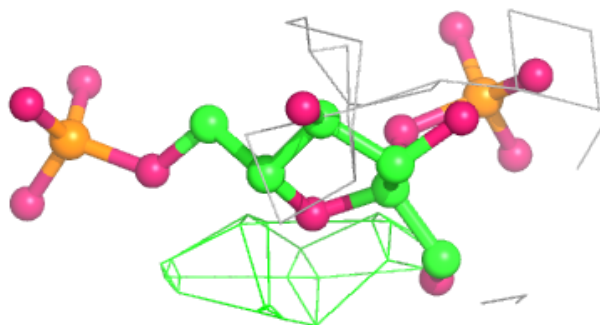
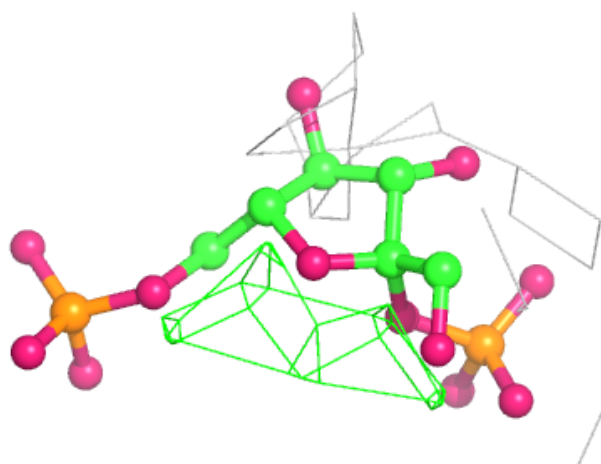
**Electron density around FDP Q 700:**

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and green (positive)



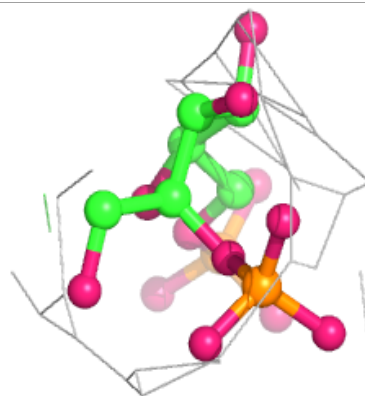
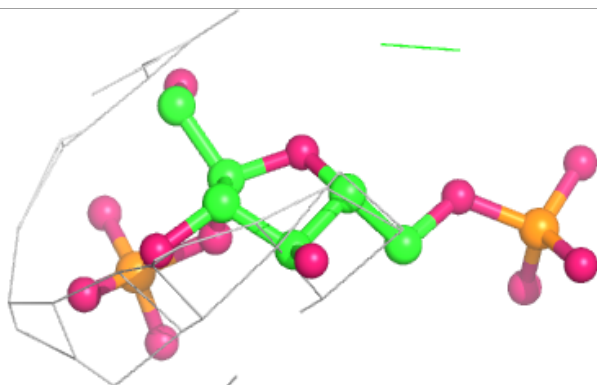
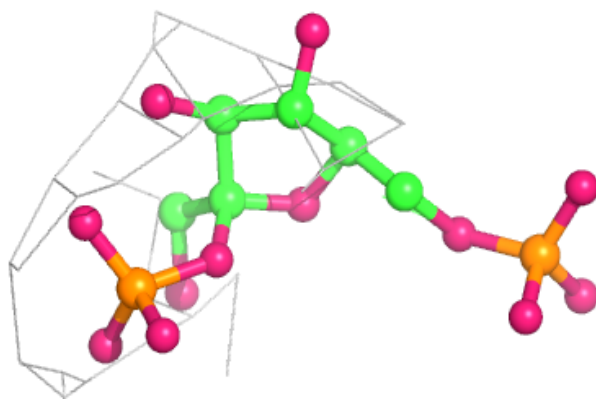
Electron density around FDP R 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

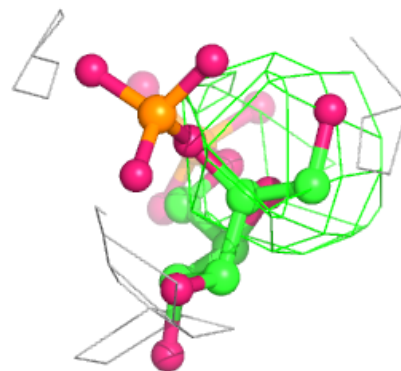
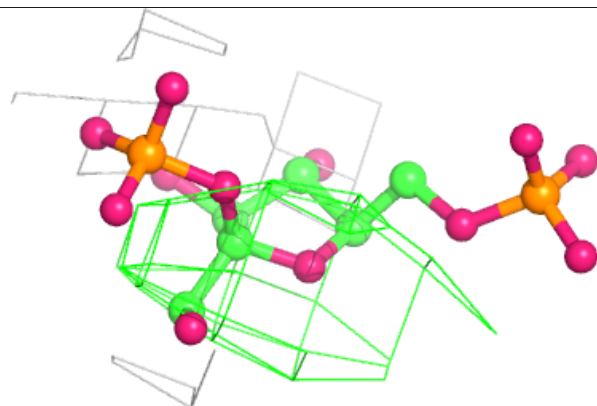
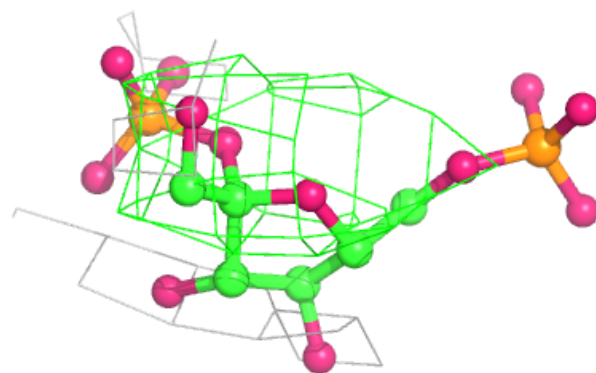


Electron density around FDP G 700:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

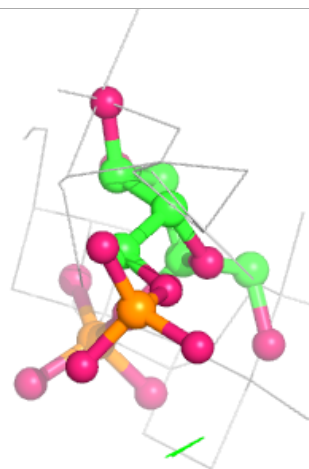
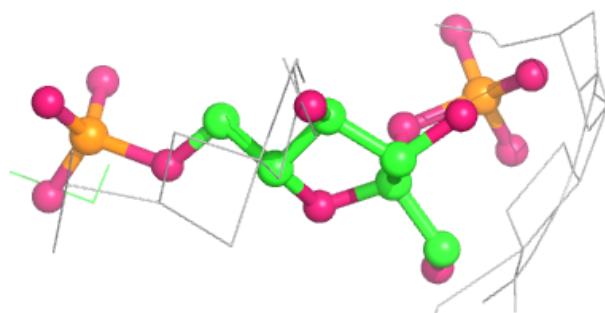
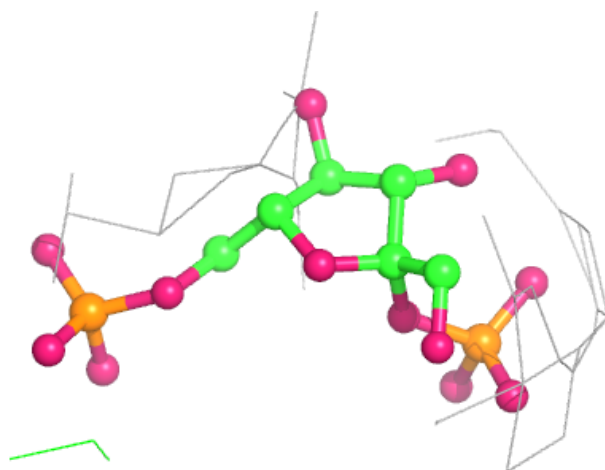
**Electron density around FDP F 700:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



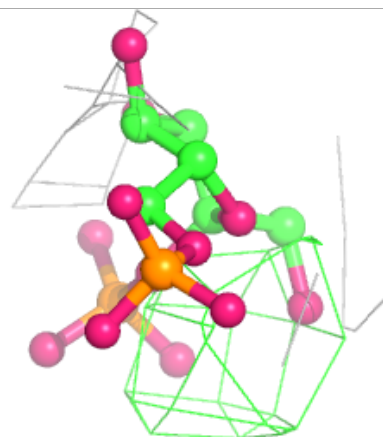
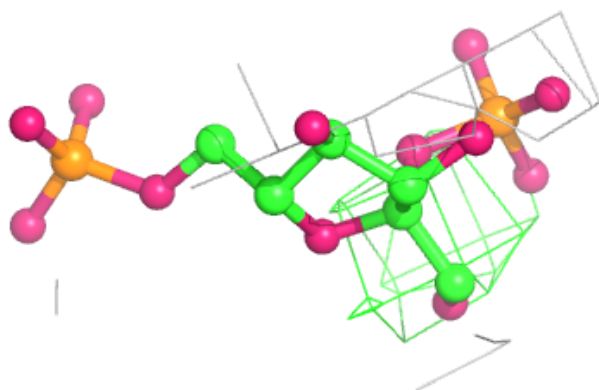
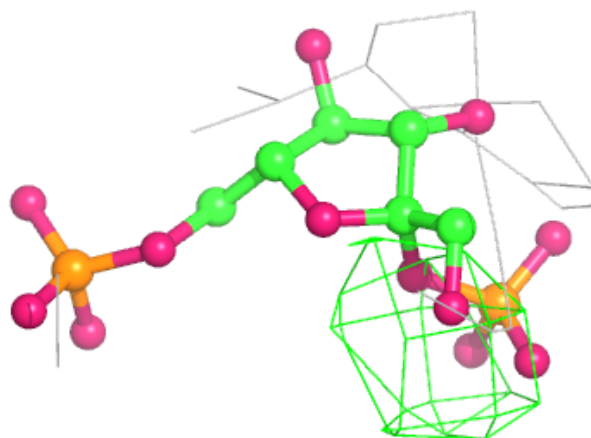
Electron density around FDP B 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



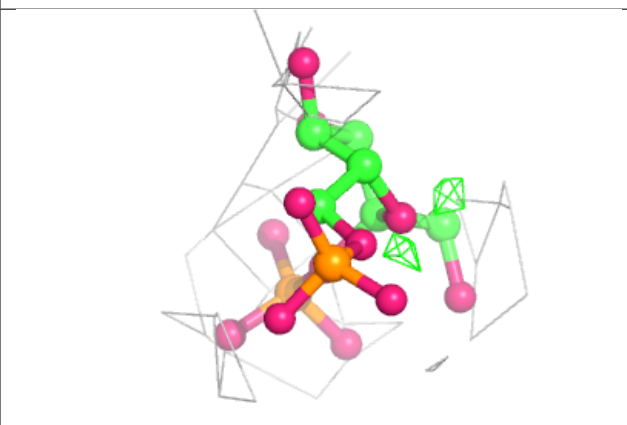
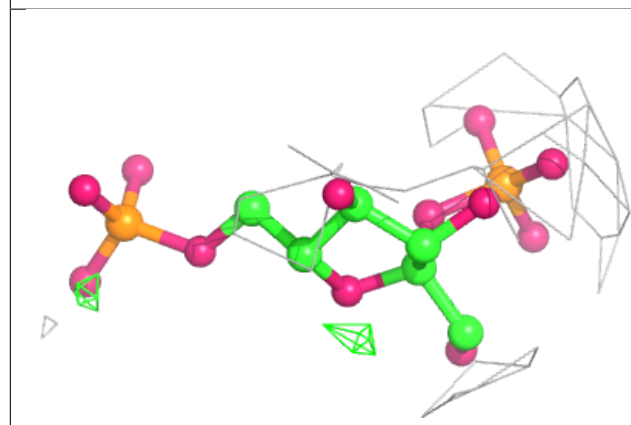
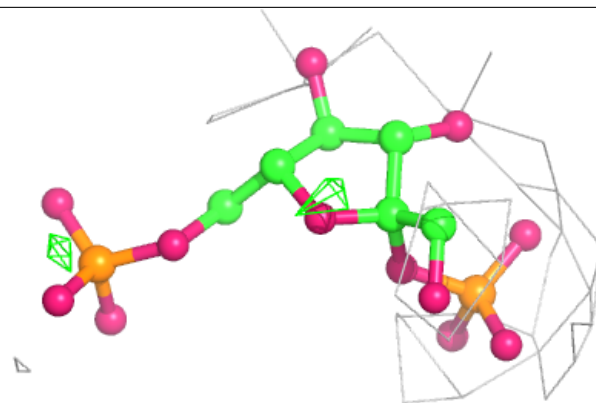
Electron density around FDP V 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

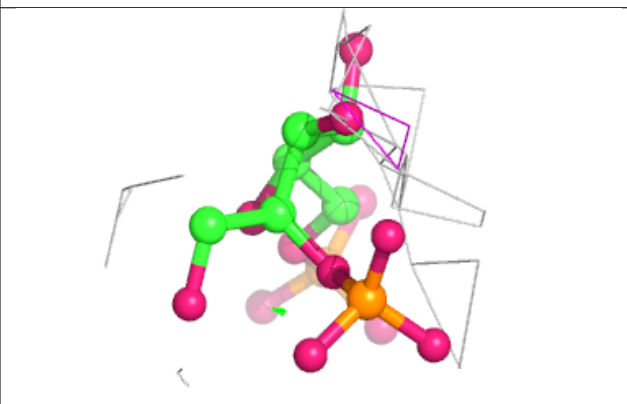
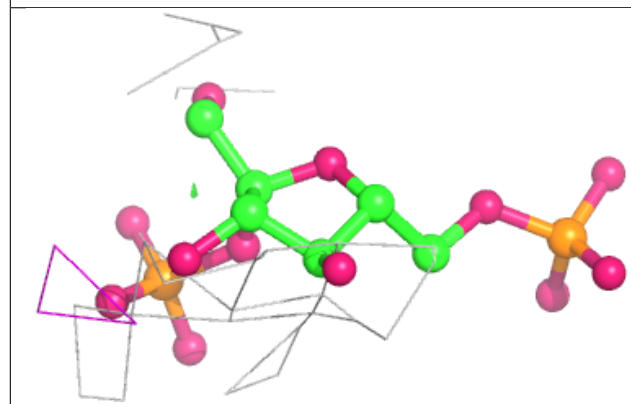
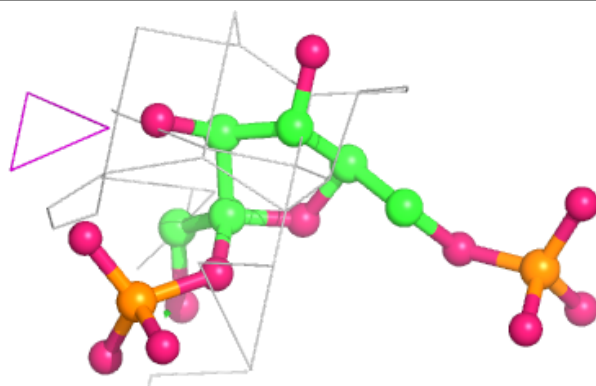


Electron density around FDP W 700:

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

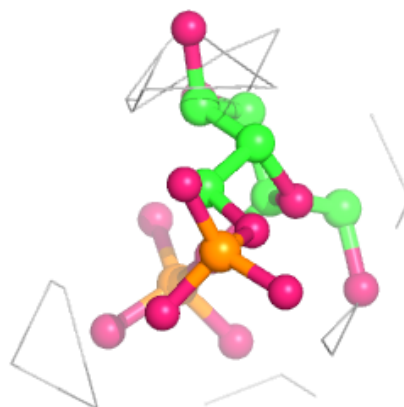
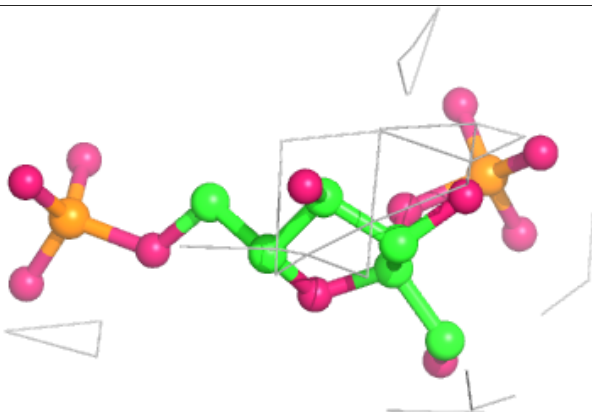
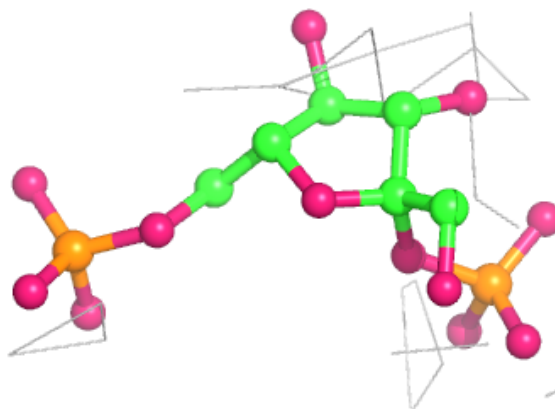
**Electron density around FDP N 700:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

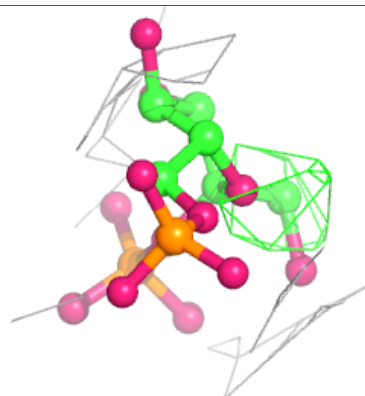
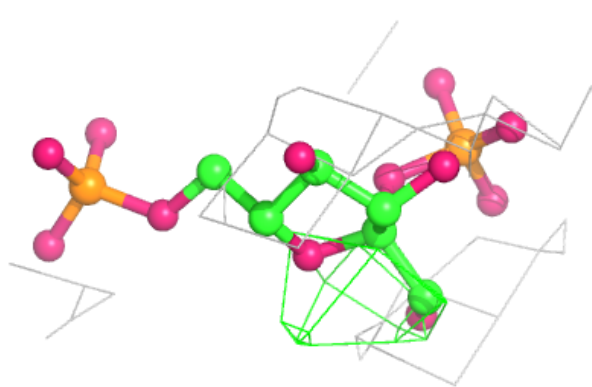
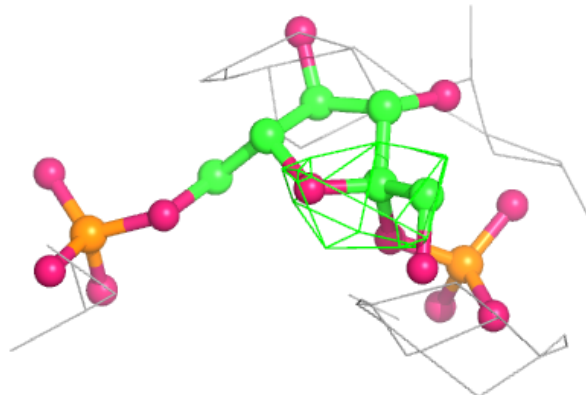


Electron density around FDP A 700:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

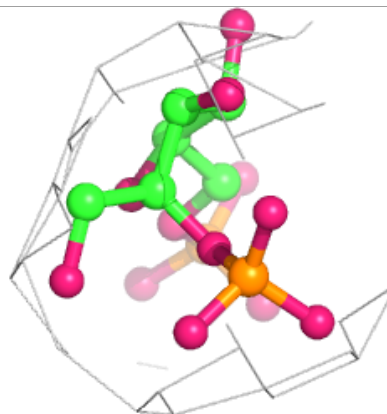
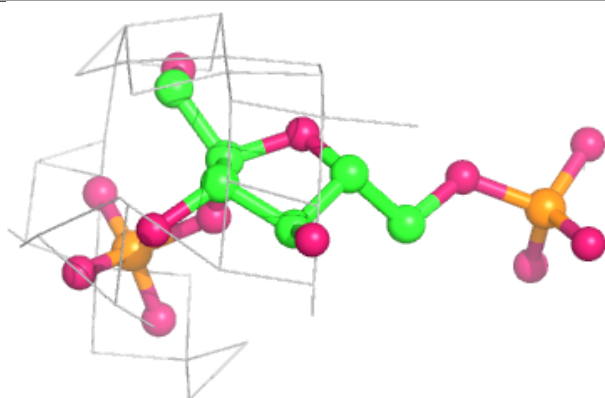
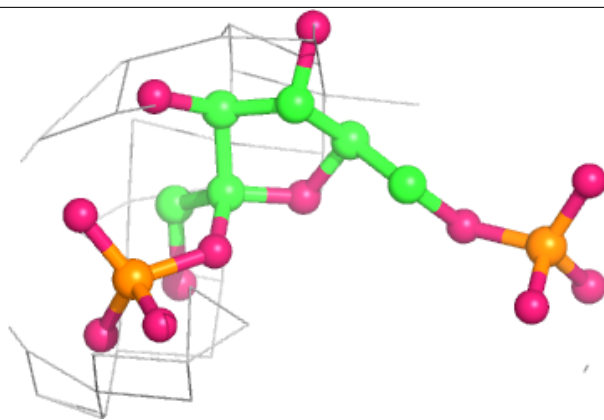
**Electron density around FDP I 700:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



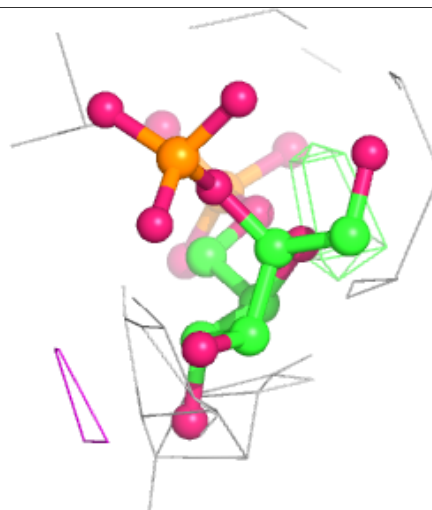
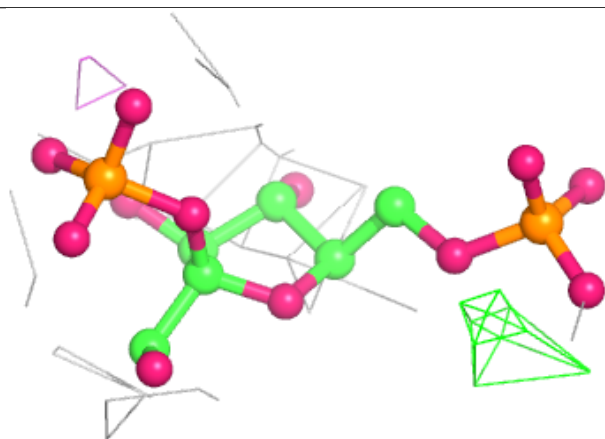
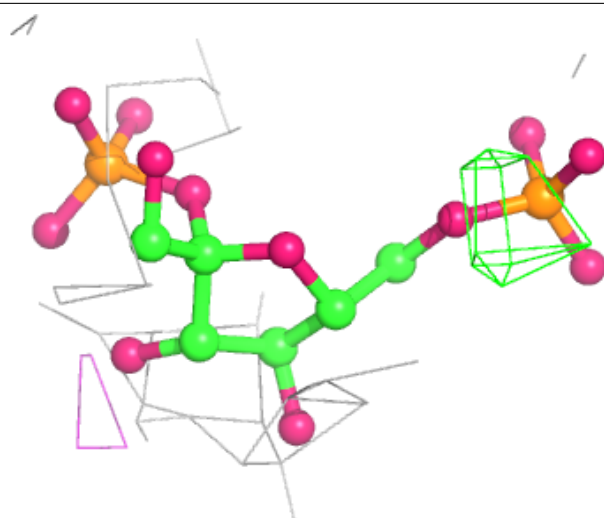
Electron density around FDP O 700:

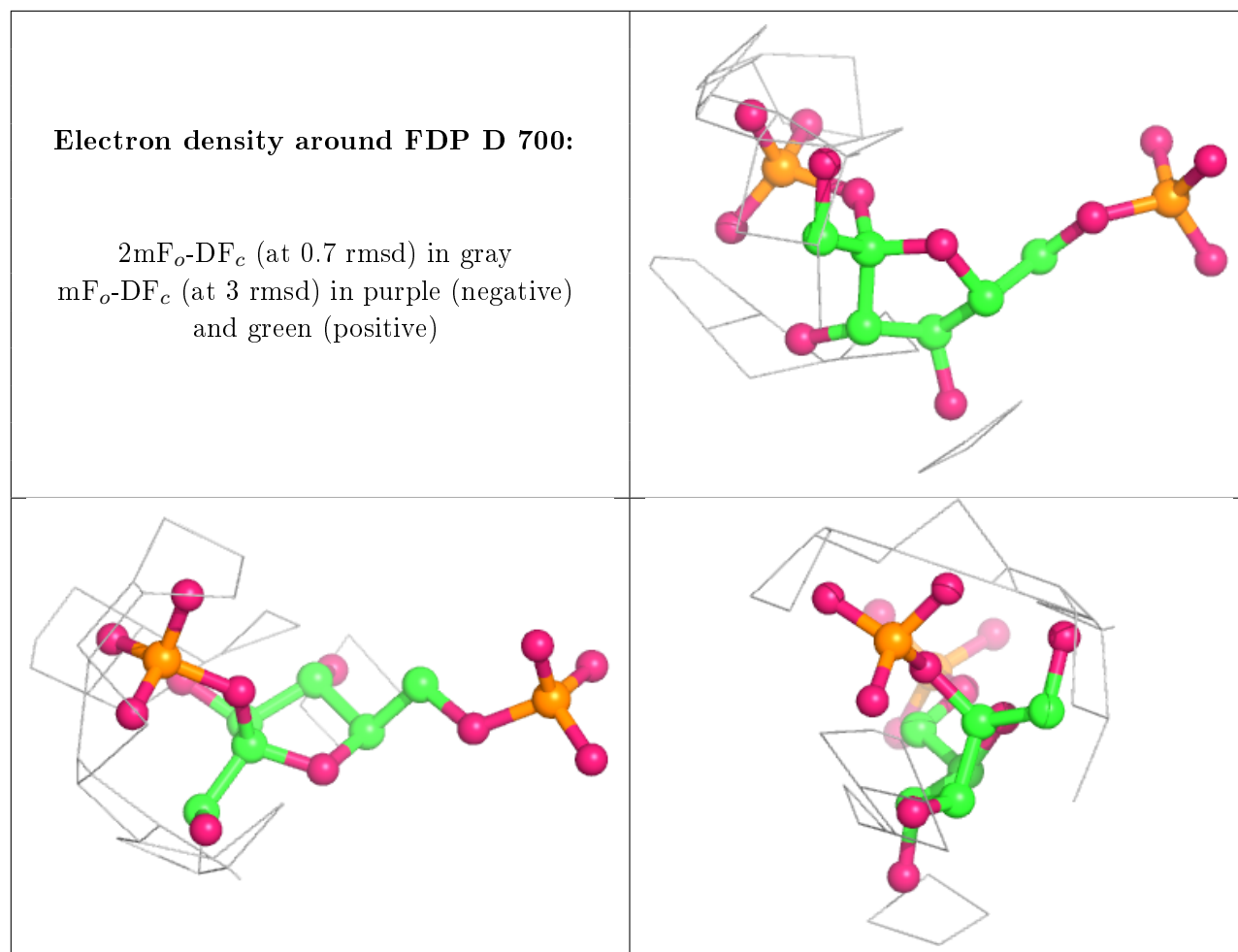
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FDP M 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.