



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:51 pm BST

PDB ID : 3WST
Title : Crystal structure of C.elegans PRMT7 in complex with SAH(P31)
Authors : Hasegawa, M.; Toma-fukai, S.; Shimizu, T.
Deposited on : 2014-03-21
Resolution : 2.39 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

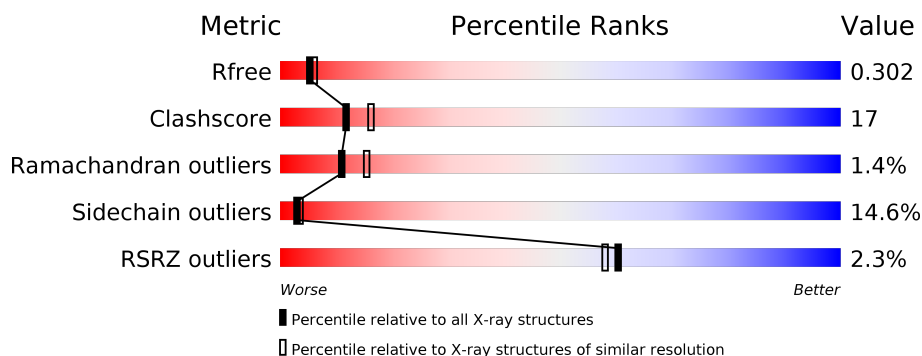
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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 | 3907 (2.40-2.40) |
| Clashscore | 141614 | 4398 (2.40-2.40) |
| Ramachandran outliers | 138981 | 4318 (2.40-2.40) |
| Sidechain outliers | 138945 | 4319 (2.40-2.40) |
| RSRZ outliers | 127900 | 3811 (2.40-2.40) |

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 | 655 | <div> <div>69%</div> <div>23%</div> <div>6%</div> <div>•</div> </div> |
| 1 | B | 655 | <div> <div>%</div> <div>61%</div> <div>29%</div> <div>8%</div> <div>•</div> </div> |
| 1 | C | 655 | <div> <div>63%</div> <div>30%</div> <div>•</div> <div>•</div> </div> |
| 1 | D | 655 | <div> <div>69%</div> <div>24%</div> <div>•</div> <div>•</div> </div> |
| 1 | E | 655 | <div> <div>%</div> <div>62%</div> <div>27%</div> <div>7%</div> <div>•</div> </div> |
| 1 | F | 655 | <div> <div>2%</div> <div>62%</div> <div>28%</div> <div>7%</div> <div>•</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | G | 655 | |
| 1 | H | 655 | |
| 1 | I | 655 | |
| 1 | J | 655 | |
| 1 | K | 655 | |
| 1 | L | 655 | |
| 1 | M | 655 | |
| 1 | N | 655 | |
| 1 | O | 655 | |
| 1 | P | 655 | |
| 1 | Q | 655 | |
| 1 | R | 655 | |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 92645 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 Protein arginine N-methyltransferase 7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 641 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5106 | 3247 | 857 | 975 | 27 | | | |
| 1 | D | 637 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5078 | 3231 | 852 | 968 | 27 | | | |
| 1 | B | 638 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5084 | 3234 | 853 | 970 | 27 | | | |
| 1 | C | 639 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5091 | 3239 | 854 | 971 | 27 | | | |
| 1 | F | 638 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5084 | 3234 | 853 | 970 | 27 | | | |
| 1 | E | 636 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5069 | 3226 | 850 | 966 | 27 | | | |
| 1 | G | 636 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5070 | 3227 | 850 | 966 | 27 | | | |
| 1 | H | 639 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5091 | 3239 | 854 | 971 | 27 | | | |
| 1 | I | 644 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5122 | 3257 | 860 | 978 | 27 | | | |
| 1 | M | 633 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5049 | 3216 | 844 | 962 | 27 | | | |
| 1 | N | 638 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5084 | 3234 | 853 | 970 | 27 | | | |
| 1 | O | 641 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5106 | 3247 | 857 | 975 | 27 | | | |
| 1 | P | 636 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5069 | 3226 | 850 | 966 | 27 | | | |
| 1 | Q | 632 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5039 | 3209 | 845 | 958 | 27 | | | |
| 1 | R | 638 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5084 | 3234 | 853 | 970 | 27 | | | |
| 1 | J | 644 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5122 | 3257 | 860 | 978 | 27 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | K | 641 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5106 | 3247 | 857 | 975 | 27 | | | |
| 1 | L | 644 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5122 | 3257 | 860 | 978 | 27 | | | |

There are 144 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| A | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| A | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| A | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| A | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| A | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| A | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| A | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| D | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| D | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| D | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| D | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| D | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| D | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| D | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| D | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| B | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| B | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| B | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| B | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| B | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| B | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| B | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| B | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| C | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| C | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| C | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| C | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| C | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| C | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| C | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| C | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| F | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| F | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| F | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| F | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| F | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| F | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| F | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| F | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| E | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| E | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| E | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| E | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| E | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| E | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| E | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| E | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| G | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| G | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| G | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| G | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| G | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| G | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| G | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| G | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| H | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| H | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| H | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| H | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| H | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| H | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| H | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| H | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| I | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| I | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| I | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| I | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| I | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| I | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| I | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| I | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| M | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| M | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| M | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| M | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |

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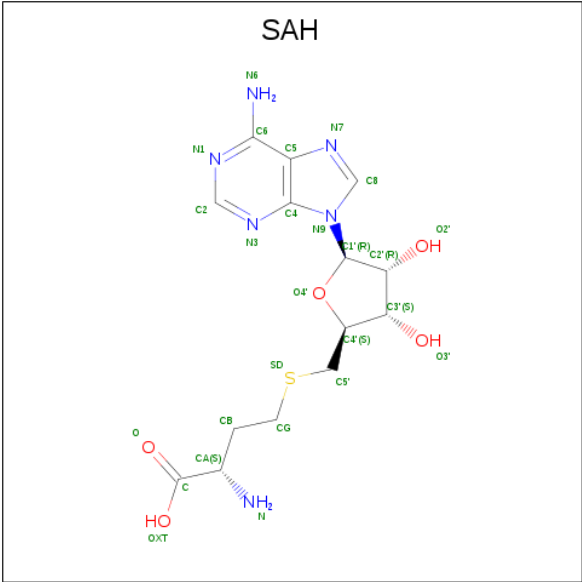
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| M | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| M | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| M | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| M | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| N | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| N | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| N | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| N | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| N | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| N | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| N | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| N | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| O | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| O | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| O | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| O | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| O | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| O | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| O | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| O | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| P | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| P | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| P | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| P | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| P | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| P | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| P | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| P | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| Q | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| Q | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| Q | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| Q | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| Q | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| Q | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| Q | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| Q | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| R | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| R | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| R | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| R | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| R | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| R | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| R | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| R | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| J | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| J | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| J | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| J | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| J | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| J | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| J | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| J | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| K | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| K | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| K | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| K | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| K | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| K | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| K | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| K | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| L | -7 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| L | -6 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |
| L | -5 | LEU | - | EXPRESSION TAG | UNP Q9XW42 |
| L | -4 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| L | -3 | SER | - | EXPRESSION TAG | UNP Q9XW42 |
| L | -2 | GLY | - | EXPRESSION TAG | UNP Q9XW42 |
| L | -1 | ILE | - | EXPRESSION TAG | UNP Q9XW42 |
| L | 0 | PRO | - | EXPRESSION TAG | UNP Q9XW42 |

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



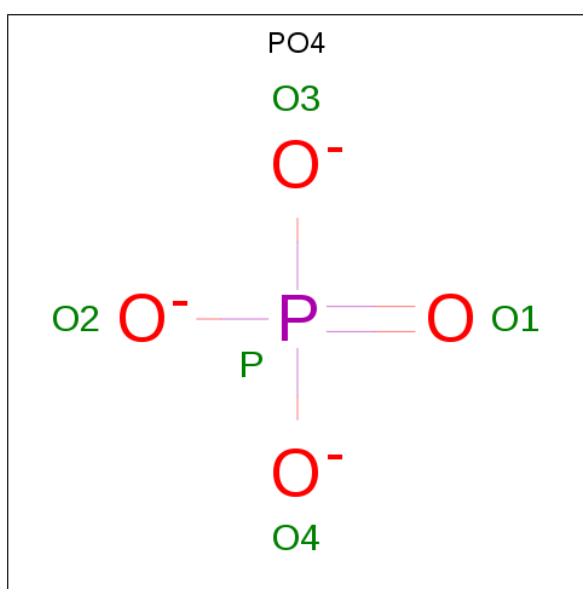
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 2 | A | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | D | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | B | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | C | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | F | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | E | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | G | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | H | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | I | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | M | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | N | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | O | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | P | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | Q | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 2 | R | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | J | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | K | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |
| 2 | L | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 26 | 14 | 6 | 5 | 1 | | |

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3 | A | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | D | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | B | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | C | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | F | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | E | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | G | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3 | H | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | I | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | M | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | N | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | O | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | P | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | Q | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | R | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | J | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | K | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 3 | L | 1 | Total | O | P | 0 | 0 |
| | | | 5 | 4 | 1 | | |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4 | A | 105 | Total | O | 0 | 0 |
| | | | 105 | 105 | | |
| 4 | D | 93 | Total | O | 0 | 0 |
| | | | 93 | 93 | | |
| 4 | B | 26 | Total | O | 0 | 0 |
| | | | 26 | 26 | | |
| 4 | C | 16 | Total | O | 0 | 0 |
| | | | 16 | 16 | | |
| 4 | F | 12 | Total | O | 0 | 0 |
| | | | 12 | 12 | | |
| 4 | E | 41 | Total | O | 0 | 0 |
| | | | 41 | 41 | | |
| 4 | G | 19 | Total | O | 0 | 0 |
| | | | 19 | 19 | | |
| 4 | H | 59 | Total | O | 0 | 0 |
| | | | 59 | 59 | | |

Continued on next page...

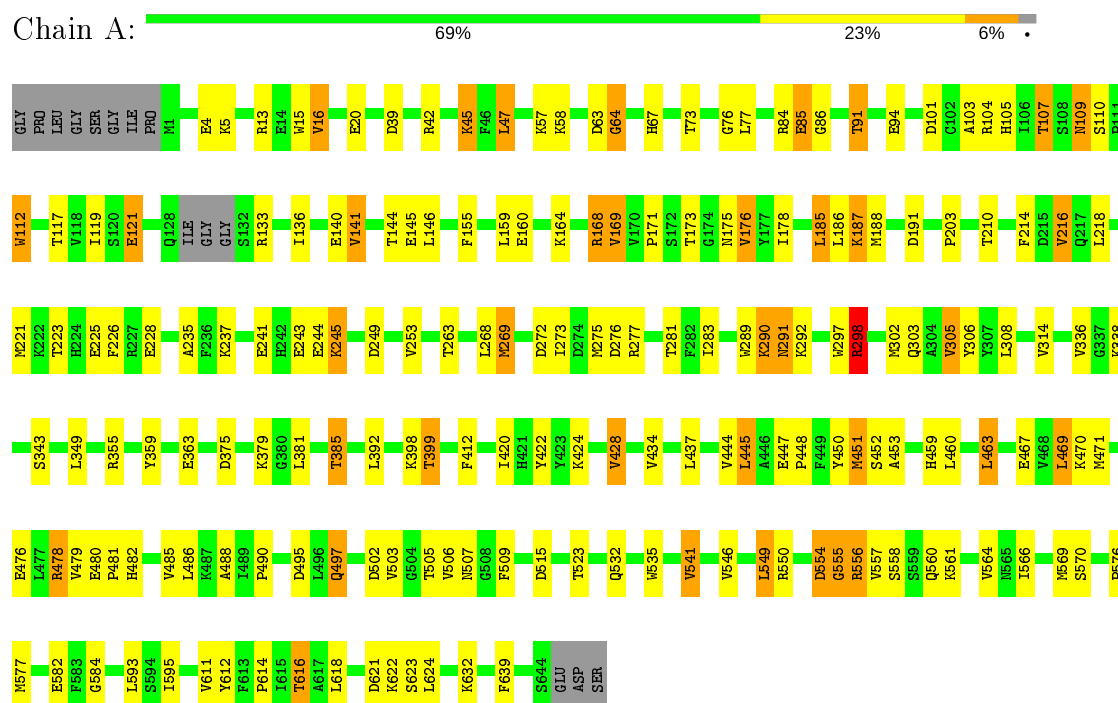
Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4 | I | 21 | Total 21 | O 21 | 0 | 0 |
| 4 | M | 2 | Total 2 | O 2 | 0 | 0 |
| 4 | P | 10 | Total 10 | O 10 | 0 | 0 |
| 4 | Q | 2 | Total 2 | O 2 | 0 | 0 |
| 4 | R | 2 | Total 2 | O 2 | 0 | 0 |
| 4 | J | 12 | Total 12 | O 12 | 0 | 0 |
| 4 | K | 6 | Total 6 | O 6 | 0 | 0 |
| 4 | L | 85 | Total 85 | O 85 | 0 | 0 |

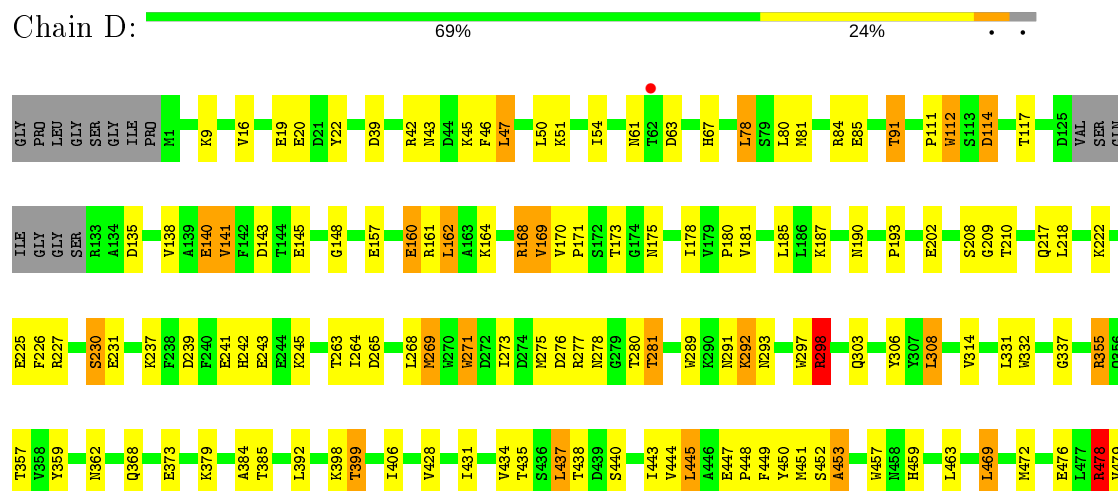
3 Residue-property plots

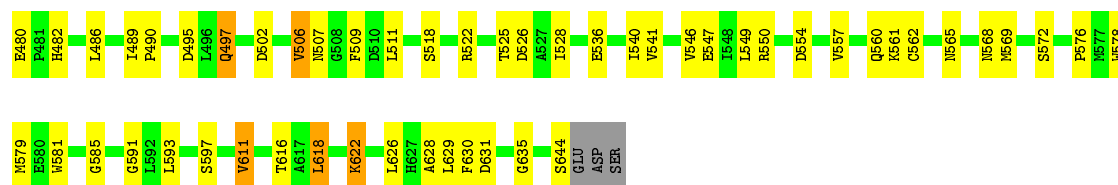
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Protein arginine N-methyltransferase 7

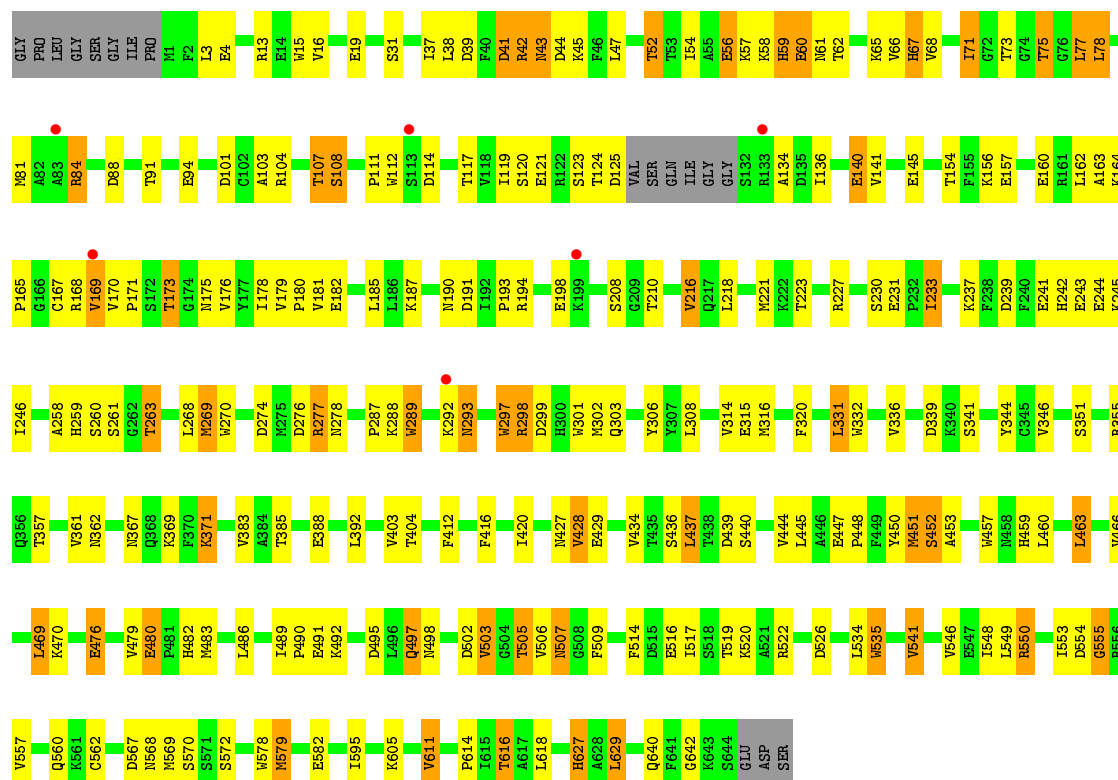


- Molecule 1: Protein arginine N-methyltransferase 7

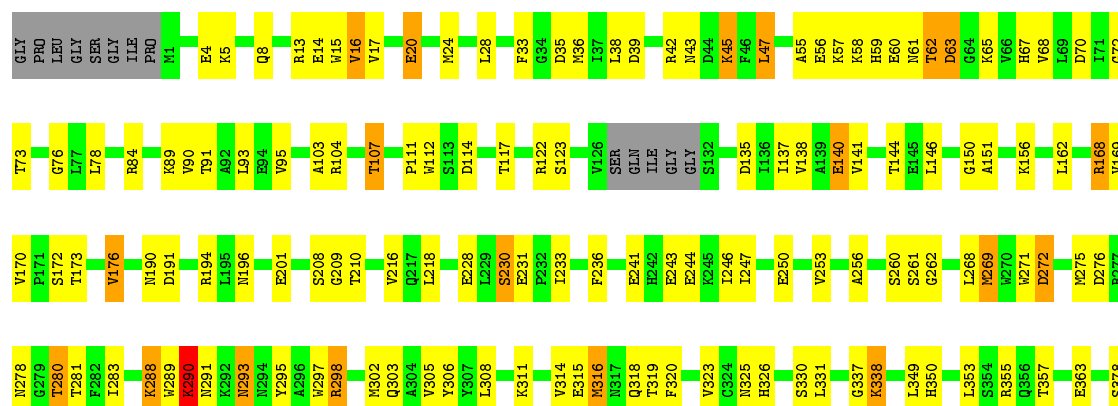


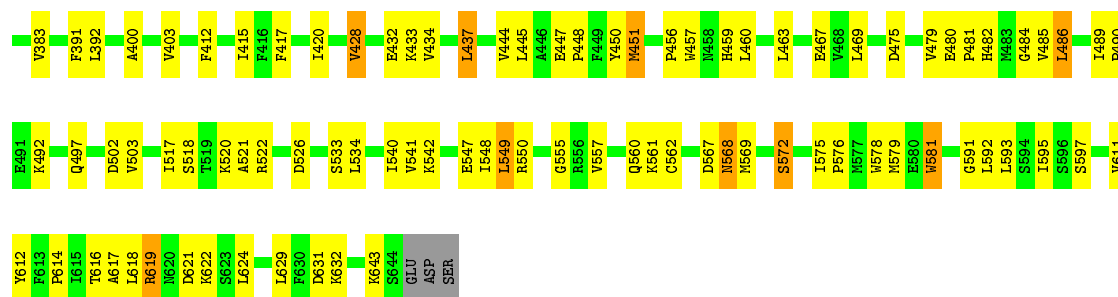


• Molecule 1: Protein arginine N-methyltransferase 7



• Molecule 1: Protein arginine N-methyltransferase 7

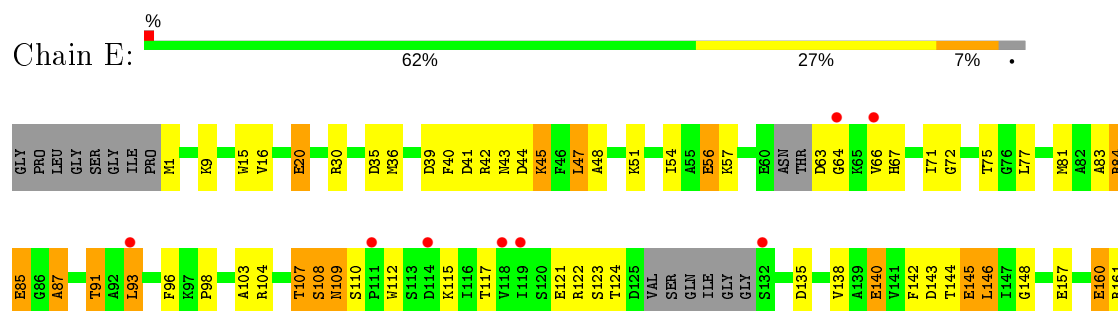


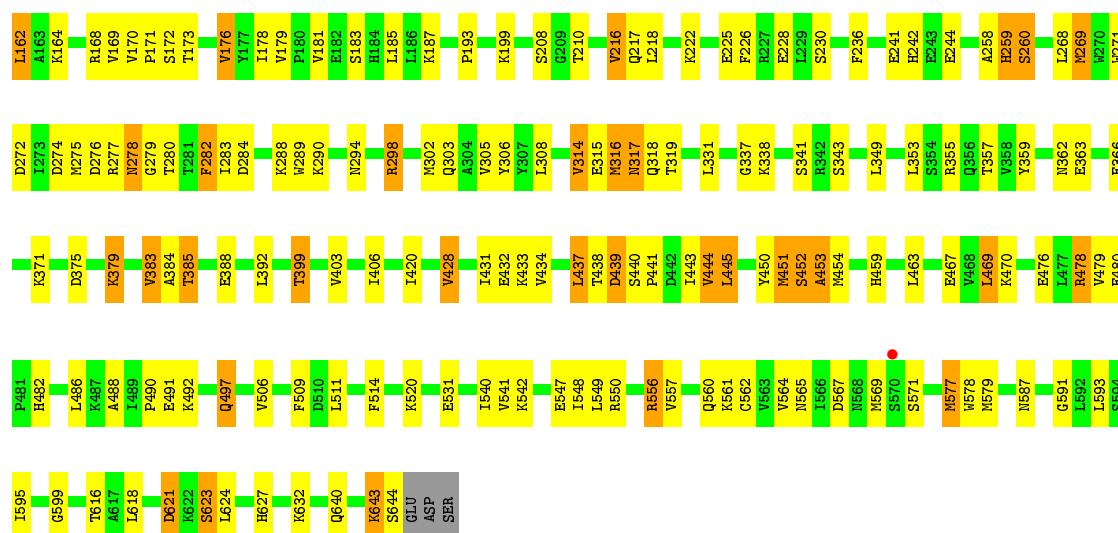


• Molecule 1: Protein arginine N-methyltransferase 7

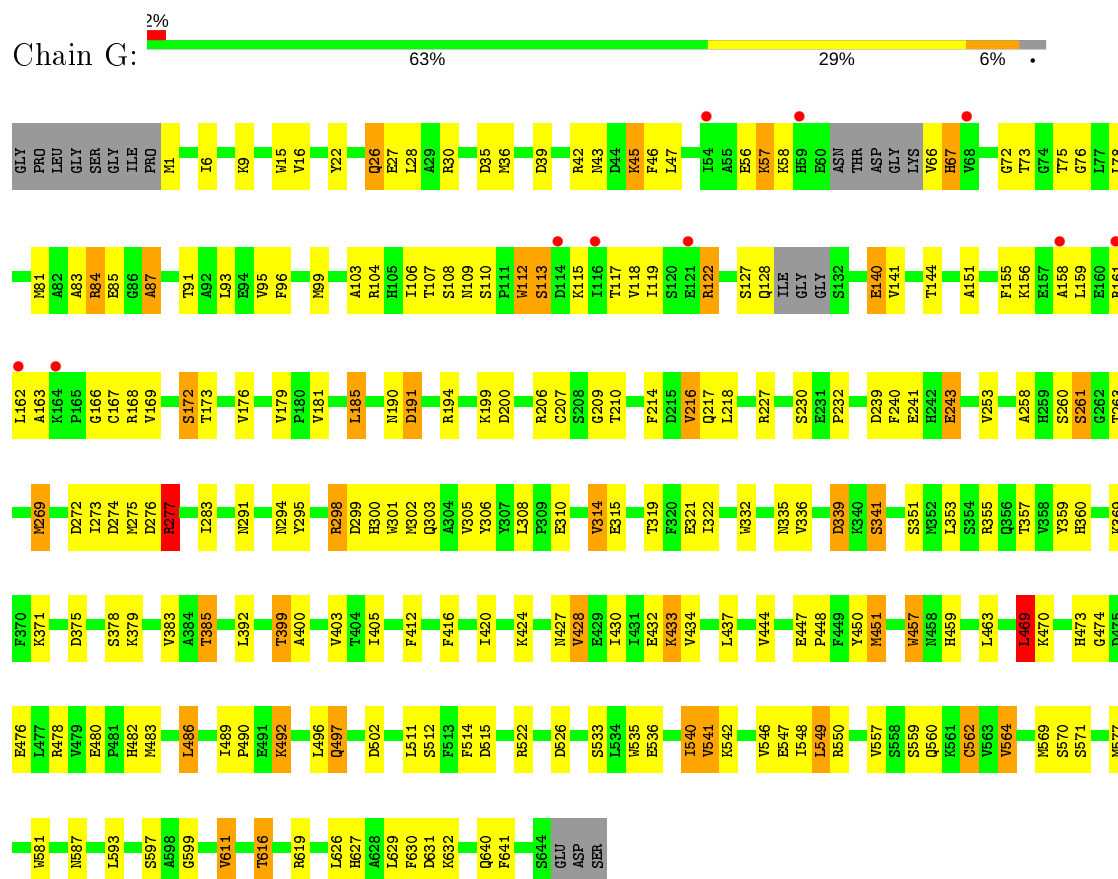


• Molecule 1: Protein arginine N-methyltransferase 7

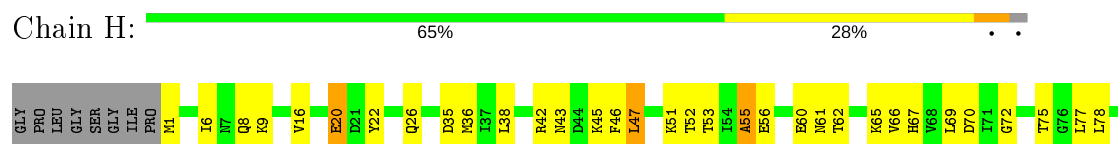




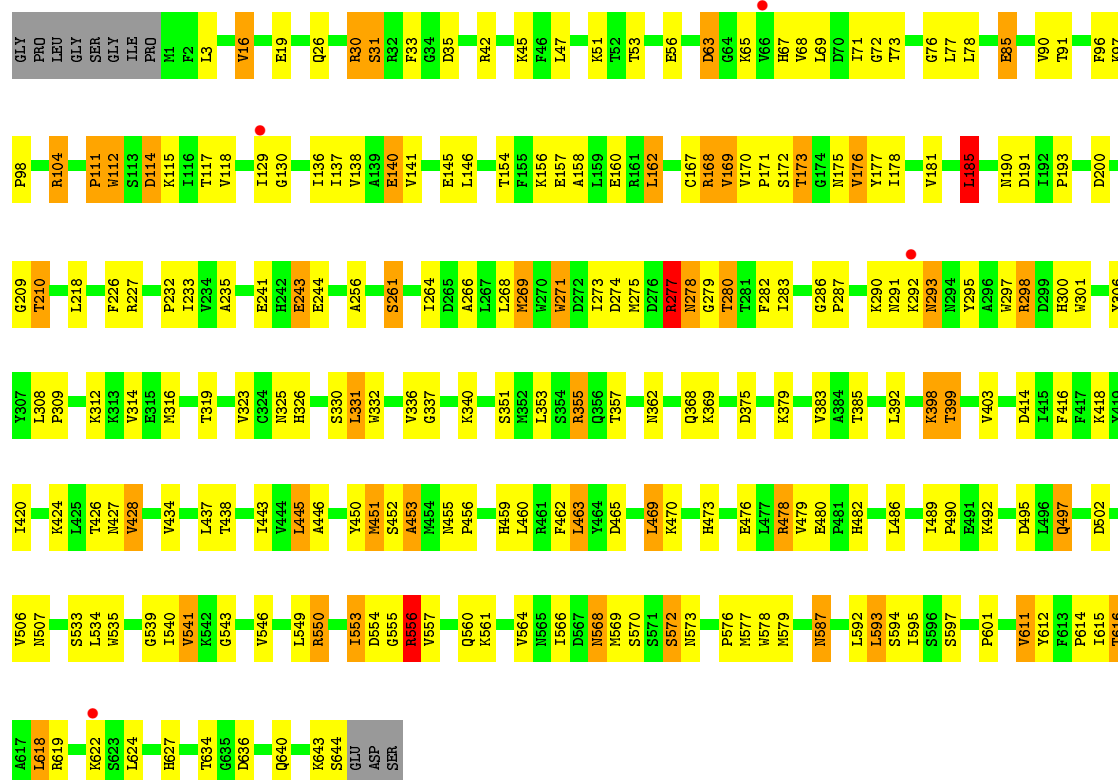
• Molecule 1: Protein arginine N-methyltransferase 7



• Molecule 1: Protein arginine N-methyltransferase 7

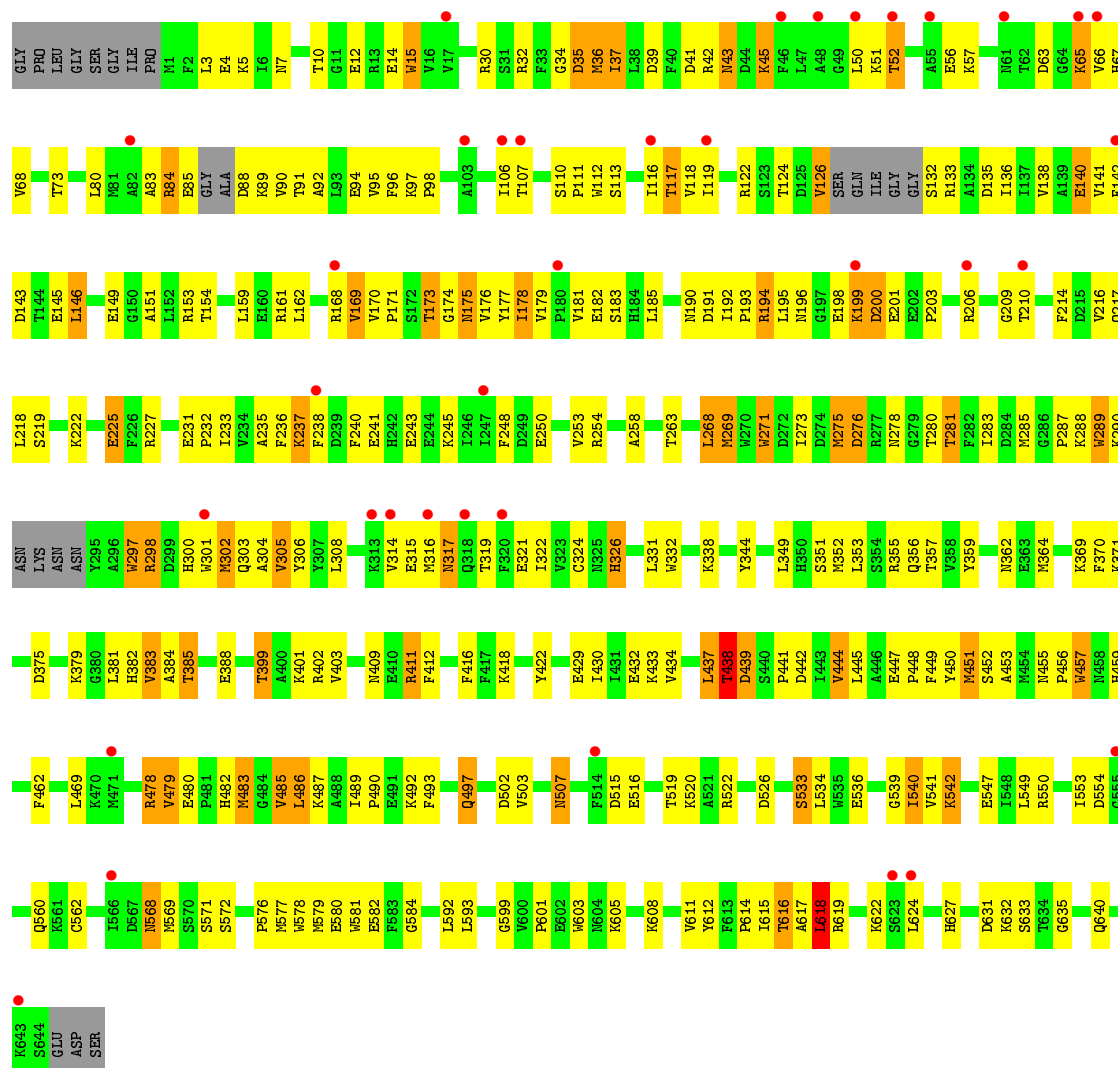


- Molecule 1: Protein arginine N-methyltransferase 7

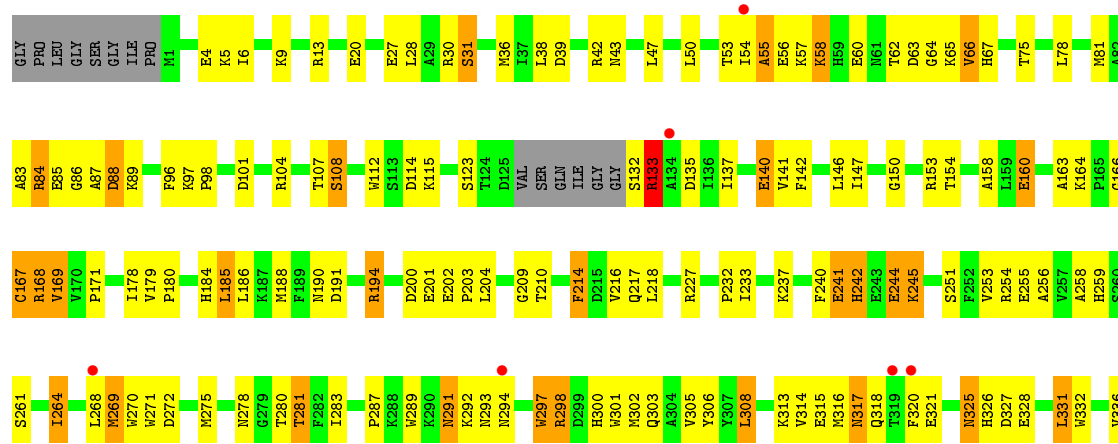


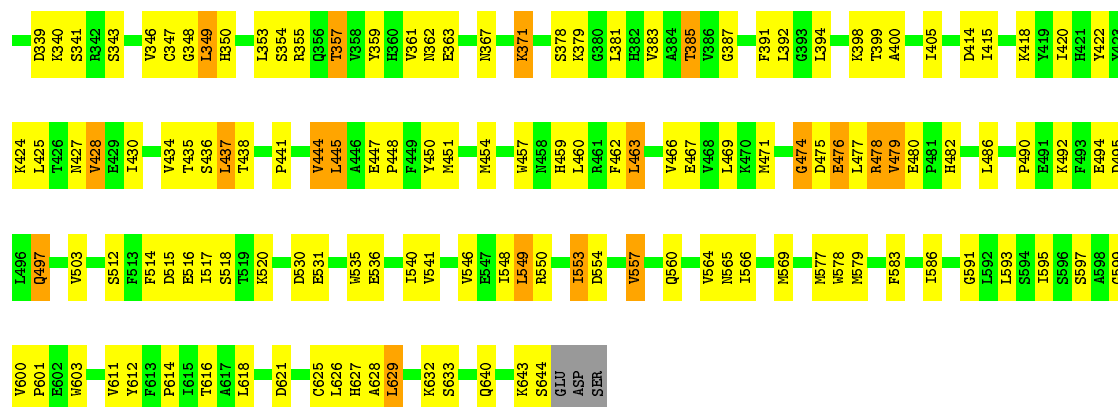
- Molecule 1: Protein arginine N-methyltransferase 7



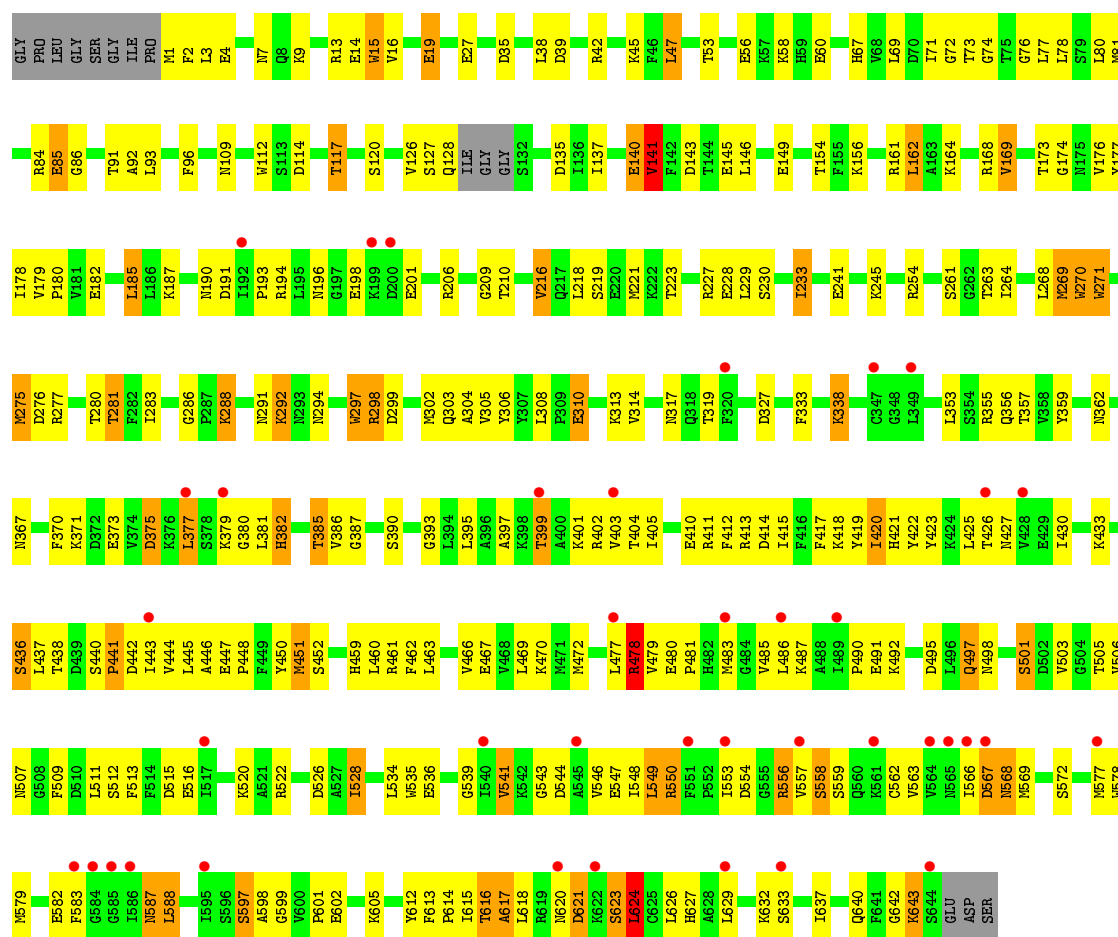


• Molecule 1: Protein arginine N-methyltransferase 7

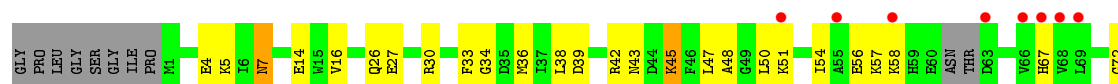


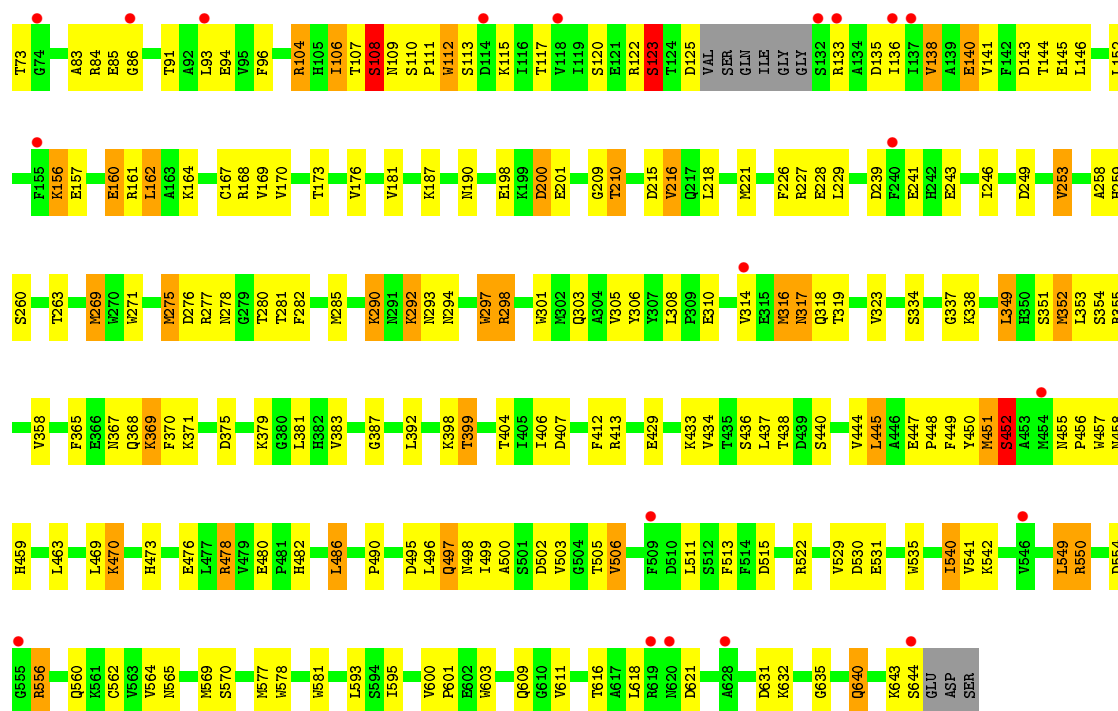


• Molecule 1: Protein arginine N-methyltransferase 7

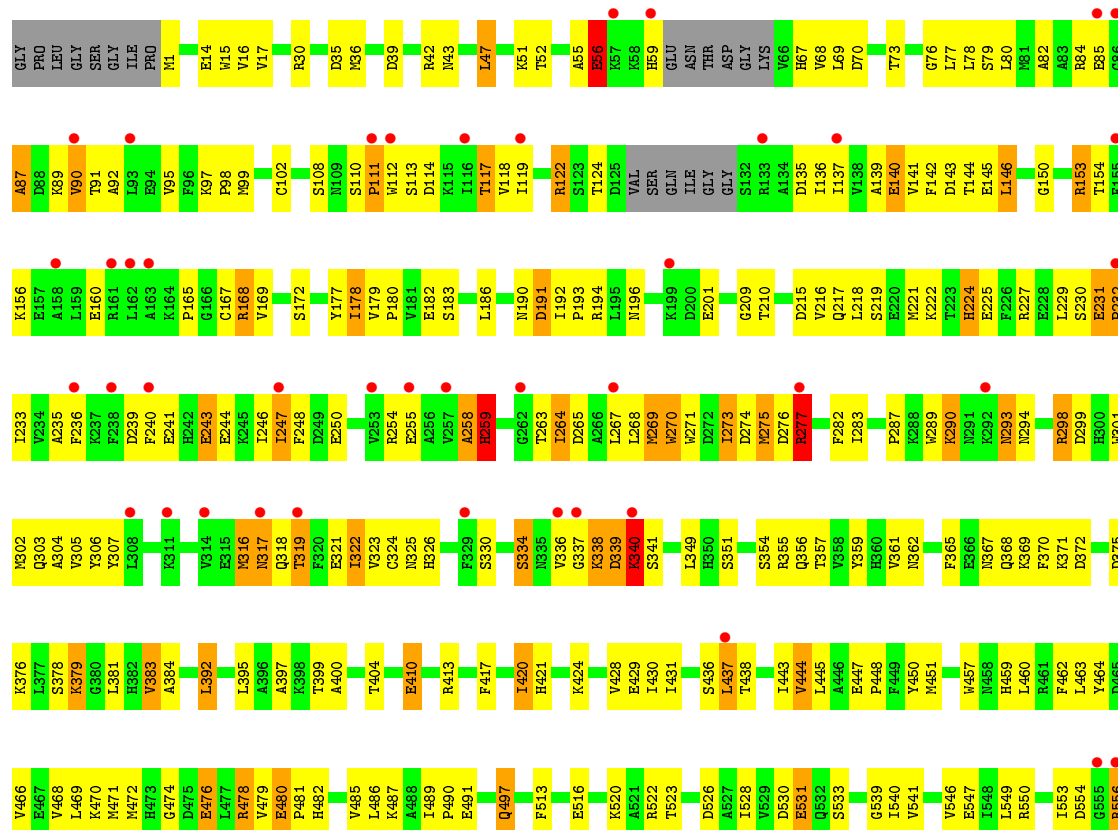


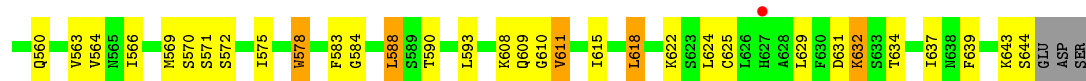
• Molecule 1: Protein arginine N-methyltransferase 7



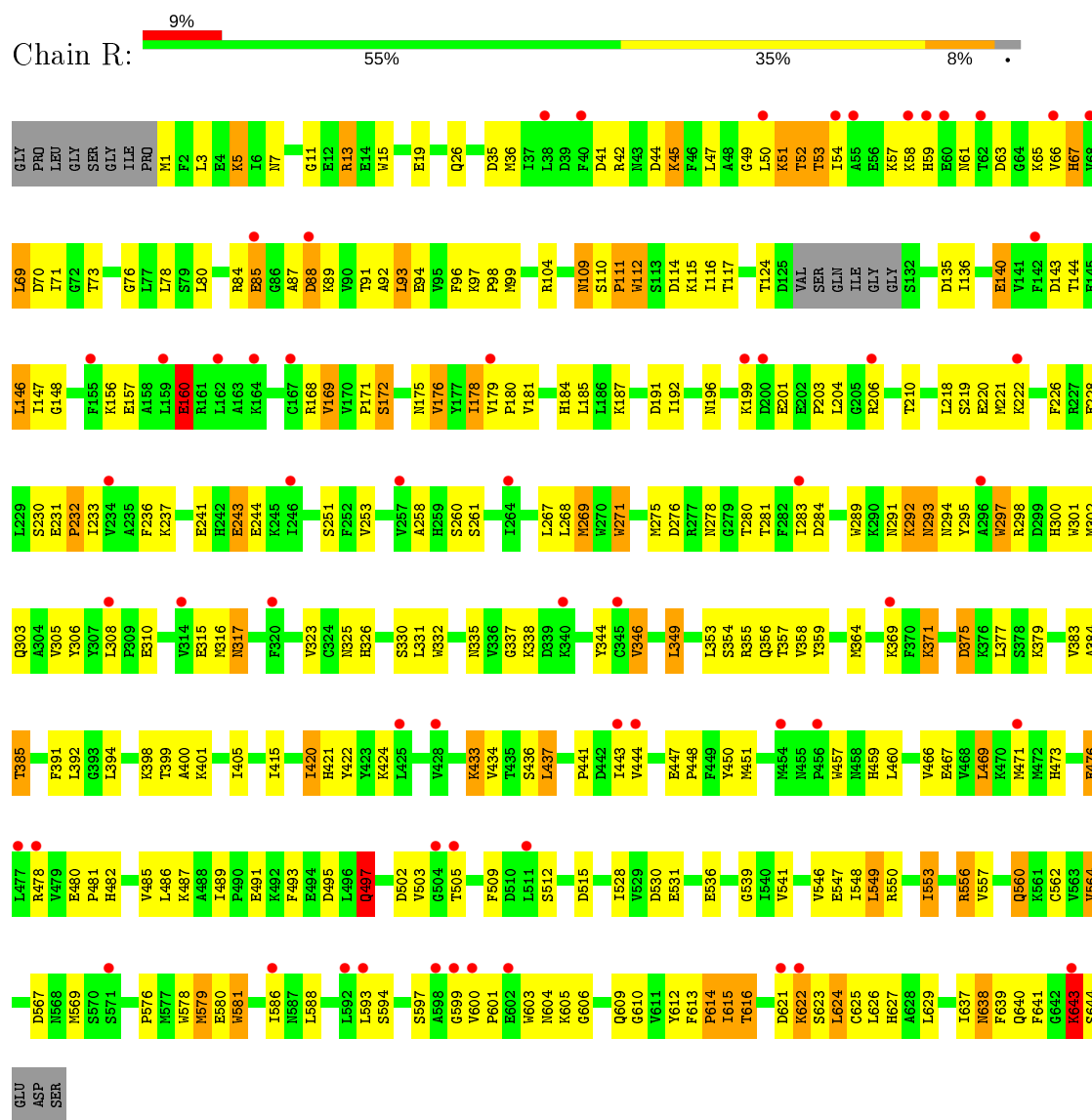


• Molecule 1: Protein arginine N-methyltransferase 7

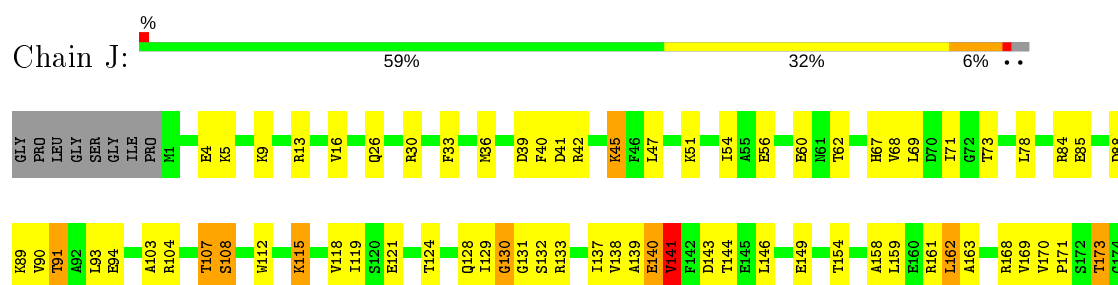


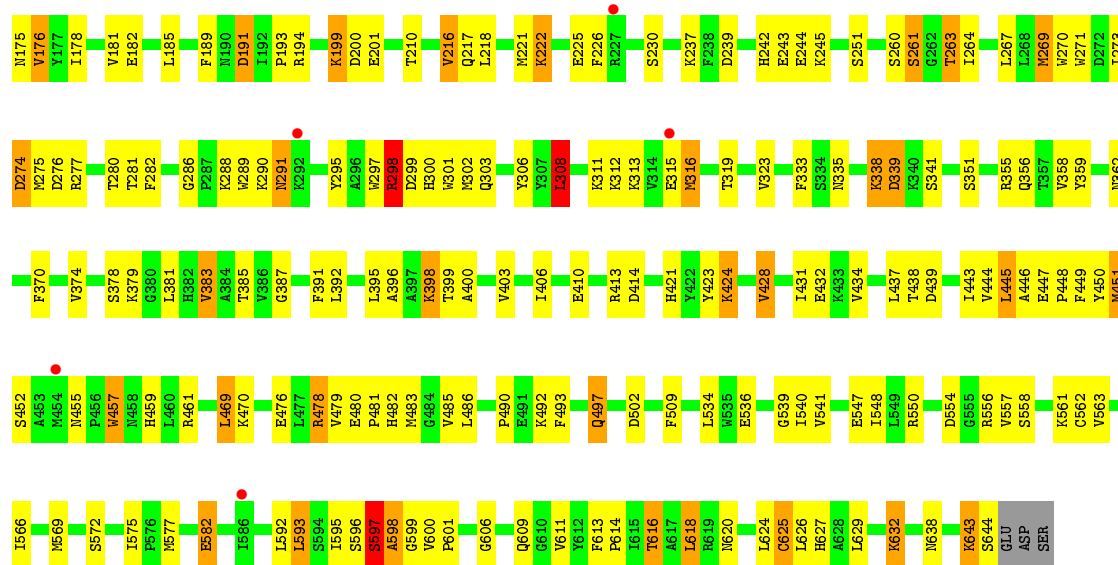


• Molecule 1: Protein arginine N-methyltransferase 7

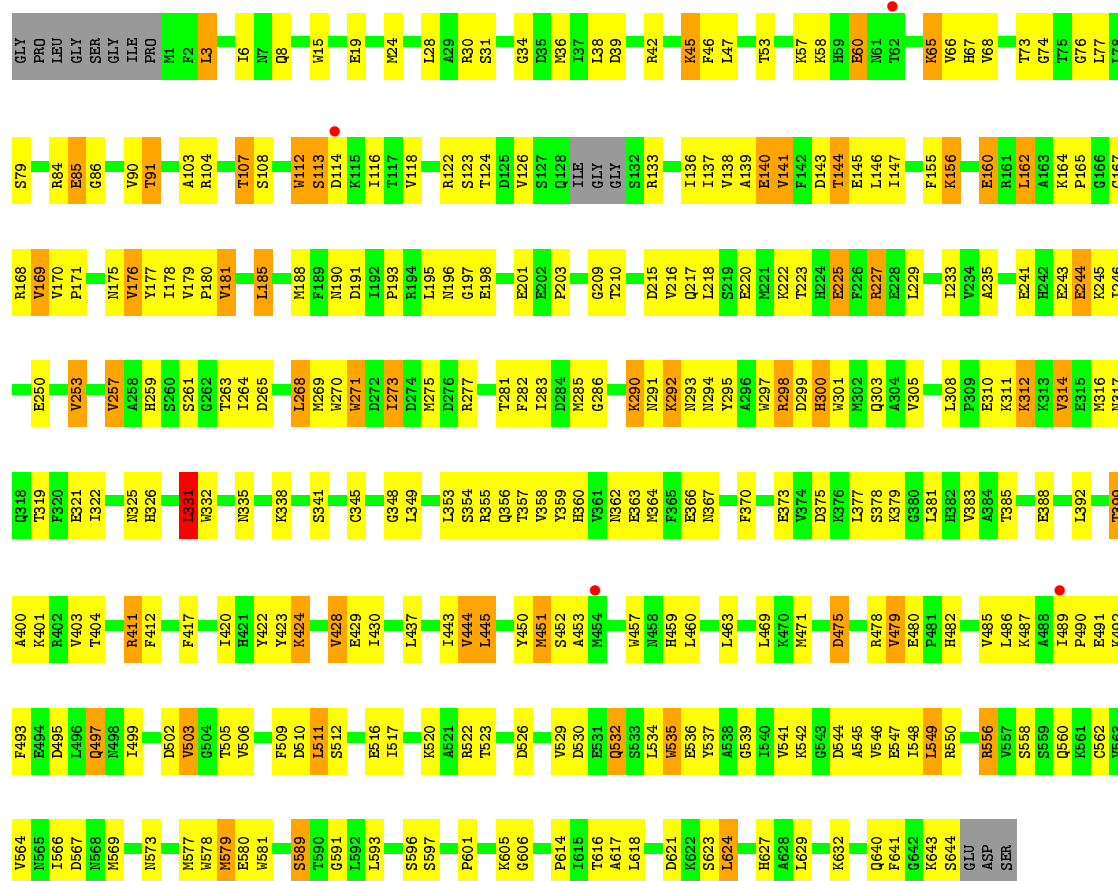


• Molecule 1: Protein arginine N-methyltransferase 7



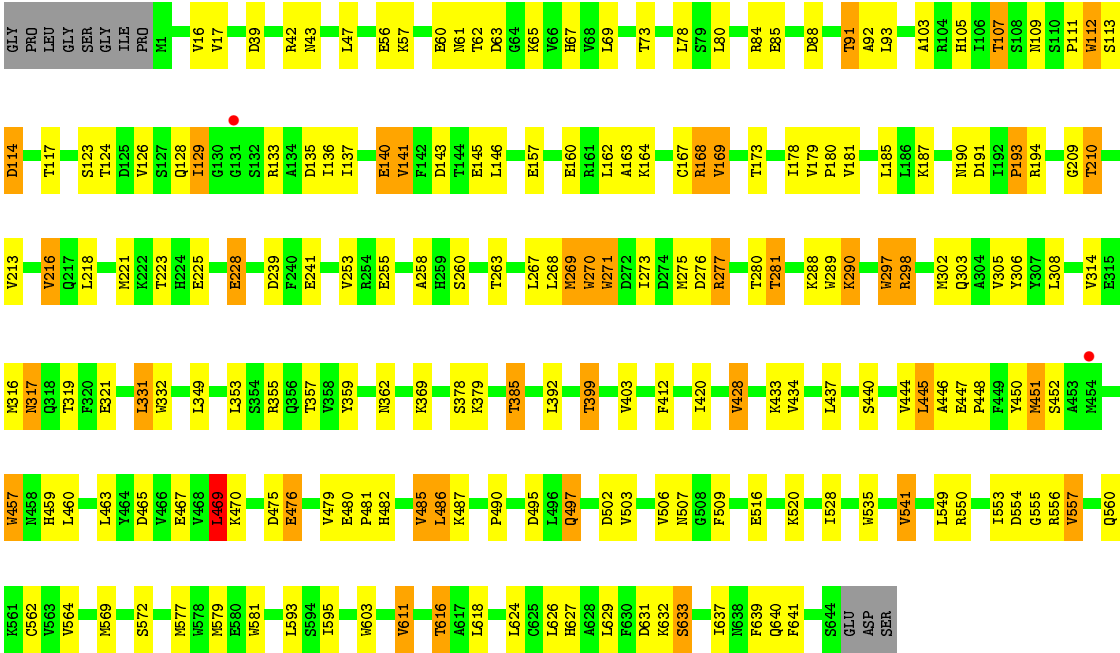


• Molecule 1: Protein arginine N-methyltransferase 7



• Molecule 1: Protein arginine N-methyltransferase 7





4 Data and refinement statistics

| Property | Value | Source |
|---|--|------------------|
| Space group | P 31 | Depositor |
| Cell constants a, b, c, α , β , γ | 190.70Å 190.70Å 373.09Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 47.41 – 2.39 47.41 – 2.39 | Depositor EDS |
| % Data completeness (in resolution range) | 98.9 (47.41-2.39) 98.9 (47.41-2.39) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.12 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.14 (at 2.39Å) | Xtriage |
| Refinement program | REFMAC 5.6.0117 | Depositor |
| R, R_{free} | 0.234 , 0.303 0.233 , 0.302 | Depositor DCC |
| R_{free} test set | 29764 reflections (5.02%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 44.9 | Xtriage |
| Anisotropy | 0.006 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 15.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | 0.019 for -h,-k,l 0.069 for h,-h-k,-l 0.023 for -k,-h,-l | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 92645 | wwPDB-VP |
| Average B, all atoms (Å ²) | 50.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: PO4, SAH

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.85 | 4/5217 (0.1%) | 0.95 | 5/7044 (0.1%) |
| 1 | B | 0.79 | 7/5195 (0.1%) | 0.88 | 0/7014 |
| 1 | C | 0.77 | 2/5202 (0.0%) | 0.88 | 3/7024 (0.0%) |
| 1 | D | 0.81 | 6/5189 (0.1%) | 0.96 | 8/7006 (0.1%) |
| 1 | E | 0.79 | 2/5179 (0.0%) | 0.94 | 3/6990 (0.0%) |
| 1 | F | 0.73 | 4/5195 (0.1%) | 0.88 | 7/7014 (0.1%) |
| 1 | G | 0.77 | 6/5180 (0.1%) | 0.90 | 5/6993 (0.1%) |
| 1 | H | 0.81 | 5/5202 (0.1%) | 0.92 | 3/7024 (0.0%) |
| 1 | I | 0.76 | 4/5234 (0.1%) | 0.86 | 3/7068 (0.0%) |
| 1 | J | 0.74 | 2/5234 (0.0%) | 0.88 | 6/7068 (0.1%) |
| 1 | K | 0.73 | 4/5217 (0.1%) | 0.85 | 5/7044 (0.1%) |
| 1 | L | 0.86 | 9/5234 (0.2%) | 0.99 | 8/7068 (0.1%) |
| 1 | M | 0.70 | 7/5158 (0.1%) | 0.81 | 3/6962 (0.0%) |
| 1 | N | 0.70 | 4/5195 (0.1%) | 0.84 | 4/7014 (0.1%) |
| 1 | O | 0.66 | 5/5217 (0.1%) | 0.78 | 3/7044 (0.0%) |
| 1 | P | 0.74 | 7/5179 (0.1%) | 0.85 | 4/6990 (0.1%) |
| 1 | Q | 0.68 | 5/5149 (0.1%) | 0.81 | 1/6951 (0.0%) |
| 1 | R | 0.65 | 8/5195 (0.2%) | 0.77 | 0/7014 |
| All | All | 0.76 | 91/93571 (0.1%) | 0.88 | 71/126332 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 1 | E | 0 | 2 |
| 1 | H | 0 | 1 |
| 1 | J | 0 | 2 |
| All | All | 0 | 6 |

All (91) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1 | L | 332 | TRP | CD2-CE2 | 7.16 | 1.50 | 1.41 |
| 1 | M | 271 | TRP | CD2-CE2 | 6.90 | 1.49 | 1.41 |
| 1 | L | 297 | TRP | CD2-CE2 | 6.63 | 1.49 | 1.41 |
| 1 | D | 332 | TRP | CD2-CE2 | 6.55 | 1.49 | 1.41 |
| 1 | A | 289 | TRP | CD2-CE2 | 6.37 | 1.49 | 1.41 |
| 1 | H | 332 | TRP | CD2-CE2 | 6.34 | 1.49 | 1.41 |
| 1 | P | 578 | TRP | CD2-CE2 | 6.32 | 1.49 | 1.41 |
| 1 | G | 535 | TRP | CD2-CE2 | 6.27 | 1.48 | 1.41 |
| 1 | A | 535 | TRP | CD2-CE2 | 6.25 | 1.48 | 1.41 |
| 1 | O | 271 | TRP | CD2-CE2 | 6.18 | 1.48 | 1.41 |
| 1 | D | 581 | TRP | CD2-CE2 | 6.16 | 1.48 | 1.41 |
| 1 | M | 581 | TRP | CD2-CE2 | 6.15 | 1.48 | 1.41 |
| 1 | G | 581 | TRP | CD2-CE2 | 6.11 | 1.48 | 1.41 |
| 1 | B | 578 | TRP | CD2-CE2 | 6.10 | 1.48 | 1.41 |
| 1 | G | 457 | TRP | CD2-CE2 | 6.09 | 1.48 | 1.41 |
| 1 | B | 270 | TRP | CD2-CE2 | 6.08 | 1.48 | 1.41 |
| 1 | H | 457 | TRP | CD2-CE2 | 6.04 | 1.48 | 1.41 |
| 1 | E | 289 | TRP | CD2-CE2 | 6.04 | 1.48 | 1.41 |
| 1 | F | 457 | TRP | CD2-CE2 | 6.00 | 1.48 | 1.41 |
| 1 | L | 535 | TRP | CD2-CE2 | 5.99 | 1.48 | 1.41 |
| 1 | J | 457 | TRP | CD2-CE2 | 5.97 | 1.48 | 1.41 |
| 1 | R | 603 | TRP | CD2-CE2 | 5.94 | 1.48 | 1.41 |
| 1 | G | 332 | TRP | CD2-CE2 | 5.93 | 1.48 | 1.41 |
| 1 | K | 332 | TRP | CD2-CE2 | 5.92 | 1.48 | 1.41 |
| 1 | K | 457 | TRP | CD2-CE2 | 5.83 | 1.48 | 1.41 |
| 1 | P | 535 | TRP | CD2-CE2 | 5.79 | 1.48 | 1.41 |
| 1 | Q | 578 | TRP | CD2-CE2 | 5.79 | 1.48 | 1.41 |
| 1 | B | 289 | TRP | CD2-CE2 | 5.79 | 1.48 | 1.41 |
| 1 | B | 332 | TRP | CD2-CE2 | 5.78 | 1.48 | 1.41 |
| 1 | D | 289 | TRP | CD2-CE2 | 5.76 | 1.48 | 1.41 |
| 1 | P | 457 | TRP | CD2-CE2 | 5.74 | 1.48 | 1.41 |
| 1 | N | 270 | TRP | CD2-CE2 | 5.73 | 1.48 | 1.41 |
| 1 | N | 603 | TRP | CD2-CE2 | 5.68 | 1.48 | 1.41 |
| 1 | P | 603 | TRP | CD2-CE2 | 5.65 | 1.48 | 1.41 |
| 1 | L | 112 | TRP | CD2-CE2 | 5.65 | 1.48 | 1.41 |
| 1 | M | 457 | TRP | CD2-CE2 | 5.64 | 1.48 | 1.41 |
| 1 | N | 457 | TRP | CD2-CE2 | 5.62 | 1.48 | 1.41 |
| 1 | L | 289 | TRP | CD2-CE2 | 5.60 | 1.48 | 1.41 |
| 1 | R | 581 | TRP | CD2-CE2 | 5.57 | 1.48 | 1.41 |
| 1 | K | 581 | TRP | CD2-CE2 | 5.56 | 1.48 | 1.41 |
| 1 | F | 332 | TRP | CD2-CE2 | 5.55 | 1.48 | 1.41 |
| 1 | Q | 270 | TRP | CD2-CE2 | 5.53 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1 | A | 15 | TRP | CD2-CE2 | 5.53 | 1.48 | 1.41 |
| 1 | N | 297 | TRP | CD2-CE2 | 5.51 | 1.48 | 1.41 |
| 1 | B | 535 | TRP | CD2-CE2 | 5.49 | 1.48 | 1.41 |
| 1 | I | 332 | TRP | CD2-CE2 | 5.47 | 1.48 | 1.41 |
| 1 | P | 297 | TRP | CD2-CE2 | 5.45 | 1.47 | 1.41 |
| 1 | B | 457 | TRP | CD2-CE2 | 5.45 | 1.47 | 1.41 |
| 1 | P | 301 | TRP | CD2-CE2 | 5.44 | 1.47 | 1.41 |
| 1 | R | 457 | TRP | CD2-CE2 | 5.44 | 1.47 | 1.41 |
| 1 | I | 112 | TRP | CD2-CE2 | 5.38 | 1.47 | 1.41 |
| 1 | Q | 301 | TRP | CD2-CE2 | 5.38 | 1.47 | 1.41 |
| 1 | M | 297 | TRP | CD2-CE2 | 5.36 | 1.47 | 1.41 |
| 1 | H | 301 | TRP | CD2-CE2 | 5.34 | 1.47 | 1.41 |
| 1 | R | 112 | TRP | CD2-CE2 | 5.34 | 1.47 | 1.41 |
| 1 | L | 271 | TRP | CD2-CE2 | 5.34 | 1.47 | 1.41 |
| 1 | G | 112 | TRP | CD2-CE2 | 5.33 | 1.47 | 1.41 |
| 1 | M | 603 | TRP | CD2-CE2 | 5.33 | 1.47 | 1.41 |
| 1 | H | 581 | TRP | CD2-CE2 | 5.32 | 1.47 | 1.41 |
| 1 | G | 15 | TRP | CD2-CE2 | 5.31 | 1.47 | 1.41 |
| 1 | P | 581 | TRP | CD2-CE2 | 5.31 | 1.47 | 1.41 |
| 1 | A | 112 | TRP | CD2-CE2 | 5.30 | 1.47 | 1.41 |
| 1 | Q | 15 | TRP | CD2-CE2 | 5.29 | 1.47 | 1.41 |
| 1 | Q | 457 | TRP | CD2-CE2 | 5.28 | 1.47 | 1.41 |
| 1 | F | 271 | TRP | CD2-CE2 | 5.28 | 1.47 | 1.41 |
| 1 | O | 297 | TRP | CD2-CE2 | 5.23 | 1.47 | 1.41 |
| 1 | D | 271 | TRP | CD2-CE2 | 5.22 | 1.47 | 1.41 |
| 1 | I | 535 | TRP | CD2-CE2 | 5.22 | 1.47 | 1.41 |
| 1 | E | 112 | TRP | CD2-CE2 | 5.21 | 1.47 | 1.41 |
| 1 | R | 289 | TRP | CD2-CE2 | 5.21 | 1.47 | 1.41 |
| 1 | M | 332 | TRP | CD2-CE2 | 5.21 | 1.47 | 1.41 |
| 1 | K | 271 | TRP | CD2-CE2 | 5.18 | 1.47 | 1.41 |
| 1 | R | 271 | TRP | CD2-CE2 | 5.18 | 1.47 | 1.41 |
| 1 | I | 271 | TRP | CD2-CE2 | 5.16 | 1.47 | 1.41 |
| 1 | O | 15 | TRP | CD2-CE2 | 5.16 | 1.47 | 1.41 |
| 1 | J | 271 | TRP | CD2-CE2 | 5.16 | 1.47 | 1.41 |
| 1 | R | 297 | TRP | CD2-CE2 | 5.15 | 1.47 | 1.41 |
| 1 | M | 15 | TRP | CD2-CE2 | 5.15 | 1.47 | 1.41 |
| 1 | H | 289 | TRP | CD2-CE2 | 5.13 | 1.47 | 1.41 |
| 1 | C | 297 | TRP | CD2-CE2 | 5.13 | 1.47 | 1.41 |
| 1 | C | 581 | TRP | CD2-CE2 | 5.12 | 1.47 | 1.41 |
| 1 | F | 289 | TRP | CD2-CE2 | 5.12 | 1.47 | 1.41 |
| 1 | L | 457 | TRP | CD2-CE2 | 5.12 | 1.47 | 1.41 |
| 1 | O | 270 | TRP | CD2-CE2 | 5.09 | 1.47 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1 | D | 112 | TRP | CD2-CE2 | 5.09 | 1.47 | 1.41 |
| 1 | L | 603 | TRP | CD2-CE2 | 5.07 | 1.47 | 1.41 |
| 1 | O | 578 | TRP | CD2-CE2 | 5.05 | 1.47 | 1.41 |
| 1 | L | 270 | TRP | CD2-CE2 | 5.05 | 1.47 | 1.41 |
| 1 | B | 297 | TRP | CD2-CE2 | 5.04 | 1.47 | 1.41 |
| 1 | D | 457 | TRP | CD2-CE2 | 5.03 | 1.47 | 1.41 |
| 1 | R | 332 | TRP | CD2-CE2 | 5.03 | 1.47 | 1.41 |

All (71) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | L | 277 | ARG | NE-CZ-NH2 | -9.40 | 115.60 | 120.30 |
| 1 | F | 331 | LEU | CA-CB-CG | 9.32 | 136.75 | 115.30 |
| 1 | L | 611 | VAL | CB-CA-C | -8.32 | 95.60 | 111.40 |
| 1 | L | 277 | ARG | NE-CZ-NH1 | 8.29 | 124.45 | 120.30 |
| 1 | D | 611 | VAL | CB-CA-C | -7.93 | 96.34 | 111.40 |
| 1 | K | 331 | LEU | CA-CB-CG | 7.65 | 132.90 | 115.30 |
| 1 | Q | 611 | VAL | CB-CA-C | -7.34 | 97.45 | 111.40 |
| 1 | J | 298 | ARG | NE-CZ-NH2 | -7.28 | 116.66 | 120.30 |
| 1 | E | 579 | MET | CG-SD-CE | -7.25 | 88.59 | 100.20 |
| 1 | C | 437 | LEU | CA-CB-CG | 7.22 | 131.91 | 115.30 |
| 1 | N | 241 | GLU | N-CA-C | 7.17 | 130.36 | 111.00 |
| 1 | H | 611 | VAL | CB-CA-C | -6.76 | 98.55 | 111.40 |
| 1 | H | 241 | GLU | C-N-CA | 6.58 | 138.16 | 121.70 |
| 1 | O | 624 | LEU | CA-CB-CG | 6.50 | 130.24 | 115.30 |
| 1 | A | 298 | ARG | NE-CZ-NH2 | -6.18 | 117.21 | 120.30 |
| 1 | L | 554 | ASP | CB-CA-C | -6.05 | 98.30 | 110.40 |
| 1 | D | 579 | MET | CG-SD-CE | -6.05 | 90.52 | 100.20 |
| 1 | F | 215 | ASP | CB-CG-OD2 | -5.99 | 112.91 | 118.30 |
| 1 | K | 549 | LEU | CA-CB-CG | 5.99 | 129.08 | 115.30 |
| 1 | F | 331 | LEU | CB-CG-CD1 | 5.91 | 121.05 | 111.00 |
| 1 | L | 469 | LEU | CA-CB-CG | 5.88 | 128.81 | 115.30 |
| 1 | P | 215 | ASP | CB-CG-OD1 | 5.87 | 123.58 | 118.30 |
| 1 | P | 486 | LEU | CA-CB-CG | 5.83 | 128.70 | 115.30 |
| 1 | J | 162 | LEU | CA-CB-CG | 5.76 | 128.54 | 115.30 |
| 1 | I | 185 | LEU | CA-CB-CG | 5.66 | 128.31 | 115.30 |
| 1 | M | 84 | ARG | NE-CZ-NH2 | -5.62 | 117.49 | 120.30 |
| 1 | I | 611 | VAL | CB-CA-C | -5.60 | 100.76 | 111.40 |
| 1 | G | 486 | LEU | CA-CB-CG | 5.60 | 128.17 | 115.30 |
| 1 | G | 469 | LEU | CA-CB-CG | 5.59 | 128.17 | 115.30 |
| 1 | G | 611 | VAL | CB-CA-C | -5.59 | 100.77 | 111.40 |
| 1 | G | 631 | ASP | CB-CG-OD1 | 5.59 | 123.33 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | N | 185 | LEU | CA-CB-CG | 5.56 | 128.09 | 115.30 |
| 1 | A | 86 | GLY | N-CA-C | 5.55 | 126.97 | 113.10 |
| 1 | D | 308 | LEU | CB-CG-CD1 | 5.55 | 120.43 | 111.00 |
| 1 | C | 486 | LEU | CA-CB-CG | 5.52 | 128.00 | 115.30 |
| 1 | H | 241 | GLU | CA-C-N | 5.52 | 129.34 | 117.20 |
| 1 | E | 145 | GLU | C-N-CA | 5.47 | 135.37 | 121.70 |
| 1 | N | 629 | LEU | CA-CB-CG | 5.44 | 127.81 | 115.30 |
| 1 | J | 298 | ARG | NE-CZ-NH1 | 5.43 | 123.01 | 120.30 |
| 1 | M | 84 | ARG | NE-CZ-NH1 | 5.42 | 123.01 | 120.30 |
| 1 | A | 549 | LEU | CA-CB-CG | 5.42 | 127.75 | 115.30 |
| 1 | D | 162 | LEU | CA-CB-CG | 5.40 | 127.72 | 115.30 |
| 1 | D | 208 | SER | CB-CA-C | -5.40 | 99.84 | 110.10 |
| 1 | K | 215 | ASP | CB-CG-OD1 | 5.37 | 123.14 | 118.30 |
| 1 | L | 486 | LEU | CB-CG-CD2 | 5.34 | 120.08 | 111.00 |
| 1 | F | 611 | VAL | CB-CA-C | -5.32 | 101.29 | 111.40 |
| 1 | D | 618 | LEU | CB-CG-CD1 | 5.31 | 120.03 | 111.00 |
| 1 | J | 274 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 1 | K | 411 | ARG | NE-CZ-NH2 | -5.30 | 117.65 | 120.30 |
| 1 | F | 70 | ASP | CB-CG-OD1 | 5.29 | 123.06 | 118.30 |
| 1 | L | 331 | LEU | CA-CB-CG | 5.28 | 127.44 | 115.30 |
| 1 | D | 298 | ARG | NE-CZ-NH2 | -5.27 | 117.66 | 120.30 |
| 1 | A | 47 | LEU | CA-CB-CG | 5.26 | 127.41 | 115.30 |
| 1 | D | 478 | ARG | NE-CZ-NH2 | 5.26 | 122.93 | 120.30 |
| 1 | C | 331 | LEU | CA-CB-CG | 5.26 | 127.40 | 115.30 |
| 1 | O | 327 | ASP | CB-CG-OD1 | 5.24 | 123.01 | 118.30 |
| 1 | G | 207 | CYS | N-CA-C | -5.22 | 96.90 | 111.00 |
| 1 | N | 579 | MET | CG-SD-CE | -5.20 | 91.88 | 100.20 |
| 1 | J | 308 | LEU | CA-CB-CG | 5.19 | 127.24 | 115.30 |
| 1 | A | 249 | ASP | CB-CG-OD2 | 5.17 | 122.95 | 118.30 |
| 1 | K | 411 | ARG | NE-CZ-NH1 | 5.16 | 122.88 | 120.30 |
| 1 | F | 215 | ASP | CB-CG-OD1 | 5.15 | 122.93 | 118.30 |
| 1 | L | 476 | GLU | CB-CA-C | -5.13 | 100.13 | 110.40 |
| 1 | J | 387 | GLY | N-CA-C | -5.13 | 100.28 | 113.10 |
| 1 | F | 272 | ASP | CB-CG-OD1 | 5.11 | 122.90 | 118.30 |
| 1 | I | 465 | ASP | CB-CG-OD2 | 5.06 | 122.85 | 118.30 |
| 1 | E | 375 | ASP | CB-CG-OD2 | 5.05 | 122.85 | 118.30 |
| 1 | M | 618 | LEU | CA-CB-CG | 5.05 | 126.91 | 115.30 |
| 1 | P | 145 | GLU | C-N-CA | 5.02 | 134.25 | 121.70 |
| 1 | P | 162 | LEU | CA-CB-CG | 5.01 | 126.83 | 115.30 |
| 1 | O | 162 | LEU | CA-CB-CG | 5.01 | 126.81 | 115.30 |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 85 | GLU | Peptide |
| 1 | E | 282 | PHE | Peptide |
| 1 | E | 316 | MET | Peptide |
| 1 | H | 282 | PHE | Peptide |
| 1 | J | 291 | ASN | Peptide |
| 1 | J | 597 | SER | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 5106 | 0 | 4989 | 129 | 0 |
| 1 | B | 5084 | 0 | 4967 | 174 | 0 |
| 1 | C | 5091 | 0 | 4976 | 158 | 1 |
| 1 | D | 5078 | 0 | 4962 | 138 | 1 |
| 1 | E | 5069 | 0 | 4953 | 160 | 0 |
| 1 | F | 5084 | 0 | 4967 | 153 | 0 |
| 1 | G | 5070 | 0 | 4955 | 145 | 0 |
| 1 | H | 5091 | 0 | 4976 | 136 | 0 |
| 1 | I | 5122 | 0 | 5007 | 173 | 0 |
| 1 | J | 5122 | 0 | 5007 | 184 | 0 |
| 1 | K | 5106 | 0 | 4989 | 212 | 0 |
| 1 | L | 5122 | 0 | 5007 | 136 | 0 |
| 1 | M | 5049 | 0 | 4935 | 270 | 0 |
| 1 | N | 5084 | 0 | 4967 | 225 | 1 |
| 1 | O | 5106 | 0 | 4989 | 214 | 0 |
| 1 | P | 5069 | 0 | 4953 | 158 | 1 |
| 1 | Q | 5039 | 0 | 4927 | 233 | 0 |
| 1 | R | 5084 | 0 | 4967 | 202 | 0 |
| 2 | A | 26 | 0 | 19 | 0 | 0 |
| 2 | B | 26 | 0 | 19 | 2 | 0 |
| 2 | C | 26 | 0 | 19 | 1 | 0 |
| 2 | D | 26 | 0 | 19 | 0 | 0 |
| 2 | E | 26 | 0 | 19 | 3 | 0 |
| 2 | F | 26 | 0 | 19 | 2 | 0 |
| 2 | G | 26 | 0 | 19 | 2 | 0 |
| 2 | H | 26 | 0 | 19 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | I | 26 | 0 | 19 | 1 | 0 |
| 2 | J | 26 | 0 | 19 | 0 | 0 |
| 2 | K | 26 | 0 | 19 | 3 | 0 |
| 2 | L | 26 | 0 | 19 | 0 | 0 |
| 2 | M | 26 | 0 | 19 | 2 | 0 |
| 2 | N | 26 | 0 | 19 | 1 | 0 |
| 2 | O | 26 | 0 | 19 | 0 | 0 |
| 2 | P | 26 | 0 | 19 | 3 | 0 |
| 2 | Q | 26 | 0 | 19 | 1 | 0 |
| 2 | R | 26 | 0 | 19 | 1 | 0 |
| 3 | A | 5 | 0 | 0 | 0 | 0 |
| 3 | B | 5 | 0 | 0 | 0 | 0 |
| 3 | C | 5 | 0 | 0 | 0 | 0 |
| 3 | D | 5 | 0 | 0 | 0 | 0 |
| 3 | E | 5 | 0 | 0 | 0 | 0 |
| 3 | F | 5 | 0 | 0 | 0 | 0 |
| 3 | G | 5 | 0 | 0 | 0 | 0 |
| 3 | H | 5 | 0 | 0 | 0 | 0 |
| 3 | I | 5 | 0 | 0 | 1 | 0 |
| 3 | J | 5 | 0 | 0 | 0 | 0 |
| 3 | K | 5 | 0 | 0 | 0 | 0 |
| 3 | L | 5 | 0 | 0 | 0 | 0 |
| 3 | M | 5 | 0 | 0 | 0 | 0 |
| 3 | N | 5 | 0 | 0 | 0 | 0 |
| 3 | O | 5 | 0 | 0 | 0 | 0 |
| 3 | P | 5 | 0 | 0 | 0 | 0 |
| 3 | Q | 5 | 0 | 0 | 1 | 0 |
| 3 | R | 5 | 0 | 0 | 0 | 0 |
| 4 | A | 105 | 0 | 0 | 0 | 0 |
| 4 | B | 26 | 0 | 0 | 0 | 0 |
| 4 | C | 16 | 0 | 0 | 1 | 0 |
| 4 | D | 93 | 0 | 0 | 3 | 0 |
| 4 | E | 41 | 0 | 0 | 0 | 0 |
| 4 | F | 12 | 0 | 0 | 1 | 0 |
| 4 | G | 19 | 0 | 0 | 1 | 0 |
| 4 | H | 59 | 0 | 0 | 1 | 0 |
| 4 | I | 21 | 0 | 0 | 3 | 0 |
| 4 | J | 12 | 0 | 0 | 1 | 0 |
| 4 | K | 6 | 0 | 0 | 0 | 0 |
| 4 | L | 85 | 0 | 0 | 4 | 0 |
| 4 | M | 2 | 0 | 0 | 2 | 0 |
| 4 | P | 10 | 0 | 0 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | Q | 2 | 0 | 0 | 0 | 0 |
| 4 | R | 2 | 0 | 0 | 0 | 0 |
| All | All | 92645 | 0 | 89835 | 3158 | 2 |

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 17.

All (3158) 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:L:490:PRO:HB3 | 1:L:569:MET:CE | 1.55 | 1.36 |
| 1:G:490:PRO:HB3 | 1:G:569:MET:CE | 1.58 | 1.32 |
| 1:F:490:PRO:HB3 | 1:F:569:MET:CE | 1.60 | 1.28 |
| 1:M:569:MET:HG3 | 1:M:624:LEU:CD1 | 1.67 | 1.23 |
| 1:B:490:PRO:HB3 | 1:B:569:MET:CE | 1.71 | 1.20 |
| 1:D:497:GLN:NE2 | 1:D:497:GLN:H | 1.42 | 1.18 |
| 1:N:379:LYS:HA | 1:N:399:THR:HG22 | 1.28 | 1.16 |
| 1:A:490:PRO:HB3 | 1:A:569:MET:CE | 1.76 | 1.16 |
| 1:E:478:ARG:HH21 | 1:E:478:ARG:HG2 | 0.99 | 1.15 |
| 1:Q:375:ASP:HA | 1:Q:399:THR:HG21 | 1.28 | 1.14 |
| 1:O:393:GLY:HA3 | 1:O:405:ILE:CD1 | 1.77 | 1.13 |
| 1:Q:153:ARG:HG3 | 1:Q:153:ARG:HH11 | 1.04 | 1.12 |
| 1:Q:218:LEU:H | 1:Q:303:GLN:NE2 | 1.44 | 1.12 |
| 1:J:597:SER:HB2 | 1:J:598:ALA:HB2 | 1.32 | 1.12 |
| 1:O:627:HIS:HB2 | 1:O:640:GLN:HB2 | 1.13 | 1.11 |
| 1:H:490:PRO:HB3 | 1:H:569:MET:CE | 1.81 | 1.11 |
| 1:L:67:HIS:CE1 | 1:L:91:THR:HG23 | 1.86 | 1.11 |
| 1:F:218:LEU:H | 1:F:303:GLN:NE2 | 1.49 | 1.10 |
| 1:Q:68:VAL:HG13 | 1:Q:90:VAL:HG13 | 1.30 | 1.10 |
| 1:C:490:PRO:HB3 | 1:C:569:MET:CE | 1.82 | 1.10 |
| 1:H:490:PRO:HB3 | 1:H:569:MET:HE2 | 1.30 | 1.10 |
| 1:J:490:PRO:HB3 | 1:J:569:MET:HE3 | 1.24 | 1.09 |
| 1:F:50:LEU:O | 1:F:54:ILE:HD12 | 1.52 | 1.09 |
| 1:K:67:HIS:CE1 | 1:K:91:THR:HG22 | 1.85 | 1.09 |
| 1:L:490:PRO:HB3 | 1:L:569:MET:HE1 | 1.27 | 1.08 |
| 1:L:67:HIS:HE1 | 1:L:91:THR:HG23 | 0.96 | 1.08 |
| 1:M:280:THR:HG23 | 1:M:281:THR:HG22 | 1.35 | 1.08 |
| 1:C:169:VAL:HG22 | 1:C:241:GLU:HG2 | 1.14 | 1.08 |
| 1:I:26:GLN:HG2 | 1:I:30:ARG:HH12 | 1.12 | 1.08 |
| 1:J:490:PRO:HB3 | 1:J:569:MET:CE | 1.84 | 1.08 |
| 1:G:169:VAL:HG12 | 1:G:241:GLU:HG3 | 1.25 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:490:PRO:HB3 | 1:A:569:MET:HE2 | 1.36 | 1.08 |
| 1:Q:264:ILE:HG12 | 1:Q:264:ILE:O | 1.44 | 1.07 |
| 1:R:433:LYS:HE2 | 1:R:433:LYS:H | 1.20 | 1.06 |
| 1:M:569:MET:HG3 | 1:M:624:LEU:HD12 | 1.32 | 1.06 |
| 1:N:54:ILE:CA | 1:N:58:LYS:HZ3 | 1.69 | 1.06 |
| 1:O:227:ARG:NH2 | 1:O:261:SER:O | 1.88 | 1.06 |
| 1:M:91:THR:HG22 | 1:M:117:THR:HG23 | 1.32 | 1.05 |
| 1:K:67:HIS:HE1 | 1:K:91:THR:HG22 | 0.94 | 1.05 |
| 1:Q:39:ASP:OD2 | 1:Q:298:ARG:HD3 | 1.56 | 1.05 |
| 1:C:168:ARG:HG2 | 1:C:168:ARG:HH11 | 0.90 | 1.05 |
| 1:H:273:ILE:HG13 | 1:H:275:MET:HE3 | 1.39 | 1.04 |
| 1:A:168:ARG:HG2 | 1:A:168:ARG:HH11 | 0.89 | 1.03 |
| 1:G:490:PRO:HB3 | 1:G:569:MET:HE3 | 1.36 | 1.03 |
| 1:N:55:ALA:N | 1:N:58:LYS:HZ2 | 1.54 | 1.03 |
| 1:K:67:HIS:HE1 | 1:K:91:THR:CG2 | 1.69 | 1.03 |
| 1:I:51:LYS:HE2 | 1:I:85:GLU:OE2 | 1.56 | 1.03 |
| 1:N:269:MET:HG2 | 1:N:306:TYR:HE1 | 1.24 | 1.03 |
| 1:Q:168:ARG:HH11 | 1:Q:168:ARG:HG2 | 1.24 | 1.03 |
| 1:M:478:ARG:HG2 | 1:M:478:ARG:HH21 | 1.20 | 1.03 |
| 1:N:444:VAL:HG13 | 1:N:479:VAL:HB | 1.40 | 1.03 |
| 1:A:103:ALA:O | 1:A:107:THR:HB | 1.57 | 1.02 |
| 1:N:54:ILE:HA | 1:N:58:LYS:NZ | 1.75 | 1.02 |
| 1:C:450:TYR:H | 1:C:459:HIS:HD2 | 1.08 | 1.02 |
| 1:N:54:ILE:HA | 1:N:58:LYS:HZ3 | 0.87 | 1.02 |
| 1:I:210:THR:HG21 | 4:I:809:HOH:O | 1.60 | 1.02 |
| 1:N:63:ASP:HB2 | 1:N:65:LYS:H | 1.23 | 1.02 |
| 1:D:490:PRO:HB3 | 1:D:569:MET:HE3 | 1.37 | 1.02 |
| 1:H:547:GLU:OE2 | 1:H:550:ARG:NH1 | 1.92 | 1.01 |
| 1:I:497:GLN:HE21 | 1:I:497:GLN:N | 1.56 | 1.01 |
| 1:G:490:PRO:CB | 1:G:569:MET:CE | 2.38 | 1.01 |
| 1:F:490:PRO:HB3 | 1:F:569:MET:HE1 | 1.38 | 1.01 |
| 1:A:420:ILE:HD11 | 1:A:428:VAL:HG22 | 1.43 | 1.01 |
| 1:B:490:PRO:HB3 | 1:B:569:MET:HE1 | 1.42 | 1.00 |
| 1:C:168:ARG:HG2 | 1:C:168:ARG:NH1 | 1.72 | 1.00 |
| 1:I:67:HIS:HE1 | 1:I:91:THR:HG23 | 1.26 | 1.00 |
| 1:P:241:GLU:HG3 | 1:P:277:ARG:HH21 | 1.26 | 1.00 |
| 1:J:490:PRO:CB | 1:J:569:MET:CE | 2.39 | 1.00 |
| 1:Q:137:ILE:HG13 | 1:Q:169:VAL:HG12 | 1.44 | 1.00 |
| 1:K:68:VAL:HG22 | 1:K:136:ILE:HB | 1.43 | 0.99 |
| 1:O:393:GLY:HA3 | 1:O:405:ILE:HD11 | 1.03 | 0.99 |
| 1:A:478:ARG:HH21 | 1:A:478:ARG:HG2 | 1.26 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:39:ASP:OD2 | 1:J:298:ARG:HD3 | 1.61 | 0.98 |
| 1:H:497:GLN:NE2 | 1:H:497:GLN:H | 1.60 | 0.98 |
| 1:H:478:ARG:HH21 | 1:H:478:ARG:HG2 | 1.29 | 0.98 |
| 1:F:490:PRO:HB3 | 1:F:569:MET:HE3 | 1.44 | 0.98 |
| 1:H:497:GLN:H | 1:H:497:GLN:HE21 | 1.09 | 0.98 |
| 1:Q:68:VAL:HG13 | 1:Q:90:VAL:CG1 | 1.94 | 0.98 |
| 1:I:26:GLN:HG2 | 1:I:30:ARG:NH1 | 1.76 | 0.98 |
| 1:K:67:HIS:CE1 | 1:K:91:THR:CG2 | 2.47 | 0.97 |
| 1:R:450:TYR:H | 1:R:459:HIS:CD2 | 1.82 | 0.97 |
| 1:H:480:GLU:OE2 | 1:H:482:HIS:HD2 | 1.44 | 0.97 |
| 1:R:556:ARG:HG3 | 1:R:556:ARG:HH11 | 1.29 | 0.97 |
| 1:A:67:HIS:HE1 | 1:A:91:THR:CG2 | 1.77 | 0.96 |
| 1:C:169:VAL:CG2 | 1:C:241:GLU:HG2 | 1.95 | 0.96 |
| 1:A:168:ARG:NH1 | 1:A:168:ARG:HG2 | 1.69 | 0.96 |
| 1:I:497:GLN:NE2 | 1:I:497:GLN:H | 1.63 | 0.96 |
| 1:R:450:TYR:H | 1:R:459:HIS:HD2 | 1.04 | 0.96 |
| 1:E:317:ASN:HD22 | 1:E:317:ASN:H | 0.99 | 0.96 |
| 1:M:478:ARG:HH21 | 1:M:478:ARG:CG | 1.79 | 0.96 |
| 1:Q:42:ARG:NH1 | 1:Q:140:GLU:HG2 | 1.80 | 0.96 |
| 1:E:67:HIS:HE1 | 1:E:91:THR:HG23 | 1.30 | 0.96 |
| 1:J:597:SER:HB2 | 1:J:598:ALA:CB | 1.94 | 0.96 |
| 1:A:497:GLN:NE2 | 1:A:497:GLN:H | 1.63 | 0.95 |
| 1:N:438:THR:HG21 | 1:O:629:LEU:HD21 | 1.48 | 0.95 |
| 1:Q:218:LEU:N | 1:Q:303:GLN:HE21 | 1.63 | 0.95 |
| 1:D:280:THR:HG23 | 1:D:281:THR:HG22 | 1.46 | 0.95 |
| 1:N:169:VAL:HG11 | 1:N:240:PHE:O | 1.68 | 0.94 |
| 1:D:168:ARG:HG2 | 1:D:168:ARG:HH11 | 1.32 | 0.94 |
| 1:O:73:THR:HB | 1:O:92:ALA:HB1 | 1.49 | 0.94 |
| 1:A:497:GLN:HE21 | 1:A:497:GLN:H | 1.08 | 0.94 |
| 1:B:39:ASP:OD2 | 1:B:298:ARG:HD3 | 1.66 | 0.94 |
| 1:L:577:MET:HE3 | 1:L:641:PHE:HZ | 1.30 | 0.94 |
| 1:A:502:ASP:OD2 | 1:A:616:THR:HG21 | 1.66 | 0.94 |
| 1:H:480:GLU:OE2 | 1:H:482:HIS:CD2 | 2.21 | 0.94 |
| 1:J:490:PRO:CB | 1:J:569:MET:HE3 | 1.97 | 0.94 |
| 1:F:42:ARG:NH1 | 1:F:140:GLU:HG2 | 1.83 | 0.94 |
| 1:M:450:TYR:H | 1:M:459:HIS:HD2 | 1.01 | 0.94 |
| 1:E:67:HIS:CE1 | 1:E:91:THR:HG23 | 2.03 | 0.93 |
| 1:P:450:TYR:H | 1:P:459:HIS:HD2 | 1.07 | 0.93 |
| 1:D:497:GLN:HE21 | 1:D:497:GLN:N | 1.64 | 0.93 |
| 1:D:490:PRO:HB3 | 1:D:569:MET:CE | 1.97 | 0.93 |
| 1:J:158:ALA:HA | 1:J:162:LEU:HD23 | 1.50 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:168:ARG:HG2 | 1:N:168:ARG:HH11 | 1.34 | 0.93 |
| 1:N:255:GLU:HG2 | 1:N:321:GLU:HG2 | 1.51 | 0.92 |
| 1:A:228:GLU:OE2 | 1:A:290:LYS:NZ | 2.02 | 0.92 |
| 1:C:490:PRO:HB3 | 1:C:569:MET:HE3 | 1.47 | 0.92 |
| 1:J:168:ARG:HG2 | 1:J:168:ARG:HH11 | 1.33 | 0.92 |
| 1:B:450:TYR:H | 1:B:459:HIS:HD2 | 0.99 | 0.92 |
| 1:E:259:HIS:HD2 | 1:E:260:SER:OG | 1.51 | 0.92 |
| 1:P:157:GLU:HA | 1:P:160:GLU:HG3 | 1.51 | 0.92 |
| 1:H:87:ALA:O | 1:H:115:LYS:HE3 | 1.67 | 0.92 |
| 1:A:133:ARG:HB2 | 1:A:164:LYS:HG3 | 1.51 | 0.92 |
| 1:E:490:PRO:HB3 | 1:E:569:MET:CE | 1.99 | 0.92 |
| 1:I:490:PRO:HB3 | 1:I:569:MET:HE2 | 1.52 | 0.92 |
| 1:O:218:LEU:H | 1:O:303:GLN:NE2 | 1.68 | 0.92 |
| 1:E:169:VAL:HG12 | 1:E:241:GLU:HG2 | 1.52 | 0.92 |
| 1:J:497:GLN:H | 1:J:497:GLN:HE21 | 1.16 | 0.92 |
| 1:D:478:ARG:HG2 | 1:D:478:ARG:HH21 | 1.35 | 0.91 |
| 1:E:478:ARG:NH2 | 1:E:478:ARG:HG2 | 1.79 | 0.91 |
| 1:L:42:ARG:NH1 | 1:L:140:GLU:HG2 | 1.85 | 0.91 |
| 1:L:490:PRO:CB | 1:L:569:MET:HE1 | 2.00 | 0.91 |
| 1:D:168:ARG:NH2 | 1:D:276:ASP:O | 2.03 | 0.91 |
| 1:E:42:ARG:NH1 | 1:E:140:GLU:HG2 | 1.84 | 0.91 |
| 1:F:218:LEU:H | 1:F:303:GLN:HE21 | 1.13 | 0.91 |
| 1:H:273:ILE:HG13 | 1:H:275:MET:CE | 2.00 | 0.91 |
| 1:H:117:THR:OG1 | 1:J:131:GLY:HA3 | 1.70 | 0.91 |
| 1:P:478:ARG:HH21 | 1:P:478:ARG:HG2 | 1.36 | 0.91 |
| 1:P:490:PRO:HB3 | 1:P:569:MET:CE | 2.00 | 0.91 |
| 1:Q:180:PRO:HG2 | 1:Q:230:SER:HB3 | 1.52 | 0.91 |
| 1:C:137:ILE:HB | 1:C:169:VAL:HG12 | 1.50 | 0.91 |
| 1:D:497:GLN:HE21 | 1:D:497:GLN:H | 0.97 | 0.91 |
| 1:D:480:GLU:OE2 | 1:D:482:HIS:HD2 | 1.54 | 0.91 |
| 1:G:490:PRO:CB | 1:G:569:MET:HE1 | 2.01 | 0.90 |
| 1:O:39:ASP:OD2 | 1:O:298:ARG:HD3 | 1.71 | 0.90 |
| 1:L:168:ARG:HH11 | 1:L:168:ARG:HG2 | 1.35 | 0.90 |
| 1:P:42:ARG:NH1 | 1:P:140:GLU:HG2 | 1.86 | 0.90 |
| 1:C:168:ARG:HH11 | 1:C:168:ARG:CG | 1.81 | 0.90 |
| 1:L:169:VAL:HG13 | 1:L:241:GLU:HG2 | 1.52 | 0.90 |
| 1:M:91:THR:HG22 | 1:M:117:THR:CG2 | 2.02 | 0.90 |
| 1:O:497:GLN:HE21 | 1:O:497:GLN:H | 1.14 | 0.90 |
| 1:R:196:ASN:HB2 | 1:R:201:GLU:OE2 | 1.71 | 0.90 |
| 1:M:497:GLN:NE2 | 1:M:497:GLN:H | 1.68 | 0.90 |
| 1:D:434:VAL:CG1 | 1:D:469:LEU:HD13 | 2.02 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:67:HIS:HE1 | 1:L:91:THR:CG2 | 1.81 | 0.90 |
| 1:M:42:ARG:HH11 | 1:M:140:GLU:HG3 | 1.36 | 0.90 |
| 1:P:490:PRO:HB3 | 1:P:569:MET:HE1 | 1.52 | 0.90 |
| 1:D:42:ARG:HH11 | 1:D:140:GLU:HG2 | 1.34 | 0.90 |
| 1:L:379:LYS:HA | 1:L:399:THR:HG23 | 1.53 | 0.90 |
| 1:I:450:TYR:H | 1:I:459:HIS:HD2 | 1.12 | 0.89 |
| 1:K:123:SER:HB3 | 2:K:701:SAH:HN62 | 1.34 | 0.89 |
| 1:M:178:ILE:O | 1:M:233:ILE:HG22 | 1.72 | 0.89 |
| 1:G:379:LYS:HA | 1:G:399:THR:HG23 | 1.55 | 0.89 |
| 1:C:314:VAL:HG21 | 1:C:320:PHE:CD2 | 2.06 | 0.89 |
| 1:E:379:LYS:HA | 1:E:399:THR:CG2 | 2.03 | 0.89 |
| 1:A:168:ARG:CG | 1:A:168:ARG:HH11 | 1.81 | 0.89 |
| 1:A:67:HIS:HE1 | 1:A:91:THR:HG22 | 1.37 | 0.89 |
| 1:P:42:ARG:HH11 | 1:P:140:GLU:HG2 | 1.36 | 0.89 |
| 1:I:379:LYS:HA | 1:I:399:THR:HG23 | 1.53 | 0.89 |
| 1:J:370:PHE:O | 1:J:374:VAL:HG23 | 1.72 | 0.89 |
| 1:A:434:VAL:CG1 | 1:A:469:LEU:HD13 | 2.03 | 0.88 |
| 1:N:55:ALA:N | 1:N:58:LYS:NZ | 2.20 | 0.88 |
| 1:Q:196:ASN:HB2 | 1:Q:201:GLU:OE2 | 1.72 | 0.88 |
| 1:O:490:PRO:HB3 | 1:O:569:MET:CE | 2.03 | 0.88 |
| 1:M:450:TYR:H | 1:M:459:HIS:CD2 | 1.89 | 0.88 |
| 1:G:379:LYS:HA | 1:G:399:THR:CG2 | 2.04 | 0.88 |
| 1:I:67:HIS:CE1 | 1:I:91:THR:HG23 | 2.08 | 0.88 |
| 1:F:497:GLN:HE21 | 1:F:497:GLN:H | 1.19 | 0.88 |
| 1:O:643:LYS:H | 1:O:643:LYS:HD2 | 1.37 | 0.88 |
| 1:R:291:ASN:HB3 | 1:R:295:TYR:HB2 | 1.56 | 0.88 |
| 1:Q:153:ARG:NH1 | 1:Q:153:ARG:HG3 | 1.74 | 0.88 |
| 1:J:194:ARG:HG2 | 1:J:201:GLU:HB2 | 1.54 | 0.87 |
| 1:R:547:GLU:OE2 | 1:R:550:ARG:NH2 | 2.07 | 0.87 |
| 1:Q:68:VAL:CG1 | 1:Q:90:VAL:HG13 | 2.03 | 0.87 |
| 1:D:379:LYS:HA | 1:D:399:THR:HG23 | 1.56 | 0.87 |
| 1:M:497:GLN:HE21 | 1:M:497:GLN:H | 1.19 | 0.87 |
| 1:O:373:GLU:O | 1:O:377:LEU:HD12 | 1.75 | 0.87 |
| 1:H:450:TYR:H | 1:H:459:HIS:HD2 | 1.22 | 0.87 |
| 1:M:68:VAL:HG22 | 1:M:136:ILE:HB | 1.55 | 0.87 |
| 1:Q:450:TYR:H | 1:Q:459:HIS:HD2 | 1.18 | 0.87 |
| 1:A:490:PRO:CB | 1:A:569:MET:HE2 | 2.06 | 0.86 |
| 1:N:147:ILE:HD11 | 1:N:331:LEU:HD13 | 1.57 | 0.86 |
| 1:I:570:SER:HB3 | 1:I:622:LYS:HG2 | 1.54 | 0.86 |
| 1:B:550:ARG:H | 1:B:560:GLN:HE22 | 1.23 | 0.86 |
| 1:N:478:ARG:HG2 | 1:N:478:ARG:HH21 | 1.39 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:379:LYS:HA | 1:D:399:THR:CG2 | 2.06 | 0.86 |
| 1:E:57:LYS:O | 1:E:66:VAL:HG21 | 1.75 | 0.86 |
| 1:F:379:LYS:HA | 1:F:399:THR:HG22 | 1.57 | 0.86 |
| 1:K:42:ARG:NH1 | 1:K:140:GLU:HG2 | 1.89 | 0.86 |
| 1:P:146:LEU:H | 1:P:146:LEU:HD23 | 1.40 | 0.86 |
| 1:J:483:MET:HB3 | 1:J:582:GLU:HG3 | 1.55 | 0.86 |
| 1:L:490:PRO:CB | 1:L:569:MET:CE | 2.50 | 0.86 |
| 1:M:379:LYS:HA | 1:M:399:THR:CG2 | 2.06 | 0.86 |
| 1:M:181:VAL:HG21 | 1:M:268:LEU:HD11 | 1.57 | 0.86 |
| 1:F:39:ASP:OD2 | 1:F:298:ARG:HD3 | 1.76 | 0.85 |
| 1:O:393:GLY:CA | 1:O:405:ILE:HD11 | 1.99 | 0.85 |
| 1:P:104:ARG:HB2 | 1:P:104:ARG:CZ | 2.04 | 0.85 |
| 1:F:450:TYR:H | 1:F:459:HIS:HD2 | 1.25 | 0.85 |
| 1:I:323:VAL:HG11 | 1:I:340:LYS:HD3 | 1.57 | 0.85 |
| 1:D:42:ARG:NH1 | 1:D:140:GLU:HG2 | 1.90 | 0.85 |
| 1:N:50:LEU:O | 1:N:54:ILE:HG23 | 1.77 | 0.85 |
| 1:L:168:ARG:NH1 | 1:L:241:GLU:OE2 | 2.08 | 0.85 |
| 1:Q:153:ARG:CG | 1:Q:153:ARG:HH11 | 1.89 | 0.85 |
| 1:F:218:LEU:HD12 | 1:F:303:GLN:CB | 2.06 | 0.85 |
| 1:M:478:ARG:HG2 | 1:M:478:ARG:NH2 | 1.89 | 0.85 |
| 1:C:450:TYR:H | 1:C:459:HIS:CD2 | 1.94 | 0.85 |
| 1:L:490:PRO:HB3 | 1:L:569:MET:HE3 | 1.57 | 0.85 |
| 1:K:569:MET:HG3 | 1:K:624:LEU:HD11 | 1.58 | 0.85 |
| 1:M:379:LYS:HA | 1:M:399:THR:HG23 | 1.57 | 0.85 |
| 1:N:58:LYS:HE2 | 1:N:66:VAL:HG21 | 1.57 | 0.85 |
| 1:R:622:LYS:H | 1:R:622:LYS:HD2 | 1.41 | 0.85 |
| 1:B:104:ARG:O | 1:B:108:SER:HB3 | 1.77 | 0.84 |
| 1:K:169:VAL:HG13 | 1:K:241:GLU:HG2 | 1.57 | 0.84 |
| 1:F:565:ASN:HD21 | 1:F:644:SER:HB2 | 1.42 | 0.84 |
| 1:B:163:ALA:HB1 | 1:B:167:CYS:SG | 2.17 | 0.84 |
| 1:J:438:THR:HG21 | 1:K:629:LEU:HD21 | 1.59 | 0.84 |
| 1:O:528:ILE:H | 1:O:528:ILE:HD12 | 1.41 | 0.84 |
| 1:D:434:VAL:HG12 | 1:D:469:LEU:HD13 | 1.60 | 0.84 |
| 1:G:497:GLN:HE21 | 1:G:497:GLN:H | 1.25 | 0.84 |
| 1:O:373:GLU:HG3 | 1:O:377:LEU:HD11 | 1.59 | 0.83 |
| 1:F:553:ILE:HG22 | 1:F:553:ILE:O | 1.77 | 0.83 |
| 1:P:450:TYR:H | 1:P:459:HIS:CD2 | 1.94 | 0.83 |
| 1:B:490:PRO:CB | 1:B:569:MET:HE1 | 2.08 | 0.83 |
| 1:E:87:ALA:O | 1:E:115:LYS:HE2 | 1.78 | 0.83 |
| 1:F:275:MET:HE1 | 1:F:283:ILE:HG13 | 1.59 | 0.83 |
| 1:R:51:LYS:HZ2 | 1:R:51:LYS:HB2 | 1.43 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:490:PRO:CB | 1:D:569:MET:CE | 2.56 | 0.83 |
| 1:A:67:HIS:CE1 | 1:A:91:THR:CG2 | 2.62 | 0.83 |
| 1:O:233:ILE:HD11 | 1:O:254:ARG:CB | 2.08 | 0.83 |
| 1:R:66:VAL:HA | 1:R:135:ASP:OD2 | 1.76 | 0.83 |
| 1:F:150:GLY:O | 1:F:154:THR:OG1 | 1.96 | 0.83 |
| 1:N:379:LYS:HA | 1:N:399:THR:CG2 | 2.08 | 0.83 |
| 1:N:480:GLU:OE2 | 1:N:482:HIS:HD2 | 1.60 | 0.83 |
| 1:R:379:LYS:HA | 1:R:399:THR:CG2 | 2.08 | 0.83 |
| 1:Q:378:SER:HB2 | 1:Q:399:THR:HG23 | 1.60 | 0.82 |
| 1:K:550:ARG:H | 1:K:560:GLN:HE22 | 1.24 | 0.82 |
| 1:N:254:ARG:O | 1:N:321:GLU:HA | 1.79 | 0.82 |
| 1:N:27:GLU:OE2 | 1:N:96:PHE:CE1 | 2.32 | 0.82 |
| 1:B:450:TYR:H | 1:B:459:HIS:CD2 | 1.91 | 0.82 |
| 1:M:110:SER:HB2 | 1:M:111:PRO:HD2 | 1.62 | 0.82 |
| 1:Q:254:ARG:O | 1:Q:321:GLU:HA | 1.79 | 0.82 |
| 1:G:66:VAL:HG12 | 1:G:87:ALA:HA | 1.62 | 0.82 |
| 1:O:450:TYR:H | 1:O:459:HIS:HD2 | 1.27 | 0.82 |
| 1:K:379:LYS:HA | 1:K:399:THR:HG23 | 1.60 | 0.82 |
| 1:K:388:GLU:OE1 | 1:K:452:SER:HB2 | 1.79 | 0.82 |
| 1:L:631:ASP:OD1 | 1:L:633:SER:HB2 | 1.80 | 0.82 |
| 1:A:506:VAL:HG12 | 1:A:507:ASN:HD22 | 1.45 | 0.82 |
| 1:L:577:MET:CE | 1:L:641:PHE:HZ | 1.92 | 0.82 |
| 1:J:189:PHE:CD1 | 1:J:359:TYR:HB2 | 2.14 | 0.81 |
| 1:P:104:ARG:O | 1:P:108:SER:HB2 | 1.80 | 0.81 |
| 1:F:553:ILE:O | 1:F:553:ILE:CG2 | 2.29 | 0.81 |
| 1:K:42:ARG:HH12 | 1:K:140:GLU:HG2 | 1.45 | 0.81 |
| 1:N:63:ASP:CB | 1:N:65:LYS:H | 1.93 | 0.81 |
| 1:C:314:VAL:CG2 | 1:C:320:PHE:CD2 | 2.63 | 0.81 |
| 1:Q:478:ARG:HH21 | 1:Q:478:ARG:HG2 | 1.45 | 0.81 |
| 1:B:490:PRO:HB3 | 1:B:569:MET:HE3 | 1.59 | 0.81 |
| 1:Q:183:SER:H | 1:Q:265:ASP:HB2 | 1.46 | 0.81 |
| 1:H:42:ARG:HH11 | 1:H:140:GLU:HG2 | 1.46 | 0.81 |
| 1:J:243:GLU:OE1 | 1:J:243:GLU:N | 2.12 | 0.81 |
| 1:P:259:HIS:HD2 | 1:P:260:SER:OG | 1.62 | 0.81 |
| 1:C:480:GLU:OE2 | 1:C:482:HIS:HD2 | 1.64 | 0.81 |
| 1:G:169:VAL:CG1 | 1:G:241:GLU:HG3 | 2.09 | 0.81 |
| 1:J:497:GLN:H | 1:J:497:GLN:NE2 | 1.78 | 0.81 |
| 1:M:50:LEU:HD23 | 1:M:170:VAL:HG21 | 1.62 | 0.81 |
| 1:N:269:MET:HG2 | 1:N:306:TYR:CE1 | 2.13 | 0.81 |
| 1:R:556:ARG:CG | 1:R:556:ARG:HH11 | 1.93 | 0.81 |
| 1:B:216:VAL:O | 1:B:302:MET:HG2 | 1.81 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:379:LYS:HA | 1:E:399:THR:HG23 | 1.63 | 0.80 |
| 1:M:444:VAL:HG13 | 1:M:479:VAL:HB | 1.61 | 0.80 |
| 1:D:450:TYR:H | 1:D:459:HIS:HD2 | 1.27 | 0.80 |
| 1:Q:216:VAL:O | 1:Q:302:MET:HG2 | 1.81 | 0.80 |
| 1:Q:264:ILE:HD11 | 1:Q:267:LEU:HD21 | 1.63 | 0.80 |
| 1:M:95:VAL:CG2 | 1:M:122:ARG:HG3 | 2.11 | 0.80 |
| 1:P:379:LYS:HA | 1:P:399:THR:HG23 | 1.63 | 0.80 |
| 1:E:478:ARG:HH21 | 1:E:478:ARG:CG | 1.90 | 0.80 |
| 1:Q:264:ILE:O | 1:Q:264:ILE:CG1 | 2.29 | 0.80 |
| 1:E:258:ALA:HB3 | 1:E:315:GLU:O | 1.82 | 0.79 |
| 1:E:317:ASN:H | 1:E:317:ASN:ND2 | 1.79 | 0.79 |
| 1:R:379:LYS:HA | 1:R:399:THR:HG21 | 1.64 | 0.79 |
| 1:R:567:ASP:HA | 1:R:623:SER:HB2 | 1.64 | 0.79 |
| 1:B:140:GLU:O | 1:B:140:GLU:HG3 | 1.82 | 0.79 |
| 1:M:39:ASP:OD2 | 1:M:298:ARG:HD2 | 1.81 | 0.79 |
| 1:J:450:TYR:H | 1:J:459:HIS:HD2 | 1.31 | 0.79 |
| 1:J:596:SER:O | 1:J:599:GLY:N | 2.11 | 0.79 |
| 1:I:169:VAL:HG13 | 1:I:241:GLU:HG2 | 1.65 | 0.79 |
| 1:P:5:LYS:HA | 1:R:420:ILE:HD11 | 1.65 | 0.79 |
| 1:D:169:VAL:HG13 | 1:D:241:GLU:HG2 | 1.63 | 0.79 |
| 1:F:50:LEU:O | 1:F:54:ILE:CD1 | 2.31 | 0.79 |
| 1:B:39:ASP:O | 1:B:43:ASN:ND2 | 2.16 | 0.79 |
| 1:K:141:VAL:HG13 | 1:K:141:VAL:O | 1.81 | 0.79 |
| 1:L:210:THR:HB | 4:L:815:HOH:O | 1.83 | 0.79 |
| 1:N:242:HIS:HB3 | 1:N:245:LYS:HD3 | 1.64 | 0.79 |
| 1:G:158:ALA:HA | 1:G:162:LEU:HD23 | 1.64 | 0.79 |
| 1:M:132:SER:N | 1:P:104:ARG:NH2 | 2.31 | 0.79 |
| 1:M:569:MET:CG | 1:M:624:LEU:CD1 | 2.58 | 0.78 |
| 1:Q:168:ARG:CG | 1:Q:168:ARG:HH11 | 1.96 | 0.78 |
| 1:J:239:ASP:OD2 | 1:J:242:HIS:HD2 | 1.66 | 0.78 |
| 1:A:169:VAL:HG13 | 1:A:241:GLU:HG2 | 1.63 | 0.78 |
| 1:M:41:ASP:O | 1:M:45:LYS:HB2 | 1.83 | 0.78 |
| 1:O:233:ILE:HD11 | 1:O:254:ARG:HB3 | 1.65 | 0.78 |
| 1:Q:218:LEU:N | 1:Q:303:GLN:NE2 | 2.25 | 0.78 |
| 1:M:480:GLU:OE2 | 1:M:482:HIS:HD2 | 1.67 | 0.78 |
| 1:G:497:GLN:NE2 | 1:G:497:GLN:H | 1.82 | 0.78 |
| 1:R:73:THR:OG1 | 1:R:76:GLY:HA2 | 1.83 | 0.78 |
| 1:K:76:GLY:O | 1:K:79:SER:N | 2.17 | 0.78 |
| 1:O:42:ARG:NH1 | 1:O:140:GLU:HG2 | 1.98 | 0.78 |
| 1:G:450:TYR:H | 1:G:459:HIS:HD2 | 1.31 | 0.78 |
| 1:K:450:TYR:H | 1:K:459:HIS:HD2 | 1.30 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:317:ASN:N | 1:E:317:ASN:HD22 | 1.75 | 0.78 |
| 1:L:42:ARG:HH11 | 1:L:140:GLU:HG2 | 1.48 | 0.78 |
| 1:N:142:PHE:CD1 | 1:N:146:LEU:HD12 | 2.20 | 0.77 |
| 1:K:541:VAL:HG23 | 1:K:601:PRO:HG3 | 1.66 | 0.77 |
| 1:N:133:ARG:HB3 | 1:N:133:ARG:HH21 | 1.48 | 0.77 |
| 1:Q:178:ILE:HD13 | 1:Q:235:ALA:HB2 | 1.65 | 0.77 |
| 1:F:450:TYR:H | 1:F:459:HIS:CD2 | 2.02 | 0.77 |
| 1:N:67:HIS:H | 1:N:135:ASP:HB2 | 1.49 | 0.77 |
| 1:Q:232:PRO:HG2 | 1:Q:290:LYS:HE2 | 1.65 | 0.77 |
| 1:J:480:GLU:OE2 | 1:J:482:HIS:HD2 | 1.66 | 0.77 |
| 1:C:490:PRO:CB | 1:C:569:MET:CE | 2.63 | 0.77 |
| 1:D:67:HIS:HE1 | 1:D:91:THR:CG2 | 1.96 | 0.77 |
| 1:M:280:THR:HG23 | 1:M:281:THR:CG2 | 2.14 | 0.77 |
| 1:Q:247:ILE:HG12 | 1:Q:250:GLU:OE2 | 1.84 | 0.77 |
| 1:B:243:GLU:N | 1:B:243:GLU:OE1 | 2.13 | 0.77 |
| 1:J:383:VAL:HG21 | 1:J:445:LEU:HD22 | 1.67 | 0.77 |
| 1:E:434:VAL:CG1 | 1:E:469:LEU:HD13 | 2.15 | 0.77 |
| 1:G:103:ALA:O | 1:G:107:THR:HG23 | 1.84 | 0.77 |
| 1:Q:218:LEU:H | 1:Q:303:GLN:HE21 | 0.78 | 0.77 |
| 1:B:179:VAL:HG12 | 1:B:180:PRO:O | 1.85 | 0.77 |
| 1:F:104:ARG:O | 1:F:108:SER:HB3 | 1.84 | 0.77 |
| 1:A:450:TYR:H | 1:A:459:HIS:HD2 | 1.33 | 0.77 |
| 1:G:95:VAL:HG22 | 1:G:95:VAL:O | 1.85 | 0.77 |
| 1:N:530:ASP:OD1 | 1:N:531:GLU:N | 2.17 | 0.77 |
| 1:B:42:ARG:NH1 | 1:B:140:GLU:HG2 | 2.00 | 0.76 |
| 1:F:206:ARG:HH12 | 1:F:310:GLU:HG3 | 1.50 | 0.76 |
| 1:N:566:ILE:HG22 | 1:N:569:MET:CE | 2.15 | 0.76 |
| 1:B:269:MET:HG2 | 1:B:306:TYR:HE2 | 1.50 | 0.76 |
| 1:C:489:ILE:O | 1:C:576:PRO:HD2 | 1.86 | 0.76 |
| 1:H:450:TYR:H | 1:H:459:HIS:CD2 | 2.04 | 0.76 |
| 1:O:411:ARG:O | 1:O:415:ILE:HD12 | 1.84 | 0.76 |
| 1:R:450:TYR:N | 1:R:459:HIS:HD2 | 1.80 | 0.76 |
| 1:A:67:HIS:CE1 | 1:A:91:THR:HG22 | 2.20 | 0.76 |
| 1:D:80:LEU:HB3 | 1:D:509:PHE:CE1 | 2.19 | 0.76 |
| 1:I:141:VAL:O | 1:I:141:VAL:HG12 | 1.85 | 0.76 |
| 1:L:467:GLU:HG3 | 1:L:555:GLY:O | 1.86 | 0.76 |
| 1:R:478:ARG:HH21 | 1:R:478:ARG:HG2 | 1.50 | 0.76 |
| 1:D:291:ASN:H | 1:D:292:LYS:NZ | 1.84 | 0.76 |
| 1:M:278:ASN:O | 1:M:280:THR:HG22 | 1.85 | 0.76 |
| 1:I:273:ILE:HD12 | 1:I:275:MET:HE1 | 1.67 | 0.76 |
| 1:H:497:GLN:N | 1:H:497:GLN:HE21 | 1.83 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:227:ARG:NH2 | 1:I:261:SER:O | 2.19 | 0.75 |
| 1:K:480:GLU:OE2 | 1:K:482:HIS:HD2 | 1.67 | 0.75 |
| 1:M:222:LYS:O | 1:M:225:GLU:HG2 | 1.86 | 0.75 |
| 1:F:218:LEU:HD12 | 1:F:303:GLN:HB3 | 1.67 | 0.75 |
| 1:C:4:GLU:OE2 | 1:C:13:ARG:HD3 | 1.86 | 0.75 |
| 1:Q:232:PRO:CG | 1:Q:290:LYS:HE2 | 2.17 | 0.75 |
| 1:N:566:ILE:CG2 | 1:N:569:MET:HE3 | 2.16 | 0.75 |
| 1:Q:276:ASP:O | 1:Q:277:ARG:HB2 | 1.87 | 0.75 |
| 1:I:568:ASN:O | 1:I:572:SER:OG | 2.03 | 0.75 |
| 1:M:412:PHE:HE2 | 1:M:451:MET:HG2 | 1.51 | 0.75 |
| 1:Q:480:GLU:HG3 | 1:Q:584:GLY:H | 1.52 | 0.75 |
| 1:I:434:VAL:HG12 | 1:I:469:LEU:HD13 | 1.69 | 0.75 |
| 1:C:42:ARG:NH1 | 1:C:140:GLU:HG2 | 2.02 | 0.75 |
| 1:C:616:THR:O | 1:C:619:ARG:HG2 | 1.85 | 0.75 |
| 1:H:478:ARG:HH21 | 1:H:478:ARG:CG | 2.00 | 0.75 |
| 1:O:490:PRO:HB3 | 1:O:569:MET:HE3 | 1.69 | 0.75 |
| 1:O:442:ASP:O | 1:O:478:ARG:HB2 | 1.87 | 0.75 |
| 1:I:275:MET:HA | 1:I:275:MET:HE2 | 1.69 | 0.75 |
| 1:J:168:ARG:HG2 | 1:J:168:ARG:NH1 | 2.02 | 0.75 |
| 1:N:450:TYR:H | 1:N:459:HIS:HD2 | 1.34 | 0.75 |
| 1:M:553:ILE:HG13 | 1:M:553:ILE:O | 1.84 | 0.74 |
| 1:B:169:VAL:HG13 | 1:B:241:GLU:HG2 | 1.70 | 0.74 |
| 1:E:42:ARG:HH12 | 1:E:140:GLU:HG2 | 1.49 | 0.74 |
| 1:E:450:TYR:H | 1:E:459:HIS:HD2 | 1.32 | 0.74 |
| 1:M:5:LYS:HA | 1:O:420:ILE:HD11 | 1.69 | 0.74 |
| 1:M:615:ILE:O | 1:M:617:ALA:N | 2.20 | 0.74 |
| 1:C:4:GLU:OE2 | 1:C:13:ARG:CD | 2.36 | 0.74 |
| 1:F:275:MET:CE | 1:F:283:ILE:HG13 | 2.16 | 0.74 |
| 1:E:497:GLN:NE2 | 1:E:497:GLN:H | 1.84 | 0.74 |
| 1:F:497:GLN:NE2 | 1:F:497:GLN:H | 1.86 | 0.74 |
| 1:M:95:VAL:HG21 | 1:M:122:ARG:HG3 | 1.69 | 0.74 |
| 1:O:169:VAL:HG13 | 1:O:241:GLU:HG2 | 1.68 | 0.74 |
| 1:O:566:ILE:O | 1:O:623:SER:HA | 1.85 | 0.74 |
| 1:N:150:GLY:O | 1:N:154:THR:OG1 | 2.06 | 0.74 |
| 1:R:371:LYS:O | 1:R:375:ASP:OD1 | 2.06 | 0.74 |
| 1:D:67:HIS:HE1 | 1:D:91:THR:HG23 | 1.49 | 0.74 |
| 1:M:480:GLU:OE2 | 1:M:482:HIS:CD2 | 2.41 | 0.74 |
| 1:C:67:HIS:HE1 | 1:C:91:THR:HG22 | 1.53 | 0.74 |
| 1:O:4:GLU:OE2 | 1:O:13:ARG:HD3 | 1.88 | 0.74 |
| 1:R:51:LYS:HB2 | 1:R:51:LYS:NZ | 2.02 | 0.73 |
| 1:H:66:VAL:N | 1:H:88:ASP:OD2 | 2.21 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:590:THR:O | 1:Q:609:GLN:NE2 | 2.20 | 0.73 |
| 1:R:384:ALA:HB3 | 1:R:444:VAL:HG12 | 1.70 | 0.73 |
| 1:B:314:VAL:HG22 | 1:B:315:GLU:H | 1.53 | 0.73 |
| 1:K:271:TRP:O | 1:K:285:MET:HB2 | 1.88 | 0.73 |
| 1:M:450:TYR:N | 1:M:459:HIS:HD2 | 1.81 | 0.73 |
| 1:O:382:HIS:CD2 | 1:O:441:PRO:HA | 2.23 | 0.73 |
| 1:J:36:MET:HA | 1:J:300:HIS:CD2 | 2.22 | 0.73 |
| 1:N:566:ILE:HG21 | 1:N:569:MET:HE3 | 1.71 | 0.73 |
| 1:L:273:ILE:HG13 | 1:L:275:MET:HE3 | 1.68 | 0.73 |
| 1:O:643:LYS:CD | 1:O:643:LYS:H | 1.99 | 0.73 |
| 1:N:104:ARG:O | 1:N:108:SER:OG | 2.04 | 0.73 |
| 1:K:550:ARG:N | 1:K:560:GLN:HE22 | 1.87 | 0.73 |
| 1:O:627:HIS:CB | 1:O:640:GLN:HB2 | 2.08 | 0.73 |
| 1:L:103:ALA:O | 1:L:107:THR:HB | 1.89 | 0.73 |
| 1:Q:222:LYS:HB2 | 1:Q:225:GLU:HG2 | 1.71 | 0.73 |
| 1:L:378:SER:HB2 | 1:L:399:THR:HG22 | 1.71 | 0.73 |
| 1:I:278:ASN:O | 1:I:280:THR:HG23 | 1.89 | 0.72 |
| 1:K:73:THR:OG1 | 1:K:76:GLY:HA2 | 1.89 | 0.72 |
| 1:H:42:ARG:NH1 | 1:H:140:GLU:HG2 | 2.04 | 0.72 |
| 1:H:490:PRO:CB | 1:H:569:MET:CE | 2.64 | 0.72 |
| 1:N:81:MET:O | 1:N:84:ARG:O | 2.07 | 0.72 |
| 1:B:218:LEU:H | 1:B:303:GLN:NE2 | 1.87 | 0.72 |
| 1:B:392:LEU:O | 1:B:392:LEU:HD23 | 1.89 | 0.72 |
| 1:M:42:ARG:NH1 | 1:M:140:GLU:HG3 | 2.04 | 0.72 |
| 1:M:245:LYS:HE3 | 1:R:337:GLY:HA2 | 1.70 | 0.72 |
| 1:B:43:ASN:H | 1:B:43:ASN:HD22 | 1.38 | 0.72 |
| 1:M:412:PHE:CE2 | 1:M:451:MET:HG2 | 2.24 | 0.72 |
| 1:N:87:ALA:HA | 1:N:88:ASP:HB2 | 1.69 | 0.72 |
| 1:D:39:ASP:OD2 | 1:D:298:ARG:HD3 | 1.88 | 0.72 |
| 1:H:549:LEU:HD23 | 1:H:637:ILE:HD13 | 1.70 | 0.72 |
| 1:M:126:VAL:H | 1:M:161:ARG:NH2 | 1.86 | 0.72 |
| 1:O:190:ASN:HD21 | 1:O:209:GLY:HA3 | 1.53 | 0.72 |
| 1:O:497:GLN:NE2 | 1:O:497:GLN:H | 1.87 | 0.72 |
| 1:P:365:PHE:O | 1:P:371:LYS:CE | 2.37 | 0.72 |
| 1:E:146:LEU:HB3 | 1:E:271:TRP:CD1 | 2.25 | 0.72 |
| 1:A:478:ARG:HH21 | 1:A:478:ARG:CG | 2.03 | 0.72 |
| 1:Q:570:SER:HB2 | 1:Q:622:LYS:HD3 | 1.72 | 0.72 |
| 1:I:434:VAL:CG1 | 1:I:469:LEU:HD13 | 2.20 | 0.72 |
| 1:N:39:ASP:OD2 | 1:N:298:ARG:CD | 2.38 | 0.72 |
| 1:E:41:ASP:OD1 | 1:E:41:ASP:C | 2.27 | 0.72 |
| 1:L:497:GLN:HE21 | 1:L:497:GLN:H | 1.35 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:203:PRO:HA | 1:F:422:TYR:CD2 | 2.25 | 0.71 |
| 1:F:244:GLU:OE1 | 1:F:245:LYS:HG3 | 1.90 | 0.71 |
| 1:H:169:VAL:HG12 | 1:H:241:GLU:HG2 | 1.70 | 0.71 |
| 1:I:171:PRO:HB3 | 1:I:275:MET:HE2 | 1.70 | 0.71 |
| 1:Q:450:TYR:H | 1:Q:459:HIS:CD2 | 2.07 | 0.71 |
| 1:F:616:THR:O | 1:F:619:ARG:NH1 | 2.21 | 0.71 |
| 1:P:57:LYS:HE2 | 1:P:135:ASP:HB3 | 1.71 | 0.71 |
| 1:R:176:VAL:CG1 | 1:R:236:PHE:HB2 | 2.21 | 0.71 |
| 1:E:259:HIS:CD2 | 1:E:260:SER:OG | 2.41 | 0.71 |
| 1:F:94:GLU:OE1 | 2:F:701:SAH:O2' | 2.08 | 0.71 |
| 1:P:317:ASN:O | 1:P:317:ASN:ND2 | 2.22 | 0.71 |
| 1:P:478:ARG:HH21 | 1:P:478:ARG:CG | 2.03 | 0.71 |
| 1:Q:367:ASN:OD1 | 1:Q:370:PHE:HB2 | 1.90 | 0.71 |
| 1:M:91:THR:CG2 | 1:M:117:THR:HG23 | 2.14 | 0.71 |
| 1:N:133:ARG:HG3 | 1:N:164:LYS:HG3 | 1.73 | 0.71 |
| 1:E:550:ARG:H | 1:E:560:GLN:HE22 | 1.37 | 0.71 |
| 1:I:450:TYR:H | 1:I:459:HIS:CD2 | 2.03 | 0.71 |
| 1:M:45:LYS:O | 1:M:275:MET:HG2 | 1.89 | 0.71 |
| 1:B:145:GLU:HG2 | 1:B:331:LEU:HD22 | 1.73 | 0.71 |
| 1:C:244:GLU:OE2 | 1:C:244:GLU:HA | 1.91 | 0.71 |
| 1:M:145:GLU:HG3 | 1:M:331:LEU:HD13 | 1.72 | 0.71 |
| 1:I:443:ILE:HG12 | 1:I:445:LEU:HD13 | 1.73 | 0.71 |
| 1:Q:217:GLN:NE2 | 1:Q:298:ARG:O | 2.14 | 0.71 |
| 1:N:55:ALA:HA | 1:N:58:LYS:HD2 | 1.73 | 0.71 |
| 1:Q:169:VAL:HG21 | 1:Q:240:PHE:HB2 | 1.73 | 0.71 |
| 1:J:173:THR:HG22 | 1:J:274:ASP:HB3 | 1.71 | 0.70 |
| 1:K:412:PHE:HE2 | 1:K:451:MET:HG2 | 1.56 | 0.70 |
| 1:N:566:ILE:HG22 | 1:N:569:MET:HE2 | 1.70 | 0.70 |
| 1:E:595:ILE:CG2 | 1:E:599:GLY:HA2 | 2.21 | 0.70 |
| 1:K:420:ILE:HD11 | 1:K:428:VAL:HG22 | 1.72 | 0.70 |
| 1:K:547:GLU:OE2 | 1:K:550:ARG:NH1 | 2.20 | 0.70 |
| 1:A:490:PRO:HB3 | 1:A:569:MET:HE1 | 1.71 | 0.70 |
| 1:B:497:GLN:H | 1:B:497:GLN:HE21 | 1.39 | 0.70 |
| 1:M:489:ILE:O | 1:M:576:PRO:HD2 | 1.91 | 0.70 |
| 1:B:241:GLU:HB2 | 1:B:277:ARG:HH21 | 1.56 | 0.70 |
| 1:K:138:VAL:HG23 | 1:K:170:VAL:HB | 1.71 | 0.70 |
| 1:M:321:GLU:O | 1:M:322:ILE:HD12 | 1.90 | 0.70 |
| 1:R:291:ASN:C | 1:R:292:LYS:HD2 | 2.12 | 0.70 |
| 1:B:450:TYR:N | 1:B:459:HIS:HD2 | 1.82 | 0.70 |
| 1:R:489:ILE:O | 1:R:576:PRO:HD2 | 1.91 | 0.70 |
| 1:I:490:PRO:HB3 | 1:I:569:MET:CE | 2.21 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:460:LEU:HB3 | 1:K:463:LEU:HD23 | 1.72 | 0.70 |
| 1:L:273:ILE:HG13 | 1:L:275:MET:CE | 2.22 | 0.70 |
| 1:P:269:MET:HG2 | 1:P:306:TYR:HE1 | 1.55 | 0.70 |
| 1:B:168:ARG:NH1 | 1:B:241:GLU:OE2 | 2.24 | 0.70 |
| 1:N:88:ASP:O | 1:N:89:LYS:HG3 | 1.92 | 0.70 |
| 1:B:227:ARG:NH2 | 1:B:261:SER:O | 2.25 | 0.70 |
| 1:B:66:VAL:HG12 | 1:B:67:HIS:N | 2.07 | 0.70 |
| 1:C:95:VAL:HG21 | 1:C:122:ARG:HG3 | 1.72 | 0.70 |
| 1:G:39:ASP:OD2 | 1:G:298:ARG:HD3 | 1.91 | 0.70 |
| 1:R:269:MET:HG2 | 1:R:306:TYR:HE1 | 1.57 | 0.70 |
| 1:E:84:ARG:NH1 | 1:E:509:PHE:CZ | 2.60 | 0.69 |
| 1:G:22:TYR:CE2 | 1:G:26:GLN:OE1 | 2.45 | 0.69 |
| 1:D:480:GLU:OE2 | 1:D:482:HIS:CD2 | 2.41 | 0.69 |
| 1:I:73:THR:OG1 | 1:I:76:GLY:HA2 | 1.92 | 0.69 |
| 1:R:349:LEU:HD12 | 1:R:415:ILE:HD13 | 1.74 | 0.69 |
| 1:G:547:GLU:OE2 | 1:G:550:ARG:NH2 | 2.24 | 0.69 |
| 1:H:169:VAL:CG1 | 1:H:241:GLU:HG2 | 2.22 | 0.69 |
| 1:I:550:ARG:H | 1:I:560:GLN:HE22 | 1.38 | 0.69 |
| 1:K:169:VAL:HG13 | 1:K:241:GLU:CG | 2.21 | 0.69 |
| 1:O:233:ILE:HD11 | 1:O:254:ARG:HB2 | 1.74 | 0.69 |
| 1:A:420:ILE:CD1 | 1:A:428:VAL:HG22 | 2.21 | 0.69 |
| 1:B:497:GLN:H | 1:B:497:GLN:NE2 | 1.90 | 0.69 |
| 1:D:145:GLU:HA | 1:D:269:MET:HE1 | 1.74 | 0.69 |
| 1:F:206:ARG:HH12 | 1:F:310:GLU:CG | 2.06 | 0.69 |
| 1:J:193:PRO:HA | 1:J:362:ASN:HD21 | 1.57 | 0.69 |
| 1:B:73:THR:HG22 | 1:B:94:GLU:HB2 | 1.72 | 0.69 |
| 1:K:516:GLU:O | 1:K:520:LYS:HG3 | 1.91 | 0.69 |
| 1:P:278:ASN:HB2 | 1:P:280:THR:HG22 | 1.74 | 0.69 |
| 1:B:447:GLU:N | 1:B:448:PRO:HA | 2.08 | 0.69 |
| 1:G:27:GLU:HG2 | 1:G:96:PHE:CE1 | 2.26 | 0.69 |
| 1:H:269:MET:HG2 | 1:H:306:TYR:CE1 | 2.28 | 0.69 |
| 1:J:67:HIS:HE1 | 1:J:91:THR:HG22 | 1.57 | 0.69 |
| 1:K:497:GLN:NE2 | 1:K:573:ASN:ND2 | 2.40 | 0.69 |
| 1:N:169:VAL:CG1 | 1:N:241:GLU:HG2 | 2.22 | 0.69 |
| 1:P:210:THR:HG21 | 4:P:810:HOH:O | 1.93 | 0.69 |
| 1:E:450:TYR:H | 1:E:459:HIS:CD2 | 2.09 | 0.69 |
| 1:Q:42:ARG:HH12 | 1:Q:140:GLU:HG2 | 1.58 | 0.69 |
| 1:A:269:MET:HG2 | 1:A:306:TYR:HE1 | 1.58 | 0.69 |
| 1:M:51:LYS:HG2 | 1:M:85:GLU:HG2 | 1.73 | 0.69 |
| 1:P:227:ARG:NH1 | 1:P:229:LEU:HD21 | 2.08 | 0.69 |
| 1:P:490:PRO:CB | 1:P:569:MET:HE1 | 2.22 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:210:THR:HB | 4:I:807:HOH:O | 1.92 | 0.69 |
| 1:N:87:ALA:CA | 1:N:88:ASP:HB2 | 2.22 | 0.69 |
| 1:D:67:HIS:CE1 | 1:D:91:THR:HG23 | 2.28 | 0.69 |
| 1:H:51:LYS:CG | 1:H:85:GLU:HG3 | 2.23 | 0.69 |
| 1:L:67:HIS:CE1 | 1:L:91:THR:CG2 | 2.66 | 0.69 |
| 1:M:37:ILE:HG21 | 1:M:503:VAL:CG1 | 2.23 | 0.69 |
| 1:N:27:GLU:OE2 | 1:N:96:PHE:CD1 | 2.45 | 0.69 |
| 1:A:434:VAL:HG12 | 1:A:469:LEU:HD13 | 1.74 | 0.69 |
| 1:C:39:ASP:OD2 | 1:C:298:ARG:HD3 | 1.93 | 0.69 |
| 1:N:566:ILE:CG2 | 1:N:569:MET:CE | 2.70 | 0.69 |
| 1:C:140:GLU:O | 1:C:140:GLU:HG3 | 1.92 | 0.68 |
| 1:Q:643:LYS:O | 1:Q:644:SER:HB3 | 1.93 | 0.68 |
| 1:B:412:PHE:HE2 | 1:B:451:MET:HG2 | 1.58 | 0.68 |
| 1:G:412:PHE:HE2 | 1:G:451:MET:HG2 | 1.58 | 0.68 |
| 1:O:567:ASP:O | 1:O:568:ASN:HB2 | 1.93 | 0.68 |
| 1:A:141:VAL:O | 1:A:141:VAL:HG13 | 1.92 | 0.68 |
| 1:B:42:ARG:HH11 | 1:B:140:GLU:HG2 | 1.58 | 0.68 |
| 1:B:169:VAL:CG1 | 1:B:241:GLU:HG2 | 2.24 | 0.68 |
| 1:H:269:MET:HG2 | 1:H:306:TYR:HE1 | 1.58 | 0.68 |
| 2:M:701:SAH:HB1 | 2:M:701:SAH:H4' | 1.76 | 0.68 |
| 1:K:580:GLU:HG2 | 1:K:589:SER:HB2 | 1.76 | 0.68 |
| 1:K:84:ARG:O | 1:K:85:GLU:HB2 | 1.93 | 0.68 |
| 1:M:145:GLU:CG | 1:M:331:LEU:HD13 | 2.24 | 0.68 |
| 1:P:190:ASN:HD21 | 1:P:209:GLY:HA3 | 1.59 | 0.68 |
| 1:R:433:LYS:CE | 1:R:433:LYS:H | 2.03 | 0.68 |
| 1:D:222:LYS:O | 1:D:225:GLU:HB2 | 1.93 | 0.68 |
| 1:R:433:LYS:N | 1:R:433:LYS:HE2 | 2.02 | 0.68 |
| 1:J:597:SER:CB | 1:J:598:ALA:HB2 | 2.19 | 0.68 |
| 1:N:315:GLU:HB2 | 1:N:318:GLN:HG2 | 1.75 | 0.68 |
| 1:A:39:ASP:OD2 | 1:A:298:ARG:HD3 | 1.93 | 0.68 |
| 1:M:569:MET:HG3 | 1:M:624:LEU:HD11 | 1.74 | 0.68 |
| 1:J:42:ARG:NH1 | 1:J:140:GLU:HG2 | 2.09 | 0.68 |
| 1:J:480:GLU:OE2 | 1:J:482:HIS:CD2 | 2.46 | 0.68 |
| 1:L:280:THR:HG23 | 1:L:281:THR:HG22 | 1.74 | 0.68 |
| 1:Q:480:GLU:OE2 | 1:Q:482:HIS:HD2 | 1.77 | 0.68 |
| 1:D:502:ASP:OD2 | 1:D:616:THR:HG21 | 1.94 | 0.68 |
| 1:P:42:ARG:HH21 | 1:P:43:ASN:HD21 | 1.41 | 0.68 |
| 1:D:490:PRO:CB | 1:D:569:MET:HE3 | 2.17 | 0.67 |
| 1:I:210:THR:CG2 | 4:I:809:HOH:O | 2.29 | 0.67 |
| 1:K:65:LYS:HA | 1:K:65:LYS:HE3 | 1.76 | 0.67 |
| 1:M:522:ARG:O | 1:M:526:ASP:HB2 | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:147:ILE:HD11 | 1:N:331:LEU:CD1 | 2.24 | 0.67 |
| 1:Q:264:ILE:HD11 | 1:Q:267:LEU:CD2 | 2.23 | 0.67 |
| 1:I:177:TYR:O | 1:I:269:MET:HA | 1.93 | 0.67 |
| 1:A:497:GLN:N | 1:A:497:GLN:HE21 | 1.87 | 0.67 |
| 1:B:168:ARG:HG2 | 1:B:168:ARG:HH11 | 1.59 | 0.67 |
| 1:H:244:GLU:H | 1:H:244:GLU:CD | 1.97 | 0.67 |
| 1:Q:137:ILE:CG1 | 1:Q:169:VAL:HG12 | 2.22 | 0.67 |
| 1:B:175:ASN:HD22 | 1:B:237:LYS:HG2 | 1.58 | 0.67 |
| 1:I:173:THR:HG22 | 1:I:274:ASP:HB3 | 1.76 | 0.67 |
| 1:Q:190:ASN:HD21 | 1:Q:209:GLY:HA3 | 1.59 | 0.67 |
| 1:A:480:GLU:CG | 1:A:584:GLY:H | 2.08 | 0.67 |
| 1:C:95:VAL:CG2 | 1:C:122:ARG:HG3 | 2.25 | 0.67 |
| 1:D:291:ASN:H | 1:D:292:LYS:HZ3 | 1.41 | 0.67 |
| 1:M:258:ALA:HB2 | 1:M:314:VAL:HG13 | 1.77 | 0.67 |
| 1:D:522:ARG:O | 1:D:526:ASP:HB2 | 1.95 | 0.67 |
| 1:C:618:LEU:HD23 | 1:C:624:LEU:HD22 | 1.75 | 0.67 |
| 1:D:497:GLN:NE2 | 1:D:497:GLN:N | 2.25 | 0.67 |
| 1:D:550:ARG:H | 1:D:560:GLN:HE22 | 1.43 | 0.67 |
| 1:H:478:ARG:HG2 | 1:H:478:ARG:NH2 | 2.04 | 0.67 |
| 1:M:214:PHE:CD2 | 1:M:305:VAL:HG22 | 2.30 | 0.67 |
| 1:N:63:ASP:HB2 | 1:N:65:LYS:N | 2.05 | 0.67 |
| 1:O:506:VAL:O | 1:O:509:PHE:HB2 | 1.95 | 0.67 |
| 1:P:152:LEU:HD22 | 1:P:246:ILE:HG23 | 1.76 | 0.67 |
| 1:E:565:ASN:HA | 1:E:624:LEU:O | 1.93 | 0.67 |
| 1:G:169:VAL:HG12 | 1:G:241:GLU:CG | 2.16 | 0.67 |
| 1:D:42:ARG:NH1 | 1:D:140:GLU:CG | 2.58 | 0.67 |
| 1:F:42:ARG:HH11 | 1:F:140:GLU:HG2 | 1.57 | 0.67 |
| 1:I:104:ARG:HG3 | 1:I:118:VAL:HB | 1.76 | 0.67 |
| 1:M:490:PRO:HB3 | 1:M:569:MET:CE | 2.25 | 0.67 |
| 1:N:497:GLN:HE21 | 1:N:497:GLN:H | 1.41 | 0.67 |
| 1:F:141:VAL:O | 1:F:141:VAL:HG12 | 1.94 | 0.66 |
| 1:J:218:LEU:H | 1:J:303:GLN:HE21 | 1.43 | 0.66 |
| 1:O:444:VAL:HG13 | 1:O:479:VAL:HA | 1.76 | 0.66 |
| 1:Q:480:GLU:OE2 | 1:Q:482:HIS:CD2 | 2.48 | 0.66 |
| 1:R:218:LEU:H | 1:R:303:GLN:HE21 | 1.43 | 0.66 |
| 1:R:384:ALA:HB2 | 1:R:437:LEU:HD11 | 1.76 | 0.66 |
| 1:A:434:VAL:CG1 | 1:A:469:LEU:CD1 | 2.73 | 0.66 |
| 1:E:169:VAL:CG1 | 1:E:241:GLU:HG2 | 2.24 | 0.66 |
| 1:G:42:ARG:HH21 | 1:G:43:ASN:ND2 | 1.93 | 0.66 |
| 1:N:137:ILE:HD11 | 1:N:163:ALA:HB2 | 1.77 | 0.66 |
| 1:N:163:ALA:HB1 | 1:N:167:CYS:SG | 2.35 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:50:LEU:O | 1:R:54:ILE:HB | 1.94 | 0.66 |
| 1:C:141:VAL:HG12 | 1:C:141:VAL:O | 1.94 | 0.66 |
| 1:J:490:PRO:HB2 | 1:J:569:MET:CE | 2.26 | 0.66 |
| 1:N:497:GLN:H | 1:N:497:GLN:NE2 | 1.93 | 0.66 |
| 1:D:489:ILE:HG13 | 1:D:490:PRO:HD2 | 1.78 | 0.66 |
| 1:G:478:ARG:HG3 | 1:G:478:ARG:HH21 | 1.60 | 0.66 |
| 1:J:239:ASP:OD2 | 1:J:242:HIS:CD2 | 2.49 | 0.66 |
| 1:N:478:ARG:HH21 | 1:N:478:ARG:CG | 2.09 | 0.66 |
| 1:P:506:VAL:HG23 | 1:P:511:LEU:HD12 | 1.78 | 0.66 |
| 1:Q:191:ASP:OD2 | 1:Q:194:ARG:NH1 | 2.29 | 0.66 |
| 1:R:460:LEU:HD11 | 1:R:637:ILE:HD11 | 1.78 | 0.66 |
| 1:E:318:GLN:OE1 | 1:H:368:GLN:HG2 | 1.96 | 0.66 |
| 1:I:414:ASP:O | 1:I:418:LYS:HG3 | 1.96 | 0.66 |
| 1:Q:91:THR:HG22 | 1:Q:117:THR:HG23 | 1.77 | 0.66 |
| 1:D:193:PRO:HA | 1:D:362:ASN:HD21 | 1.61 | 0.66 |
| 1:F:490:PRO:CB | 1:F:569:MET:HE1 | 2.19 | 0.66 |
| 1:G:490:PRO:HB3 | 1:G:569:MET:HE2 | 1.72 | 0.66 |
| 1:J:490:PRO:CB | 1:J:569:MET:HE2 | 2.26 | 0.66 |
| 1:I:541:VAL:HG23 | 1:I:601:PRO:HG3 | 1.78 | 0.66 |
| 1:M:83:ALA:HB1 | 1:M:112:TRP:CG | 2.30 | 0.66 |
| 1:N:480:GLU:OE2 | 1:N:482:HIS:CD2 | 2.45 | 0.66 |
| 1:O:528:ILE:HD12 | 1:O:528:ILE:N | 2.10 | 0.66 |
| 1:Q:69:LEU:HB3 | 1:Q:137:ILE:HG22 | 1.78 | 0.66 |
| 1:J:67:HIS:CE1 | 1:J:89:LYS:HD3 | 2.31 | 0.66 |
| 1:M:84:ARG:HD3 | 1:M:112:TRP:CH2 | 2.31 | 0.66 |
| 1:N:39:ASP:OD2 | 1:N:298:ARG:HD3 | 1.95 | 0.66 |
| 1:A:218:LEU:H | 1:A:303:GLN:NE2 | 1.94 | 0.66 |
| 1:J:601:PRO:HD2 | 4:J:812:HOH:O | 1.95 | 0.66 |
| 1:P:146:LEU:HB3 | 1:P:271:TRP:CD1 | 2.31 | 0.66 |
| 1:E:490:PRO:HB3 | 1:E:569:MET:HE3 | 1.77 | 0.66 |
| 1:F:171:PRO:HB3 | 1:F:273:ILE:HD12 | 1.76 | 0.66 |
| 1:K:349:LEU:HD11 | 1:K:353:LEU:HD12 | 1.78 | 0.66 |
| 1:G:559:SER:OG | 1:G:632:LYS:HB2 | 1.95 | 0.65 |
| 1:N:242:HIS:O | 1:N:245:LYS:HG2 | 1.94 | 0.65 |
| 1:A:141:VAL:O | 1:A:141:VAL:CG1 | 2.44 | 0.65 |
| 1:A:269:MET:HG2 | 1:A:306:TYR:CE1 | 2.31 | 0.65 |
| 1:G:173:THR:HB | 1:G:274:ASP:HB3 | 1.78 | 0.65 |
| 1:K:297:TRP:CD2 | 1:K:495:ASP:HB3 | 2.31 | 0.65 |
| 1:N:583:PHE:O | 1:N:586:ILE:HG12 | 1.95 | 0.65 |
| 1:O:218:LEU:HD13 | 1:O:268:LEU:HD13 | 1.78 | 0.65 |
| 1:Q:85:GLU:HG3 | 1:Q:85:GLU:O | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:73:THR:HG22 | 1:J:94:GLU:HB2 | 1.77 | 0.65 |
| 1:N:381:LEU:O | 1:N:400:ALA:HB1 | 1.95 | 0.65 |
| 1:O:126:VAL:O | 1:O:161:ARG:NH2 | 2.27 | 0.65 |
| 1:C:314:VAL:HG21 | 1:C:320:PHE:CE2 | 2.31 | 0.65 |
| 1:D:67:HIS:CE1 | 1:D:91:THR:CG2 | 2.79 | 0.65 |
| 1:O:382:HIS:ND1 | 1:O:402:ARG:HD3 | 2.12 | 0.65 |
| 1:Q:84:ARG:O | 1:Q:85:GLU:HB3 | 1.95 | 0.65 |
| 1:C:489:ILE:HD13 | 1:C:541:VAL:HG21 | 1.78 | 0.65 |
| 1:O:42:ARG:HH11 | 1:O:140:GLU:HG2 | 1.59 | 0.65 |
| 1:O:433:LYS:O | 1:O:436:SER:HB2 | 1.97 | 0.65 |
| 1:O:7:ASN:HD21 | 1:O:640:GLN:HE22 | 1.42 | 0.65 |
| 1:Q:421:HIS:O | 1:Q:424:LYS:HD3 | 1.97 | 0.65 |
| 1:R:597:SER:HA | 1:R:599:GLY:H | 1.62 | 0.65 |
| 1:D:193:PRO:HA | 1:D:362:ASN:ND2 | 2.11 | 0.65 |
| 1:D:42:ARG:HH11 | 1:D:140:GLU:CG | 2.07 | 0.65 |
| 1:L:168:ARG:NH2 | 1:L:276:ASP:O | 2.28 | 0.65 |
| 1:A:480:GLU:OE2 | 1:A:482:HIS:CD2 | 2.49 | 0.65 |
| 1:C:262:GLY:O | 1:C:314:VAL:HG12 | 1.96 | 0.65 |
| 1:H:623:SER:O | 1:H:624:LEU:HD23 | 1.97 | 0.65 |
| 1:J:273:ILE:HG13 | 1:J:275:MET:HE3 | 1.79 | 0.65 |
| 1:K:250:GLU:HB2 | 1:K:326:HIS:NE2 | 2.12 | 0.65 |
| 1:G:42:ARG:HH21 | 1:G:43:ASN:HD21 | 1.44 | 0.65 |
| 1:K:283:ILE:HG23 | 1:K:298:ARG:HH21 | 1.62 | 0.65 |
| 1:D:616:THR:HG23 | 4:D:822:HOH:O | 1.95 | 0.65 |
| 1:E:145:GLU:HG2 | 1:E:145:GLU:O | 1.95 | 0.65 |
| 1:J:159:LEU:HA | 1:J:163:ALA:HB3 | 1.79 | 0.65 |
| 1:K:217:GLN:HB2 | 1:K:536:GLU:HB3 | 1.78 | 0.65 |
| 1:C:314:VAL:CG2 | 1:C:320:PHE:HD2 | 2.10 | 0.64 |
| 1:D:169:VAL:HG22 | 1:D:171:PRO:O | 1.97 | 0.64 |
| 1:F:368:GLN:NE2 | 1:F:371:LYS:HE3 | 2.12 | 0.64 |
| 1:M:359:TYR:CE2 | 1:M:605:LYS:HB2 | 2.32 | 0.64 |
| 1:Q:143:ASP:O | 1:Q:145:GLU:N | 2.30 | 0.64 |
| 1:R:168:ARG:NH1 | 1:R:241:GLU:OE2 | 2.29 | 0.64 |
| 1:B:392:LEU:C | 1:B:392:LEU:HD23 | 2.17 | 0.64 |
| 1:D:629:LEU:HD21 | 1:E:438:THR:HG21 | 1.79 | 0.64 |
| 1:H:378:SER:HB3 | 1:H:383:VAL:HG11 | 1.79 | 0.64 |
| 1:H:502:ASP:OD2 | 1:H:616:THR:HG21 | 1.98 | 0.64 |
| 1:Q:323:VAL:HG11 | 1:Q:340:LYS:HE2 | 1.78 | 0.64 |
| 1:D:111:PRO:O | 1:D:112:TRP:HB2 | 1.97 | 0.64 |
| 1:I:277:ARG:O | 1:I:277:ARG:HG2 | 1.96 | 0.64 |
| 1:N:87:ALA:O | 1:N:115:LYS:HE3 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:352:MET:HG2 | 1:P:412:PHE:CE2 | 2.32 | 0.64 |
| 1:P:478:ARG:NH2 | 1:P:478:ARG:HG2 | 2.11 | 0.64 |
| 1:L:317:ASN:HD22 | 1:L:317:ASN:H | 1.44 | 0.64 |
| 1:N:39:ASP:OD2 | 1:N:298:ARG:HD2 | 1.98 | 0.64 |
| 1:Q:168:ARG:NH1 | 1:Q:168:ARG:HG2 | 2.02 | 0.64 |
| 1:A:63:ASP:O | 1:A:63:ASP:OD1 | 2.16 | 0.64 |
| 1:F:565:ASN:ND2 | 1:F:644:SER:HB2 | 2.12 | 0.64 |
| 1:N:550:ARG:H | 1:N:560:GLN:HE22 | 1.45 | 0.64 |
| 1:N:55:ALA:H | 1:N:58:LYS:HZ2 | 1.45 | 0.64 |
| 1:R:280:THR:HG23 | 1:R:281:THR:H | 1.63 | 0.64 |
| 1:H:61:ASN:ND2 | 1:H:65:LYS:O | 2.28 | 0.64 |
| 1:K:218:LEU:HB2 | 1:K:303:GLN:HE21 | 1.62 | 0.64 |
| 1:N:50:LEU:O | 1:N:54:ILE:CG2 | 2.46 | 0.64 |
| 1:P:4:GLU:O | 1:R:420:ILE:HD11 | 1.98 | 0.64 |
| 1:G:45:LYS:O | 1:G:275:MET:HG2 | 1.98 | 0.64 |
| 1:O:3:LEU:O | 1:O:15:TRP:HA | 1.98 | 0.64 |
| 1:N:462:PHE:O | 1:N:466:VAL:HG23 | 1.98 | 0.64 |
| 1:B:4:GLU:OE2 | 1:B:13:ARG:HD3 | 1.98 | 0.64 |
| 1:C:42:ARG:HH21 | 1:C:43:ASN:HD21 | 1.46 | 0.64 |
| 1:G:218:LEU:H | 1:G:303:GLN:NE2 | 1.96 | 0.64 |
| 1:G:474:GLY:HA3 | 1:G:476:GLU:OE2 | 1.98 | 0.64 |
| 1:J:218:LEU:H | 1:J:303:GLN:NE2 | 1.96 | 0.64 |
| 1:R:176:VAL:HG13 | 1:R:236:PHE:HB2 | 1.80 | 0.64 |
| 1:A:218:LEU:HD12 | 1:A:303:GLN:HB2 | 1.80 | 0.63 |
| 1:K:122:ARG:HD3 | 1:K:124:THR:OG1 | 1.98 | 0.63 |
| 1:P:375:ASP:O | 1:P:399:THR:HG21 | 1.97 | 0.63 |
| 1:P:38:LEU:HD13 | 1:P:498:ASN:HD22 | 1.63 | 0.63 |
| 1:C:269:MET:HG2 | 1:C:306:TYR:CE1 | 2.33 | 0.63 |
| 1:K:516:GLU:HG3 | 1:K:520:LYS:HE3 | 1.79 | 0.63 |
| 1:I:218:LEU:HD13 | 1:I:268:LEU:HD13 | 1.80 | 0.63 |
| 1:I:497:GLN:HE21 | 1:I:497:GLN:H | 0.77 | 0.63 |
| 1:L:450:TYR:H | 1:L:459:HIS:HD2 | 1.45 | 0.63 |
| 1:M:83:ALA:HB1 | 1:M:112:TRP:CB | 2.28 | 0.63 |
| 1:P:141:VAL:O | 1:P:141:VAL:HG12 | 1.96 | 0.63 |
| 1:L:168:ARG:HH11 | 1:L:168:ARG:CG | 2.11 | 0.63 |
| 1:A:480:GLU:OE2 | 1:A:482:HIS:HD2 | 1.80 | 0.63 |
| 1:K:68:VAL:CG2 | 1:K:136:ILE:HB | 2.26 | 0.63 |
| 1:K:46:PHE:CE2 | 1:K:140:GLU:HB2 | 2.33 | 0.63 |
| 1:M:43:ASN:N | 1:M:43:ASN:HD22 | 1.96 | 0.63 |
| 1:E:103:ALA:O | 1:E:107:THR:HB | 1.97 | 0.63 |
| 1:H:84:ARG:O | 1:H:85:GLU:HB2 | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:109:ASN:N | 1:A:109:ASN:HD22 | 1.96 | 0.63 |
| 1:I:543:GLY:HA3 | 1:I:568:ASN:ND2 | 2.14 | 0.63 |
| 1:K:624:LEU:H | 1:K:624:LEU:HD12 | 1.64 | 0.63 |
| 1:O:218:LEU:H | 1:O:303:GLN:HE21 | 1.43 | 0.63 |
| 1:R:497:GLN:HE21 | 1:R:497:GLN:H | 1.44 | 0.63 |
| 1:B:41:ASP:O | 1:B:44:ASP:N | 2.30 | 0.63 |
| 1:H:156:LYS:O | 1:H:160:GLU:HG2 | 1.98 | 0.63 |
| 1:L:577:MET:HE2 | 1:L:626:LEU:HD11 | 1.80 | 0.63 |
| 1:M:434:VAL:CG1 | 1:M:469:LEU:HD13 | 2.28 | 0.63 |
| 1:Q:169:VAL:HG23 | 1:Q:172:SER:HA | 1.79 | 0.63 |
| 1:Q:528:ILE:HD13 | 1:Q:639:PHE:O | 1.99 | 0.63 |
| 1:C:103:ALA:O | 1:C:107:THR:HB | 1.99 | 0.63 |
| 1:E:176:VAL:HG13 | 1:E:236:PHE:HB2 | 1.81 | 0.63 |
| 1:K:169:VAL:HG22 | 1:K:171:PRO:O | 1.99 | 0.63 |
| 1:Q:73:THR:OG1 | 1:Q:76:GLY:HA2 | 1.98 | 0.63 |
| 1:I:193:PRO:HA | 1:I:362:ASN:HD21 | 1.63 | 0.62 |
| 1:A:577:MET:HE1 | 1:A:639:PHE:CE1 | 2.33 | 0.62 |
| 1:I:171:PRO:HB3 | 1:I:275:MET:CE | 2.29 | 0.62 |
| 1:K:141:VAL:CG1 | 1:K:141:VAL:O | 2.47 | 0.62 |
| 1:C:353:LEU:HD22 | 1:C:357:THR:HG21 | 1.81 | 0.62 |
| 1:E:135:ASP:OD1 | 1:E:164:LYS:HD2 | 2.00 | 0.62 |
| 1:H:42:ARG:HH21 | 1:H:43:ASN:HD21 | 1.47 | 0.62 |
| 1:I:534:LEU:HD11 | 1:I:576:PRO:HB3 | 1.80 | 0.62 |
| 1:I:63:ASP:OD2 | 1:I:65:LYS:HB2 | 2.00 | 0.62 |
| 1:G:161:ARG:HB2 | 1:G:162:LEU:HD22 | 1.82 | 0.62 |
| 1:I:157:GLU:HA | 1:I:160:GLU:HG2 | 1.81 | 0.62 |
| 1:K:510:ASP:OD2 | 1:K:512:SER:HB3 | 1.99 | 0.62 |
| 1:I:420:ILE:CD1 | 1:I:428:VAL:HG22 | 2.29 | 0.62 |
| 1:O:112:TRP:CZ3 | 1:O:509:PHE:HE1 | 2.18 | 0.62 |
| 1:C:191:ASP:OD2 | 1:C:194:ARG:NH1 | 2.32 | 0.62 |
| 1:G:72:GLY:O | 2:G:701:SAH:N | 2.31 | 0.62 |
| 1:I:178:ILE:HA | 1:I:268:LEU:O | 1.98 | 0.62 |
| 1:M:382:HIS:CD2 | 1:M:402:ARG:HG3 | 2.34 | 0.62 |
| 1:R:467:GLU:HG3 | 1:R:556:ARG:HD2 | 1.81 | 0.62 |
| 1:F:42:ARG:HH21 | 1:F:43:ASN:HD21 | 1.48 | 0.62 |
| 1:K:108:SER:O | 1:K:113:SER:HB2 | 1.99 | 0.62 |
| 1:L:506:VAL:HG12 | 1:L:507:ASN:HD22 | 1.64 | 0.62 |
| 1:M:356:GLN:O | 1:M:359:TYR:HB3 | 1.99 | 0.62 |
| 1:N:54:ILE:HD11 | 1:N:87:ALA:N | 2.14 | 0.62 |
| 1:C:194:ARG:HB3 | 1:C:201:GLU:OE1 | 2.00 | 0.62 |
| 1:D:168:ARG:HG2 | 1:D:168:ARG:NH1 | 2.07 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:274:ASP:HA | 1:E:282:PHE:HD1 | 1.64 | 0.62 |
| 1:H:51:LYS:HG3 | 1:H:85:GLU:HG3 | 1.81 | 0.62 |
| 1:R:356:GLN:O | 1:R:606:GLY:HA2 | 2.00 | 0.62 |
| 1:I:26:GLN:CG | 1:I:30:ARG:HH12 | 1.99 | 0.62 |
| 1:J:39:ASP:OD2 | 1:J:298:ARG:CD | 2.43 | 0.62 |
| 1:N:218:LEU:H | 1:N:303:GLN:NE2 | 1.98 | 0.62 |
| 1:Q:379:LYS:HA | 1:Q:399:THR:OG1 | 2.00 | 0.62 |
| 1:Q:97:LYS:HB2 | 1:Q:98:PRO:HD3 | 1.80 | 0.62 |
| 1:D:622:LYS:H | 1:D:622:LYS:HD3 | 1.64 | 0.62 |
| 1:I:176:VAL:HG22 | 1:I:235:ALA:HB3 | 1.82 | 0.62 |
| 1:I:292:LYS:HG2 | 1:I:293:ASN:HA | 1.79 | 0.62 |
| 1:K:167:CYS:SG | 1:K:168:ARG:N | 2.73 | 0.62 |
| 1:N:379:LYS:CA | 1:N:399:THR:HG22 | 2.18 | 0.62 |
| 1:P:227:ARG:HH12 | 1:P:229:LEU:HD21 | 1.64 | 0.62 |
| 1:G:108:SER:O | 1:G:109:ASN:HB2 | 2.01 | 0.61 |
| 1:L:379:LYS:CA | 1:L:399:THR:HG23 | 2.28 | 0.61 |
| 1:N:133:ARG:CG | 1:N:164:LYS:HG3 | 2.29 | 0.61 |
| 1:C:337:GLY:O | 1:C:338:LYS:HD2 | 2.00 | 0.61 |
| 1:E:497:GLN:H | 1:E:497:GLN:HE21 | 1.46 | 0.61 |
| 1:F:259:HIS:HD2 | 1:F:260:SER:OG | 1.83 | 0.61 |
| 1:I:480:GLU:OE2 | 1:I:482:HIS:HD2 | 1.83 | 0.61 |
| 1:K:250:GLU:HB2 | 1:K:326:HIS:CD2 | 2.33 | 0.61 |
| 1:N:565:ASN:ND2 | 1:N:644:SER:OG | 2.32 | 0.61 |
| 1:D:622:LYS:N | 1:D:622:LYS:HD3 | 2.15 | 0.61 |
| 1:F:243:GLU:HA | 1:F:246:ILE:HD12 | 1.82 | 0.61 |
| 1:G:95:VAL:CG2 | 1:G:95:VAL:O | 2.47 | 0.61 |
| 1:J:563:VAL:HG13 | 1:J:625:CYS:SG | 2.40 | 0.61 |
| 1:K:445:LEU:HD12 | 1:K:480:GLU:HB2 | 1.81 | 0.61 |
| 1:P:352:MET:HG2 | 1:P:412:PHE:CZ | 2.35 | 0.61 |
| 1:J:470:LYS:HD2 | 1:J:554:ASP:O | 2.00 | 0.61 |
| 1:L:577:MET:HE3 | 1:L:641:PHE:CZ | 2.23 | 0.61 |
| 1:O:548:ILE:O | 1:O:549:LEU:HD13 | 2.01 | 0.61 |
| 1:Q:417:PHE:CZ | 1:Q:430:ILE:HB | 2.36 | 0.61 |
| 1:B:39:ASP:OD2 | 1:B:298:ARG:CD | 2.45 | 0.61 |
| 1:K:77:LEU:HD22 | 1:K:511:LEU:HD11 | 1.83 | 0.61 |
| 1:K:573:ASN:O | 1:K:614:PRO:HD2 | 1.99 | 0.61 |
| 1:N:218:LEU:HD12 | 1:N:303:GLN:HB2 | 1.81 | 0.61 |
| 1:M:3:LEU:HD22 | 1:O:418:LYS:HA | 1.83 | 0.61 |
| 1:P:550:ARG:H | 1:P:560:GLN:HE22 | 1.47 | 0.61 |
| 1:C:5:LYS:NZ | 1:C:14:GLU:OE1 | 2.34 | 0.61 |
| 1:G:218:LEU:H | 1:G:303:GLN:HE21 | 1.48 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:216:VAL:O | 1:C:302:MET:HG2 | 2.00 | 0.61 |
| 1:K:475:ASP:OD1 | 1:K:475:ASP:N | 2.33 | 0.61 |
| 1:M:42:ARG:HA | 1:M:283:ILE:HD11 | 1.82 | 0.61 |
| 1:N:444:VAL:CG1 | 1:N:479:VAL:HB | 2.24 | 0.61 |
| 1:J:189:PHE:CE1 | 1:J:359:TYR:HB2 | 2.36 | 0.61 |
| 1:K:39:ASP:O | 1:K:42:ARG:HB3 | 2.01 | 0.61 |
| 1:L:133:ARG:HB2 | 1:L:164:LYS:HG3 | 1.81 | 0.61 |
| 1:O:587:ASN:HD22 | 1:O:588:LEU:N | 1.98 | 0.61 |
| 1:Q:460:LEU:HB3 | 1:Q:463:LEU:HD23 | 1.81 | 0.61 |
| 1:Q:92:ALA:HB3 | 1:Q:118:VAL:HG23 | 1.83 | 0.61 |
| 1:R:275:MET:HE1 | 1:R:283:ILE:HG13 | 1.82 | 0.61 |
| 1:B:447:GLU:H | 1:B:448:PRO:HA | 1.64 | 0.61 |
| 1:E:241:GLU:HG3 | 1:E:277:ARG:HH21 | 1.65 | 0.61 |
| 1:J:67:HIS:HE1 | 1:J:91:THR:CG2 | 2.14 | 0.61 |
| 1:M:196:ASN:HB2 | 1:M:201:GLU:OE2 | 2.01 | 0.61 |
| 1:Q:35:ASP:OD1 | 1:Q:299:ASP:HB3 | 2.01 | 0.61 |
| 1:B:269:MET:HG2 | 1:B:306:TYR:CE2 | 2.35 | 0.60 |
| 1:F:218:LEU:N | 1:F:303:GLN:NE2 | 2.34 | 0.60 |
| 1:H:190:ASN:HD21 | 1:H:209:GLY:HA3 | 1.66 | 0.60 |
| 1:J:182:GLU:HG3 | 1:J:263:THR:O | 2.01 | 0.60 |
| 1:Q:69:LEU:HD12 | 1:Q:91:THR:OG1 | 2.02 | 0.60 |
| 1:A:480:GLU:HG3 | 1:A:481:PRO:HA | 1.84 | 0.60 |
| 1:E:511:LEU:O | 1:E:514:PHE:N | 2.30 | 0.60 |
| 1:H:420:ILE:HD11 | 1:H:428:VAL:HG22 | 1.83 | 0.60 |
| 1:O:275:MET:HE1 | 1:O:283:ILE:H | 1.66 | 0.60 |
| 1:P:5:LYS:NZ | 1:P:14:GLU:OE1 | 2.34 | 0.60 |
| 1:R:146:LEU:HB2 | 1:R:271:TRP:CD1 | 2.35 | 0.60 |
| 1:I:273:ILE:CD1 | 1:I:275:MET:HE1 | 2.31 | 0.60 |
| 1:K:241:GLU:HB2 | 1:K:277:ARG:HH21 | 1.65 | 0.60 |
| 1:M:182:GLU:OE2 | 1:M:227:ARG:NH1 | 2.34 | 0.60 |
| 1:M:478:ARG:NH2 | 1:M:478:ARG:CG | 2.50 | 0.60 |
| 1:A:291:ASN:H | 1:A:292:LYS:NZ | 1.99 | 0.60 |
| 1:C:460:LEU:HB3 | 1:C:463:LEU:HD23 | 1.83 | 0.60 |
| 1:E:258:ALA:O | 1:E:317:ASN:HA | 2.01 | 0.60 |
| 1:E:72:GLY:HA3 | 2:E:701:SAH:O4' | 2.01 | 0.60 |
| 1:I:502:ASP:OD2 | 1:I:616:THR:HG21 | 2.01 | 0.60 |
| 1:P:365:PHE:O | 1:P:371:LYS:HE3 | 2.01 | 0.60 |
| 1:R:562:CYS:SG | 1:R:564:VAL:HG13 | 2.42 | 0.60 |
| 1:A:45:LYS:O | 1:A:275:MET:HG2 | 2.02 | 0.60 |
| 1:F:196:ASN:O | 1:F:198:GLU:N | 2.33 | 0.60 |
| 1:M:143:ASP:HB3 | 1:M:149:GLU:OE1 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:114:ASP:HB3 | 1:B:65:LYS:NZ | 2.16 | 0.60 |
| 1:A:185:LEU:O | 1:A:188:MET:HB2 | 2.01 | 0.60 |
| 1:L:577:MET:CE | 1:L:626:LEU:HD11 | 2.31 | 0.60 |
| 1:R:203:PRO:HA | 1:R:422:TYR:CG | 2.37 | 0.60 |
| 1:C:168:ARG:NH2 | 1:C:276:ASP:O | 2.34 | 0.60 |
| 1:J:91:THR:HG21 | 1:J:129:ILE:CG2 | 2.32 | 0.60 |
| 1:J:597:SER:CB | 1:J:598:ALA:CB | 2.77 | 0.60 |
| 1:L:446:ALA:O | 1:L:481:PRO:HD3 | 2.01 | 0.60 |
| 1:N:54:ILE:C | 1:N:58:LYS:NZ | 2.55 | 0.60 |
| 1:O:135:ASP:OD1 | 1:O:164:LYS:HD2 | 2.02 | 0.60 |
| 1:A:577:MET:CE | 1:A:639:PHE:CE1 | 2.84 | 0.60 |
| 1:C:489:ILE:CD1 | 1:C:541:VAL:HG21 | 2.31 | 0.60 |
| 1:G:169:VAL:HG13 | 1:G:172:SER:HA | 1.82 | 0.60 |
| 1:J:141:VAL:O | 1:J:141:VAL:HG13 | 2.00 | 0.60 |
| 1:Q:583:PHE:HB3 | 1:Q:588:LEU:HD12 | 1.82 | 0.60 |
| 1:Q:95:VAL:HB | 1:Q:122:ARG:HG3 | 1.84 | 0.60 |
| 1:C:547:GLU:OE1 | 1:C:550:ARG:NH1 | 2.35 | 0.60 |
| 1:D:622:LYS:CD | 1:D:622:LYS:H | 2.15 | 0.60 |
| 1:I:470:LYS:O | 1:I:473:HIS:O | 2.20 | 0.60 |
| 1:M:218:LEU:H | 1:M:303:GLN:NE2 | 2.00 | 0.60 |
| 1:N:36:MET:HA | 1:N:300:HIS:CD2 | 2.36 | 0.60 |
| 1:Q:480:GLU:CG | 1:Q:584:GLY:H | 2.14 | 0.60 |
| 1:B:480:GLU:OE2 | 1:B:482:HIS:HD2 | 1.86 | 0.59 |
| 1:B:66:VAL:HG12 | 1:B:67:HIS:H | 1.66 | 0.59 |
| 1:J:243:GLU:H | 1:J:243:GLU:CD | 2.00 | 0.59 |
| 1:P:84:ARG:C | 1:P:86:GLY:H | 2.05 | 0.59 |
| 1:B:490:PRO:CB | 1:B:569:MET:CE | 2.60 | 0.59 |
| 1:K:373:GLU:HA | 1:K:373:GLU:OE1 | 2.02 | 0.59 |
| 1:D:434:VAL:CG1 | 1:D:469:LEU:CD1 | 2.80 | 0.59 |
| 1:F:142:PHE:CD1 | 1:F:146:LEU:HD12 | 2.37 | 0.59 |
| 1:G:22:TYR:HE2 | 1:G:26:GLN:OE1 | 1.83 | 0.59 |
| 1:N:168:ARG:HG2 | 1:N:168:ARG:NH1 | 2.13 | 0.59 |
| 1:Q:550:ARG:H | 1:Q:560:GLN:HE21 | 1.50 | 0.59 |
| 1:Q:77:LEU:HA | 1:Q:80:LEU:HD12 | 1.83 | 0.59 |
| 1:B:54:ILE:O | 1:B:58:LYS:HG2 | 2.03 | 0.59 |
| 1:G:434:VAL:CG1 | 1:G:469:LEU:HD13 | 2.32 | 0.59 |
| 1:M:492:LYS:HB2 | 1:M:572:SER:HA | 1.84 | 0.59 |
| 1:P:310:GLU:OE2 | 1:P:338:LYS:HD2 | 2.02 | 0.59 |
| 1:Q:480:GLU:HG3 | 1:Q:584:GLY:N | 2.18 | 0.59 |
| 1:R:175:ASN:HD21 | 1:R:237:LYS:HG2 | 1.66 | 0.59 |
| 1:C:291:ASN:HB3 | 1:C:295:TYR:HB2 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:143:ASP:OD2 | 1:D:148:GLY:HA3 | 2.02 | 0.59 |
| 1:D:379:LYS:CA | 1:D:399:THR:CG2 | 2.80 | 0.59 |
| 1:F:451:MET:HG3 | 1:F:452:SER:N | 2.18 | 0.59 |
| 1:L:126:VAL:HG11 | 1:L:129:ILE:HD13 | 1.85 | 0.59 |
| 1:M:84:ARG:HD3 | 1:M:112:TRP:HH2 | 1.66 | 0.59 |
| 1:P:190:ASN:ND2 | 1:P:209:GLY:HA3 | 2.17 | 0.59 |
| 1:Q:73:THR:O | 2:Q:701:SAH:HA | 2.02 | 0.59 |
| 1:A:497:GLN:N | 1:A:497:GLN:NE2 | 2.46 | 0.59 |
| 1:A:67:HIS:HE1 | 1:A:91:THR:HG23 | 1.66 | 0.59 |
| 1:B:476:GLU:H | 1:B:476:GLU:CD | 2.05 | 0.59 |
| 1:I:269:MET:HG2 | 1:I:306:TYR:HE1 | 1.68 | 0.59 |
| 1:Q:231:GLU:O | 1:Q:232:PRO:C | 2.39 | 0.59 |
| 1:R:556:ARG:CG | 1:R:556:ARG:NH1 | 2.62 | 0.59 |
| 1:H:52:THR:O | 1:H:55:ALA:HB3 | 2.02 | 0.59 |
| 1:K:190:ASN:HD21 | 1:K:209:GLY:HA3 | 1.67 | 0.59 |
| 1:N:142:PHE:CD1 | 1:N:146:LEU:CD1 | 2.85 | 0.59 |
| 1:F:42:ARG:HH12 | 1:F:140:GLU:HG2 | 1.62 | 0.59 |
| 1:N:275:MET:HE1 | 1:N:283:ILE:N | 2.17 | 0.59 |
| 1:C:84:ARG:NH1 | 1:O:280:THR:HG23 | 2.18 | 0.59 |
| 1:P:156:LYS:O | 1:P:160:GLU:HG2 | 2.02 | 0.59 |
| 1:P:138:VAL:HG23 | 1:P:170:VAL:HB | 1.83 | 0.59 |
| 1:B:41:ASP:O | 1:B:42:ARG:C | 2.41 | 0.59 |
| 1:I:35:ASP:OD1 | 1:I:300:HIS:HD2 | 1.86 | 0.59 |
| 1:M:141:VAL:HG12 | 1:M:141:VAL:O | 2.02 | 0.59 |
| 1:M:84:ARG:HG2 | 1:M:85:GLU:OE1 | 2.01 | 0.59 |
| 1:N:54:ILE:HD11 | 1:N:87:ALA:H | 1.67 | 0.59 |
| 1:Q:102:CYS:HA | 1:Q:513:PHE:HE2 | 1.68 | 0.59 |
| 1:M:32:ARG:HG3 | 1:M:34:GLY:H | 1.68 | 0.59 |
| 1:M:379:LYS:CA | 1:M:399:THR:CG2 | 2.80 | 0.59 |
| 1:N:254:ARG:O | 1:N:321:GLU:CA | 2.49 | 0.59 |
| 1:O:67:HIS:HE1 | 1:O:91:THR:OG1 | 1.86 | 0.59 |
| 1:Q:583:PHE:CB | 1:Q:588:LEU:HD12 | 2.33 | 0.59 |
| 1:P:5:LYS:CA | 1:R:420:ILE:HD11 | 2.33 | 0.59 |
| 1:B:245:LYS:HE3 | 1:E:337:GLY:HA2 | 1.85 | 0.58 |
| 1:K:53:THR:HG22 | 1:K:168:ARG:HE | 1.68 | 0.58 |
| 1:M:280:THR:HG23 | 1:M:281:THR:N | 2.18 | 0.58 |
| 1:O:373:GLU:HG3 | 1:O:377:LEU:CD1 | 2.32 | 0.58 |
| 1:Q:258:ALA:O | 1:Q:259:HIS:HB3 | 2.03 | 0.58 |
| 1:Q:365:PHE:O | 1:Q:371:LYS:HE3 | 2.03 | 0.58 |
| 1:Q:375:ASP:HA | 1:Q:399:THR:CG2 | 2.18 | 0.58 |
| 1:R:181:VAL:HG22 | 1:R:228:GLU:HA | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:486:LEU:HD12 | 1:C:548:ILE:HB | 1.85 | 0.58 |
| 1:J:4:GLU:OE2 | 1:J:13:ARG:HD3 | 2.02 | 0.58 |
| 1:L:497:GLN:NE2 | 1:L:497:GLN:H | 2.01 | 0.58 |
| 1:P:241:GLU:CG | 1:P:277:ARG:HH21 | 2.10 | 0.58 |
| 1:P:367:ASN:OD1 | 1:P:369:LYS:HG2 | 2.02 | 0.58 |
| 1:R:491:GLU:HG2 | 1:R:493:PHE:CD2 | 2.38 | 0.58 |
| 1:A:434:VAL:HG12 | 1:A:469:LEU:CD1 | 2.34 | 0.58 |
| 1:M:176:VAL:HG21 | 1:M:236:PHE:HD2 | 1.68 | 0.58 |
| 1:M:37:ILE:HG21 | 1:M:503:VAL:HG11 | 1.85 | 0.58 |
| 1:B:140:GLU:OE1 | 1:B:301:TRP:HZ2 | 1.86 | 0.58 |
| 1:K:39:ASP:OD1 | 1:K:298:ARG:NH1 | 2.36 | 0.58 |
| 1:M:110:SER:HB2 | 1:M:111:PRO:CD | 2.31 | 0.58 |
| 1:M:490:PRO:HB3 | 1:M:569:MET:HE2 | 1.85 | 0.58 |
| 1:N:490:PRO:HB3 | 1:N:569:MET:HE1 | 1.85 | 0.58 |
| 1:E:142:PHE:CD1 | 1:E:146:LEU:HD12 | 2.39 | 0.58 |
| 1:E:218:LEU:H | 1:E:303:GLN:NE2 | 2.00 | 0.58 |
| 1:J:451:MET:HG3 | 1:J:452:SER:N | 2.18 | 0.58 |
| 1:L:577:MET:CE | 1:L:641:PHE:CZ | 2.80 | 0.58 |
| 1:O:168:ARG:NH2 | 1:O:276:ASP:O | 2.33 | 0.58 |
| 1:O:245:LYS:HD3 | 1:P:337:GLY:HA2 | 1.86 | 0.58 |
| 1:P:497:GLN:NE2 | 1:P:497:GLN:H | 2.01 | 0.58 |
| 1:Q:497:GLN:H | 1:Q:497:GLN:NE2 | 2.02 | 0.58 |
| 1:F:522:ARG:O | 1:F:526:ASP:HB2 | 2.04 | 0.58 |
| 1:H:385:THR:HG22 | 4:H:820:HOH:O | 2.04 | 0.58 |
| 1:H:83:ALA:C | 1:H:84:ARG:O | 2.39 | 0.58 |
| 1:N:184:HIS:O | 1:N:188:MET:HG3 | 2.03 | 0.58 |
| 1:O:370:PHE:HE1 | 1:O:588:LEU:CD2 | 2.17 | 0.58 |
| 1:P:146:LEU:CD2 | 1:P:146:LEU:H | 2.12 | 0.58 |
| 1:R:180:PRO:HD2 | 1:R:230:SER:HB3 | 1.84 | 0.58 |
| 1:E:383:VAL:HG21 | 1:E:445:LEU:HD22 | 1.84 | 0.58 |
| 1:J:403:VAL:HB | 1:J:428:VAL:HB | 1.85 | 0.58 |
| 1:M:169:VAL:HG11 | 1:M:241:GLU:HA | 1.86 | 0.58 |
| 1:N:58:LYS:CE | 1:N:66:VAL:HG21 | 2.31 | 0.58 |
| 1:Q:222:LYS:CB | 1:Q:224:HIS:HB3 | 2.33 | 0.58 |
| 1:G:385:THR:HG21 | 1:G:405:ILE:HG23 | 1.86 | 0.58 |
| 1:H:141:VAL:O | 1:H:141:VAL:HG13 | 2.04 | 0.58 |
| 1:N:53:THR:O | 1:N:58:LYS:NZ | 2.37 | 0.58 |
| 1:P:541:VAL:HG23 | 1:P:601:PRO:HG3 | 1.84 | 0.58 |
| 1:Q:39:ASP:OD2 | 1:Q:298:ARG:HB3 | 2.04 | 0.58 |
| 1:F:168:ARG:HA | 1:F:241:GLU:OE2 | 2.04 | 0.58 |
| 1:F:206:ARG:NH1 | 1:F:310:GLU:HG3 | 2.17 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:36:MET:HB3 | 1:M:300:HIS:CG | 2.39 | 0.58 |
| 1:N:354:SER:OG | 1:N:357:THR:OG1 | 2.21 | 0.58 |
| 1:O:497:GLN:N | 1:O:497:GLN:HE21 | 1.95 | 0.58 |
| 1:P:7:ASN:HD21 | 1:P:640:GLN:HE22 | 1.51 | 0.58 |
| 1:R:530:ASP:O | 1:R:610:GLY:HA2 | 2.04 | 0.58 |
| 1:C:68:VAL:HB | 1:C:90:VAL:HG22 | 1.85 | 0.58 |
| 1:E:317:ASN:N | 1:E:317:ASN:ND2 | 2.41 | 0.58 |
| 1:F:373:GLU:OE2 | 1:F:585:GLY:N | 2.26 | 0.58 |
| 1:G:66:VAL:CG1 | 1:G:87:ALA:HA | 2.34 | 0.58 |
| 1:I:478:ARG:HH21 | 1:I:478:ARG:CG | 2.16 | 0.58 |
| 1:L:480:GLU:OE2 | 1:L:482:HIS:HD2 | 1.87 | 0.58 |
| 1:O:112:TRP:HZ3 | 1:O:509:PHE:HE1 | 1.52 | 0.58 |
| 1:Q:110:SER:HB2 | 1:Q:111:PRO:CD | 2.34 | 0.58 |
| 1:R:80:LEU:HB3 | 1:R:509:PHE:CD1 | 2.39 | 0.58 |
| 1:B:94:GLU:OE2 | 2:B:701:SAH:O3' | 2.22 | 0.57 |
| 1:E:140:GLU:HG3 | 1:E:140:GLU:O | 2.04 | 0.57 |
| 1:I:157:GLU:HA | 1:I:160:GLU:CG | 2.34 | 0.57 |
| 1:I:278:ASN:O | 1:I:280:THR:N | 2.37 | 0.57 |
| 1:M:37:ILE:HG21 | 1:M:503:VAL:HG13 | 1.85 | 0.57 |
| 1:N:242:HIS:HB3 | 1:N:245:LYS:CD | 2.34 | 0.57 |
| 1:O:80:LEU:HB3 | 1:O:509:PHE:CZ | 2.38 | 0.57 |
| 1:Q:122:ARG:HH21 | 1:Q:124:THR:HG21 | 1.69 | 0.57 |
| 1:B:480:GLU:OE2 | 1:B:482:HIS:CD2 | 2.57 | 0.57 |
| 1:K:84:ARG:HB2 | 1:K:112:TRP:CE2 | 2.39 | 0.57 |
| 1:L:403:VAL:HB | 1:L:428:VAL:HB | 1.85 | 0.57 |
| 1:M:67:HIS:CD2 | 1:M:133:ARG:O | 2.56 | 0.57 |
| 1:O:194:ARG:HG2 | 1:O:201:GLU:CB | 2.34 | 0.57 |
| 1:A:269:MET:CG | 1:A:306:TYR:HE1 | 2.17 | 0.57 |
| 1:A:490:PRO:CB | 1:A:569:MET:CE | 2.64 | 0.57 |
| 1:E:383:VAL:HB | 1:E:443:ILE:HG23 | 1.84 | 0.57 |
| 1:J:144:THR:O | 1:J:269:MET:CE | 2.53 | 0.57 |
| 1:J:618:LEU:HG | 1:J:624:LEU:HD22 | 1.86 | 0.57 |
| 1:K:179:VAL:HG21 | 1:K:270:TRP:CH2 | 2.39 | 0.57 |
| 1:P:45:LYS:HG2 | 1:P:282:PHE:O | 2.04 | 0.57 |
| 1:Q:150:GLY:O | 1:Q:154:THR:OG1 | 2.22 | 0.57 |
| 1:C:288:LYS:O | 1:C:290:LYS:N | 2.37 | 0.57 |
| 1:D:373:GLU:OE2 | 1:D:585:GLY:N | 2.26 | 0.57 |
| 1:D:50:LEU:O | 1:D:54:ILE:HG13 | 2.05 | 0.57 |
| 1:G:81:MET:O | 1:G:84:ARG:HB3 | 2.04 | 0.57 |
| 1:L:434:VAL:CG1 | 1:L:469:LEU:HD13 | 2.35 | 0.57 |
| 1:L:541:VAL:HG11 | 1:L:595:ILE:HD13 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:95:VAL:HG13 | 1:M:96:PHE:N | 2.19 | 0.57 |
| 1:O:193:PRO:HA | 1:O:362:ASN:HD21 | 1.69 | 0.57 |
| 1:P:253:VAL:O | 1:P:253:VAL:CG2 | 2.52 | 0.57 |
| 1:A:155:PHE:O | 1:A:159:LEU:HG | 2.04 | 0.57 |
| 1:D:43:ASN:HB3 | 1:D:507:ASN:HD21 | 1.68 | 0.57 |
| 1:E:439:ASP:N | 1:E:439:ASP:OD1 | 2.36 | 0.57 |
| 1:F:141:VAL:CG1 | 1:F:141:VAL:O | 2.51 | 0.57 |
| 1:H:77:LEU:HD13 | 1:H:511:LEU:HD11 | 1.86 | 0.57 |
| 1:J:158:ALA:HA | 1:J:162:LEU:CD2 | 2.30 | 0.57 |
| 1:J:274:ASP:OD2 | 1:J:277:ARG:HA | 2.04 | 0.57 |
| 1:K:548:ILE:HG22 | 1:K:549:LEU:HD22 | 1.87 | 0.57 |
| 1:M:32:ARG:HG3 | 1:M:34:GLY:N | 2.19 | 0.57 |
| 1:O:141:VAL:O | 1:O:141:VAL:HG13 | 2.05 | 0.57 |
| 1:O:557:VAL:HG22 | 1:O:632:LYS:HB2 | 1.85 | 0.57 |
| 1:Q:239:ASP:OD1 | 1:Q:241:GLU:HB2 | 2.03 | 0.57 |
| 1:A:168:ARG:NH2 | 1:A:276:ASP:O | 2.37 | 0.57 |
| 1:A:291:ASN:H | 1:A:292:LYS:HZ3 | 1.53 | 0.57 |
| 1:A:379:LYS:HA | 1:A:399:THR:HG23 | 1.86 | 0.57 |
| 1:I:169:VAL:HG22 | 1:I:171:PRO:O | 2.04 | 0.57 |
| 1:J:497:GLN:N | 1:J:497:GLN:NE2 | 2.51 | 0.57 |
| 1:L:187:LYS:O | 1:L:191:ASP:HB2 | 2.03 | 0.57 |
| 1:L:239:ASP:OD1 | 1:L:277:ARG:NH2 | 2.36 | 0.57 |
| 1:O:419:TYR:O | 1:O:420:ILE:C | 2.42 | 0.57 |
| 1:Q:236:PHE:CZ | 1:Q:324:CYS:HB3 | 2.40 | 0.57 |
| 1:C:269:MET:HG2 | 1:C:306:TYR:HE1 | 1.69 | 0.57 |
| 1:K:140:GLU:HG3 | 1:K:140:GLU:O | 2.04 | 0.57 |
| 1:M:353:LEU:HD22 | 1:M:357:THR:HG21 | 1.87 | 0.57 |
| 1:M:493:PHE:HA | 1:M:539:GLY:HA3 | 1.86 | 0.57 |
| 1:O:173:THR:CG2 | 1:O:174:GLY:N | 2.68 | 0.57 |
| 1:P:123:SER:HB3 | 2:P:701:SAH:HN62 | 1.69 | 0.57 |
| 1:F:506:VAL:HG12 | 1:F:507:ASN:HD22 | 1.70 | 0.57 |
| 1:J:129:ILE:O | 1:J:130:GLY:C | 2.43 | 0.57 |
| 1:J:67:HIS:CE1 | 1:J:91:THR:CG2 | 2.87 | 0.57 |
| 1:L:56:GLU:OE1 | 1:L:168:ARG:HD2 | 2.04 | 0.57 |
| 1:O:420:ILE:HG13 | 1:O:421:HIS:N | 2.19 | 0.57 |
| 1:O:7:ASN:HB2 | 1:O:14:GLU:CD | 2.24 | 0.57 |
| 1:P:221:MET:HG2 | 1:P:226:PHE:CD1 | 2.39 | 0.57 |
| 1:R:622:LYS:N | 1:R:622:LYS:HD2 | 2.17 | 0.57 |
| 1:J:67:HIS:HD2 | 1:J:133:ARG:O | 1.86 | 0.57 |
| 1:M:192:ILE:O | 1:M:194:ARG:HD3 | 2.05 | 0.57 |
| 1:M:541:VAL:CG2 | 1:M:601:PRO:HG3 | 2.35 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:485:VAL:HG21 | 1:O:547:GLU:HG2 | 1.87 | 0.57 |
| 1:O:56:GLU:O | 1:O:60:GLU:HG2 | 2.05 | 0.57 |
| 1:O:77:LEU:HD13 | 1:O:511:LEU:HD11 | 1.86 | 0.57 |
| 1:Q:356:GLN:NE2 | 1:Q:608:LYS:HE3 | 2.20 | 0.57 |
| 1:D:111:PRO:O | 1:D:112:TRP:CB | 2.52 | 0.57 |
| 1:G:480:GLU:OE2 | 1:G:482:HIS:HD2 | 1.88 | 0.57 |
| 1:L:193:PRO:HA | 1:L:362:ASN:HD21 | 1.70 | 0.57 |
| 1:Q:447:GLU:N | 1:Q:448:PRO:HA | 2.20 | 0.57 |
| 1:B:68:VAL:HG22 | 1:B:136:ILE:HD12 | 1.86 | 0.56 |
| 1:C:490:PRO:CB | 1:C:569:MET:HE3 | 2.30 | 0.56 |
| 1:E:67:HIS:HE1 | 1:E:91:THR:CG2 | 2.11 | 0.56 |
| 1:F:335:ASN:OD1 | 1:F:335:ASN:N | 2.37 | 0.56 |
| 1:K:283:ILE:HG23 | 1:K:298:ARG:NH2 | 2.20 | 0.56 |
| 1:K:356:GLN:O | 1:K:359:TYR:HB3 | 2.04 | 0.56 |
| 1:L:460:LEU:HD21 | 1:L:579:MET:HE1 | 1.87 | 0.56 |
| 1:N:140:GLU:OE1 | 1:N:301:TRP:HZ2 | 1.87 | 0.56 |
| 1:P:549:LEU:HD12 | 1:P:560:GLN:NE2 | 2.18 | 0.56 |
| 1:R:353:LEU:HD22 | 1:R:357:THR:HG21 | 1.87 | 0.56 |
| 1:E:490:PRO:CB | 1:E:569:MET:CE | 2.79 | 0.56 |
| 1:R:622:LYS:H | 1:R:622:LYS:CD | 2.16 | 0.56 |
| 1:B:314:VAL:HG21 | 1:B:320:PHE:CD1 | 2.40 | 0.56 |
| 1:I:460:LEU:HB3 | 1:I:463:LEU:HD22 | 1.88 | 0.56 |
| 1:K:145:GLU:HG3 | 1:K:331:LEU:HD22 | 1.87 | 0.56 |
| 1:L:317:ASN:ND2 | 1:L:317:ASN:H | 2.03 | 0.56 |
| 1:N:280:THR:OG1 | 1:N:281:THR:HG22 | 2.04 | 0.56 |
| 1:Q:491:GLU:OE1 | 1:Q:539:GLY:HA3 | 2.05 | 0.56 |
| 1:R:52:THR:HG21 | 1:R:276:ASP:HB2 | 1.87 | 0.56 |
| 1:B:534:LEU:HD21 | 1:B:611:VAL:HG11 | 1.88 | 0.56 |
| 1:F:218:LEU:N | 1:F:303:GLN:HE21 | 1.94 | 0.56 |
| 1:F:383:VAL:HG13 | 1:F:403:VAL:HG22 | 1.86 | 0.56 |
| 1:M:300:HIS:CE1 | 1:M:301:TRP:CD2 | 2.93 | 0.56 |
| 1:N:168:ARG:HH11 | 1:N:168:ARG:CG | 2.13 | 0.56 |
| 1:Q:289:TRP:O | 1:Q:289:TRP:HE3 | 1.88 | 0.56 |
| 1:Q:255:GLU:OE1 | 1:Q:319:THR:HG22 | 2.05 | 0.56 |
| 1:R:181:VAL:HG11 | 1:R:226:PHE:HB2 | 1.88 | 0.56 |
| 1:R:45:LYS:O | 1:R:275:MET:HG2 | 2.05 | 0.56 |
| 1:R:297:TRP:CE3 | 1:R:495:ASP:HB3 | 2.40 | 0.56 |
| 1:E:379:LYS:CA | 1:E:399:THR:CG2 | 2.81 | 0.56 |
| 1:L:480:GLU:OE2 | 1:L:482:HIS:CD2 | 2.58 | 0.56 |
| 1:O:616:THR:OG1 | 1:O:617:ALA:N | 2.39 | 0.56 |
| 1:Q:516:GLU:O | 1:Q:520:LYS:HG3 | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:80:LEU:HD13 | 1:R:509:PHE:HB3 | 1.88 | 0.56 |
| 1:J:556:ARG:HG2 | 1:J:556:ARG:O | 2.04 | 0.56 |
| 1:K:133:ARG:HB2 | 1:K:164:LYS:HG3 | 1.87 | 0.56 |
| 1:K:218:LEU:CD1 | 1:K:268:LEU:HD22 | 2.36 | 0.56 |
| 1:L:114:ASP:N | 1:L:114:ASP:OD1 | 2.35 | 0.56 |
| 1:L:168:ARG:HH12 | 1:L:241:GLU:CD | 2.08 | 0.56 |
| 1:M:169:VAL:CG1 | 1:M:241:GLU:HA | 2.35 | 0.56 |
| 1:M:37:ILE:CG2 | 1:M:503:VAL:HG13 | 2.36 | 0.56 |
| 1:M:3:LEU:O | 1:M:15:TRP:HA | 2.05 | 0.56 |
| 1:O:444:VAL:CG1 | 1:O:479:VAL:HA | 2.35 | 0.56 |
| 1:O:624:LEU:HB2 | 1:O:643:LYS:HA | 1.86 | 0.56 |
| 1:Q:356:GLN:HE22 | 1:Q:608:LYS:HE3 | 1.71 | 0.56 |
| 1:C:288:LYS:C | 1:C:290:LYS:H | 2.08 | 0.56 |
| 1:F:145:GLU:HG2 | 1:F:331:LEU:HD22 | 1.87 | 0.56 |
| 1:I:141:VAL:O | 1:I:141:VAL:CG1 | 2.52 | 0.56 |
| 1:K:354:SER:O | 1:K:358:VAL:HG23 | 2.05 | 0.56 |
| 1:N:179:VAL:HG22 | 1:N:232:PRO:HA | 1.87 | 0.56 |
| 1:A:73:THR:HG22 | 1:A:94:GLU:HB2 | 1.87 | 0.56 |
| 1:C:490:PRO:HB3 | 1:C:569:MET:HE2 | 1.84 | 0.56 |
| 1:C:522:ARG:O | 1:C:526:ASP:HB2 | 2.05 | 0.56 |
| 1:J:273:ILE:HG13 | 1:J:275:MET:CE | 2.36 | 0.56 |
| 1:K:502:ASP:CG | 1:K:616:THR:HG21 | 2.25 | 0.56 |
| 1:K:30:ARG:NH1 | 1:K:526:ASP:OD1 | 2.39 | 0.56 |
| 1:M:7:ASN:HB2 | 1:M:14:GLU:OE1 | 2.05 | 0.56 |
| 1:R:310:GLU:OE1 | 1:R:338:LYS:HG3 | 2.06 | 0.56 |
| 1:R:437:LEU:O | 1:R:473:HIS:NE2 | 2.38 | 0.56 |
| 1:A:218:LEU:H | 1:A:303:GLN:HE21 | 1.52 | 0.56 |
| 1:C:517:ILE:HG13 | 1:C:518:SER:N | 2.19 | 0.56 |
| 1:H:273:ILE:CG1 | 1:H:275:MET:CE | 2.81 | 0.56 |
| 1:I:643:LYS:O | 1:I:644:SER:CB | 2.54 | 0.56 |
| 1:L:191:ASP:OD2 | 1:L:194:ARG:NH1 | 2.38 | 0.56 |
| 1:N:57:LYS:NZ | 1:N:166:GLY:O | 2.39 | 0.56 |
| 1:O:505:THR:HA | 1:O:509:PHE:O | 2.05 | 0.56 |
| 1:C:42:ARG:HH11 | 1:C:140:GLU:HG2 | 1.71 | 0.56 |
| 1:F:291:ASN:HB3 | 1:F:295:TYR:HB2 | 1.88 | 0.56 |
| 1:F:443:ILE:HG12 | 1:F:445:LEU:HD13 | 1.87 | 0.56 |
| 1:G:489:ILE:HD13 | 1:G:541:VAL:HG21 | 1.87 | 0.56 |
| 1:K:241:GLU:HB2 | 1:K:277:ARG:NH2 | 2.21 | 0.56 |
| 1:M:138:VAL:HG23 | 1:M:170:VAL:HB | 1.88 | 0.56 |
| 1:A:39:ASP:OD2 | 1:A:298:ARG:CD | 2.54 | 0.56 |
| 1:N:378:SER:HB3 | 1:N:400:ALA:HB2 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:69:LEU:HD12 | 1:R:70:ASP:N | 2.20 | 0.56 |
| 1:E:480:GLU:OE2 | 1:E:482:HIS:HD2 | 1.89 | 0.55 |
| 1:F:163:ALA:HB1 | 1:F:167:CYS:SG | 2.46 | 0.55 |
| 1:F:478:ARG:HH21 | 1:F:478:ARG:HG2 | 1.71 | 0.55 |
| 1:Q:569:MET:HE1 | 1:Q:575:ILE:HG12 | 1.88 | 0.55 |
| 1:F:35:ASP:O | 1:F:36:MET:C | 2.45 | 0.55 |
| 1:M:198:GLU:HB2 | 1:M:201:GLU:OE2 | 2.06 | 0.55 |
| 1:Q:370:PHE:HE2 | 1:Q:588:LEU:HD21 | 1.71 | 0.55 |
| 1:R:369:LYS:HE3 | 1:R:586:ILE:HG21 | 1.89 | 0.55 |
| 1:G:434:VAL:HG12 | 1:G:469:LEU:HD13 | 1.89 | 0.55 |
| 1:K:156:LYS:O | 1:K:160:GLU:HG2 | 2.06 | 0.55 |
| 1:Q:222:LYS:HB2 | 1:Q:224:HIS:HB3 | 1.87 | 0.55 |
| 1:R:481:PRO:HG2 | 1:R:581:TRP:CE3 | 2.41 | 0.55 |
| 1:B:344:TYR:O | 1:B:346:VAL:HG13 | 2.07 | 0.55 |
| 1:E:275:MET:HE1 | 1:E:283:ILE:HG13 | 1.88 | 0.55 |
| 1:L:502:ASP:OD2 | 1:L:616:THR:HG21 | 2.07 | 0.55 |
| 1:M:126:VAL:H | 1:M:161:ARG:HH22 | 1.51 | 0.55 |
| 1:M:66:VAL:O | 1:M:88:ASP:HB2 | 2.06 | 0.55 |
| 1:N:348:GLY:O | 1:N:415:ILE:HD11 | 2.07 | 0.55 |
| 1:N:58:LYS:N | 1:N:58:LYS:HE3 | 2.21 | 0.55 |
| 1:O:615:ILE:O | 1:O:616:THR:C | 2.45 | 0.55 |
| 1:Q:180:PRO:CG | 1:Q:230:SER:HB3 | 2.31 | 0.55 |
| 1:B:38:LEU:HD21 | 1:B:503:VAL:HA | 1.87 | 0.55 |
| 1:B:483:MET:HB3 | 1:B:582:GLU:HG3 | 1.87 | 0.55 |
| 1:D:180:PRO:HB3 | 1:D:264:ILE:HD13 | 1.89 | 0.55 |
| 1:E:72:GLY:CA | 2:E:701:SAH:O4' | 2.54 | 0.55 |
| 1:R:434:VAL:HG12 | 1:R:469:LEU:HD13 | 1.88 | 0.55 |
| 1:C:460:LEU:HD22 | 1:C:463:LEU:HD21 | 1.88 | 0.55 |
| 1:F:385:THR:HB | 1:F:405:ILE:HA | 1.88 | 0.55 |
| 1:G:36:MET:HA | 1:G:300:HIS:CD2 | 2.41 | 0.55 |
| 1:I:478:ARG:HH21 | 1:I:478:ARG:HG2 | 1.70 | 0.55 |
| 1:J:137:ILE:HD11 | 1:J:163:ALA:HB2 | 1.89 | 0.55 |
| 1:K:145:GLU:CG | 1:K:331:LEU:HD22 | 2.37 | 0.55 |
| 1:N:123:SER:OG | 2:N:701:SAH:N6 | 2.38 | 0.55 |
| 1:A:379:LYS:HA | 1:A:399:THR:CG2 | 2.36 | 0.55 |
| 1:B:506:VAL:O | 1:B:507:ASN:C | 2.44 | 0.55 |
| 1:F:218:LEU:H | 1:F:303:GLN:HE22 | 1.48 | 0.55 |
| 1:K:38:LEU:HD21 | 1:K:503:VAL:HA | 1.89 | 0.55 |
| 1:L:136:ILE:HA | 1:L:168:ARG:O | 2.07 | 0.55 |
| 1:L:627:HIS:HB2 | 1:L:640:GLN:HB2 | 1.88 | 0.55 |
| 1:O:643:LYS:N | 1:O:643:LYS:HD2 | 2.14 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:210:THR:HB | 4:P:804:HOH:O | 2.05 | 0.55 |
| 1:Q:354:SER:HB2 | 3:Q:702:PO4:O3 | 2.07 | 0.55 |
| 1:B:239:ASP:OD2 | 1:B:242:HIS:HD2 | 1.89 | 0.55 |
| 1:G:412:PHE:CE2 | 1:G:451:MET:HG2 | 2.40 | 0.55 |
| 1:J:222:LYS:HB2 | 1:J:225:GLU:HG2 | 1.89 | 0.55 |
| 1:M:145:GLU:HG2 | 1:M:331:LEU:CD1 | 2.36 | 0.55 |
| 1:R:379:LYS:HA | 1:R:399:THR:HG22 | 1.89 | 0.55 |
| 1:R:80:LEU:HB3 | 1:R:509:PHE:CE1 | 2.41 | 0.55 |
| 1:C:522:ARG:HG2 | 1:C:526:ASP:OD2 | 2.07 | 0.55 |
| 1:E:359:TYR:C | 1:E:359:TYR:CD1 | 2.81 | 0.55 |
| 1:H:218:LEU:H | 1:H:303:GLN:HE21 | 1.55 | 0.55 |
| 1:J:497:GLN:N | 1:J:497:GLN:HE21 | 1.96 | 0.55 |
| 1:N:367:ASN:O | 1:N:371:LYS:HD3 | 2.07 | 0.55 |
| 1:C:550:ARG:H | 1:C:560:GLN:HE22 | 1.54 | 0.55 |
| 1:F:143:ASP:OD1 | 1:F:143:ASP:N | 2.37 | 0.55 |
| 1:J:383:VAL:CG2 | 1:J:445:LEU:HD22 | 2.37 | 0.55 |
| 1:M:434:VAL:CG1 | 1:M:469:LEU:CD1 | 2.85 | 0.55 |
| 1:N:315:GLU:HB2 | 1:N:318:GLN:CG | 2.35 | 0.55 |
| 1:Q:42:ARG:HH11 | 1:Q:140:GLU:HG2 | 1.67 | 0.55 |
| 1:C:502:ASP:OD2 | 1:C:616:THR:CG2 | 2.55 | 0.54 |
| 1:D:157:GLU:HA | 1:D:160:GLU:HG3 | 1.90 | 0.54 |
| 1:D:42:ARG:HH21 | 1:D:43:ASN:HD21 | 1.54 | 0.54 |
| 1:L:297:TRP:CD2 | 1:L:495:ASP:HB3 | 2.42 | 0.54 |
| 1:M:568:ASN:HD22 | 1:M:568:ASN:N | 2.05 | 0.54 |
| 1:N:142:PHE:HD1 | 1:N:146:LEU:HD12 | 1.69 | 0.54 |
| 1:N:132:SER:HB2 | 1:R:104:ARG:CZ | 2.36 | 0.54 |
| 1:R:460:LEU:HD21 | 1:R:579:MET:CE | 2.37 | 0.54 |
| 1:B:241:GLU:HB2 | 1:B:277:ARG:NH2 | 2.21 | 0.54 |
| 1:B:550:ARG:H | 1:B:560:GLN:NE2 | 1.99 | 0.54 |
| 1:B:554:ASP:O | 1:B:555:GLY:O | 2.26 | 0.54 |
| 1:D:565:ASN:HD21 | 1:D:644:SER:HB3 | 1.71 | 0.54 |
| 1:E:420:ILE:HD11 | 1:E:428:VAL:HG22 | 1.90 | 0.54 |
| 1:I:353:LEU:HD22 | 1:I:357:THR:HG21 | 1.88 | 0.54 |
| 1:M:402:ARG:NH2 | 1:M:429:GLU:OE1 | 2.28 | 0.54 |
| 1:C:84:ARG:NH1 | 1:O:280:THR:CG2 | 2.70 | 0.54 |
| 1:B:218:LEU:H | 1:B:303:GLN:HE21 | 1.52 | 0.54 |
| 1:B:534:LEU:HD11 | 1:B:611:VAL:HG13 | 1.90 | 0.54 |
| 1:E:39:ASP:OD2 | 1:E:298:ARG:HD3 | 2.07 | 0.54 |
| 1:J:339:ASP:OD1 | 1:J:341:SER:HB2 | 2.06 | 0.54 |
| 1:J:71:ILE:HG21 | 1:J:154:THR:CG2 | 2.37 | 0.54 |
| 1:M:486:LEU:HD22 | 1:M:578:TRP:O | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:156:LYS:HG3 | 1:R:157:GLU:N | 2.22 | 0.54 |
| 1:I:534:LEU:CD1 | 1:I:576:PRO:HB3 | 2.37 | 0.54 |
| 1:K:578:TRP:CG | 1:K:591:GLY:HA3 | 2.43 | 0.54 |
| 1:M:485:VAL:HG13 | 1:M:487:LYS:HG3 | 1.88 | 0.54 |
| 1:O:182:GLU:OE1 | 1:O:263:THR:HG22 | 2.07 | 0.54 |
| 1:O:180:PRO:HB2 | 1:O:264:ILE:HG12 | 1.89 | 0.54 |
| 1:P:470:LYS:O | 1:P:473:HIS:O | 2.26 | 0.54 |
| 1:P:50:LEU:O | 1:P:54:ILE:HB | 2.06 | 0.54 |
| 1:B:43:ASN:N | 1:B:43:ASN:ND2 | 2.55 | 0.54 |
| 1:B:505:THR:HA | 1:B:509:PHE:O | 2.06 | 0.54 |
| 1:C:467:GLU:HG3 | 1:C:555:GLY:O | 2.07 | 0.54 |
| 1:C:55:ALA:HB1 | 1:O:292:LYS:HE3 | 1.90 | 0.54 |
| 1:H:420:ILE:CD1 | 1:H:428:VAL:HG22 | 2.37 | 0.54 |
| 1:I:129:ILE:HG22 | 1:I:130:GLY:O | 2.06 | 0.54 |
| 1:I:269:MET:HG2 | 1:I:306:TYR:CE1 | 2.42 | 0.54 |
| 1:K:485:VAL:HG13 | 1:K:487:LYS:HG3 | 1.90 | 0.54 |
| 1:K:556:ARG:CZ | 1:K:556:ARG:H | 2.20 | 0.54 |
| 1:N:169:VAL:CG1 | 1:N:240:PHE:O | 2.51 | 0.54 |
| 1:P:5:LYS:HA | 1:R:420:ILE:CD1 | 2.36 | 0.54 |
| 1:R:179:VAL:HG22 | 1:R:232:PRO:HA | 1.88 | 0.54 |
| 1:E:216:VAL:HG23 | 1:E:217:GLN:N | 2.21 | 0.54 |
| 1:G:432:GLU:HG2 | 1:G:433:LYS:HG3 | 1.89 | 0.54 |
| 1:I:497:GLN:CD | 1:I:573:ASN:ND2 | 2.59 | 0.54 |
| 1:I:539:GLY:O | 1:I:540:ILE:HD13 | 2.07 | 0.54 |
| 1:K:84:ARG:O | 1:K:85:GLU:CB | 2.56 | 0.54 |
| 1:B:123:SER:O | 1:B:125:ASP:N | 2.41 | 0.54 |
| 1:B:194:ARG:HD2 | 1:B:198:GLU:O | 2.08 | 0.54 |
| 1:N:84:ARG:HB3 | 1:N:112:TRP:CZ2 | 2.43 | 0.54 |
| 1:P:379:LYS:HA | 1:P:399:THR:CG2 | 2.37 | 0.54 |
| 1:M:169:VAL:HG11 | 1:M:240:PHE:O | 2.08 | 0.54 |
| 1:P:110:SER:HB2 | 1:P:112:TRP:CE3 | 2.43 | 0.54 |
| 1:P:33:PHE:HB2 | 1:P:36:MET:HE2 | 1.89 | 0.54 |
| 1:A:245:LYS:HD3 | 1:D:337:GLY:HA2 | 1.90 | 0.54 |
| 1:D:291:ASN:O | 1:D:292:LYS:HD3 | 2.08 | 0.54 |
| 1:D:46:PHE:CZ | 1:D:140:GLU:HB2 | 2.42 | 0.54 |
| 1:L:168:ARG:NH1 | 1:L:168:ARG:HG2 | 2.15 | 0.54 |
| 1:M:190:ASN:HD21 | 1:M:209:GLY:HA3 | 1.73 | 0.54 |
| 1:M:533:SER:O | 1:M:536:GLU:HB2 | 2.08 | 0.54 |
| 1:N:137:ILE:O | 1:N:169:VAL:HA | 2.08 | 0.54 |
| 1:O:417:PHE:CZ | 1:O:430:ILE:HB | 2.43 | 0.54 |
| 1:R:447:GLU:N | 1:R:448:PRO:HA | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:45:LYS:O | 1:C:275:MET:HG2 | 2.08 | 0.54 |
| 1:K:179:VAL:HG21 | 1:K:270:TRP:HH2 | 1.72 | 0.54 |
| 1:M:434:VAL:HG13 | 1:M:469:LEU:HD13 | 1.90 | 0.54 |
| 1:N:490:PRO:HB3 | 1:N:569:MET:CE | 2.38 | 0.54 |
| 1:Q:178:ILE:CD1 | 1:Q:235:ALA:HB2 | 2.35 | 0.54 |
| 1:Q:276:ASP:O | 1:Q:277:ARG:CB | 2.56 | 0.54 |
| 1:I:489:ILE:O | 1:I:576:PRO:HD2 | 2.08 | 0.53 |
| 1:J:592:LEU:HD21 | 1:J:595:ILE:HD11 | 1.90 | 0.53 |
| 1:Q:530:ASP:O | 1:Q:610:GLY:HA2 | 2.09 | 0.53 |
| 1:B:297:TRP:CZ2 | 1:B:299:ASP:HB2 | 2.43 | 0.53 |
| 1:E:138:VAL:HG23 | 1:E:170:VAL:HB | 1.89 | 0.53 |
| 1:I:42:ARG:HH11 | 1:I:140:GLU:HG3 | 1.72 | 0.53 |
| 1:O:4:GLU:OE2 | 1:O:13:ARG:NH1 | 2.42 | 0.53 |
| 1:O:73:THR:OG1 | 1:O:76:GLY:HA2 | 2.08 | 0.53 |
| 1:P:297:TRP:CE3 | 1:P:495:ASP:HB3 | 2.44 | 0.53 |
| 1:B:627:HIS:CD2 | 1:B:627:HIS:N | 2.76 | 0.53 |
| 1:D:243:GLU:N | 1:D:243:GLU:OE1 | 2.30 | 0.53 |
| 1:G:141:VAL:O | 1:G:141:VAL:HG12 | 2.08 | 0.53 |
| 1:I:193:PRO:HA | 1:I:362:ASN:ND2 | 2.23 | 0.53 |
| 1:J:88:ASP:O | 1:J:115:LYS:HG2 | 2.08 | 0.53 |
| 1:O:229:LEU:HD13 | 1:O:314:VAL:HG12 | 1.89 | 0.53 |
| 1:A:176:VAL:HG22 | 1:A:235:ALA:HB3 | 1.90 | 0.53 |
| 1:D:242:HIS:HB2 | 1:D:245:LYS:HG3 | 1.90 | 0.53 |
| 1:F:91:THR:HG22 | 1:F:117:THR:HG22 | 1.89 | 0.53 |
| 1:K:505:THR:HA | 1:K:509:PHE:O | 2.08 | 0.53 |
| 1:M:132:SER:N | 1:P:104:ARG:HH21 | 2.06 | 0.53 |
| 1:M:375:ASP:O | 1:M:399:THR:HG21 | 2.09 | 0.53 |
| 1:Q:179:VAL:HG22 | 1:Q:232:PRO:HA | 1.89 | 0.53 |
| 1:A:214:PHE:CD2 | 1:A:305:VAL:HG22 | 2.44 | 0.53 |
| 1:E:241:GLU:CG | 1:E:277:ARG:HH21 | 2.20 | 0.53 |
| 1:E:274:ASP:HA | 1:E:282:PHE:CD1 | 2.43 | 0.53 |
| 1:F:277:ARG:C | 1:F:279:GLY:H | 2.12 | 0.53 |
| 1:G:490:PRO:HB2 | 1:G:569:MET:HE1 | 1.84 | 0.53 |
| 1:G:6:ILE:HG13 | 1:I:426:THR:HB | 1.91 | 0.53 |
| 1:I:68:VAL:O | 1:I:90:VAL:HA | 2.08 | 0.53 |
| 1:K:36:MET:HA | 1:K:300:HIS:CD2 | 2.43 | 0.53 |
| 1:L:528:ILE:HD13 | 1:L:639:PHE:O | 2.08 | 0.53 |
| 1:M:258:ALA:CB | 1:M:314:VAL:HG13 | 2.38 | 0.53 |
| 1:M:92:ALA:HB3 | 1:M:118:VAL:HG22 | 1.90 | 0.53 |
| 1:N:55:ALA:CA | 1:N:58:LYS:HZ2 | 2.22 | 0.53 |
| 1:R:489:ILE:HD11 | 1:R:541:VAL:HG11 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:250:GLU:HB2 | 1:H:326:HIS:NE2 | 2.23 | 0.53 |
| 1:K:534:LEU:O | 1:K:536:GLU:N | 2.42 | 0.53 |
| 1:P:198:GLU:HB2 | 1:P:201:GLU:HG3 | 1.90 | 0.53 |
| 1:Q:447:GLU:H | 1:Q:448:PRO:HA | 1.73 | 0.53 |
| 1:R:300:HIS:CE1 | 1:R:301:TRP:CD2 | 2.97 | 0.53 |
| 1:B:75:THR:HG22 | 1:B:77:LEU:H | 1.73 | 0.53 |
| 1:D:178:ILE:HA | 1:D:268:LEU:O | 2.09 | 0.53 |
| 1:D:78:LEU:O | 1:D:81:MET:HB2 | 2.09 | 0.53 |
| 1:E:434:VAL:HG13 | 1:E:469:LEU:HD13 | 1.91 | 0.53 |
| 1:I:379:LYS:HA | 1:I:399:THR:CG2 | 2.33 | 0.53 |
| 1:K:122:ARG:O | 1:K:123:SER:C | 2.45 | 0.53 |
| 1:K:123:SER:HB3 | 2:K:701:SAH:N6 | 2.13 | 0.53 |
| 1:N:450:TYR:H | 1:N:459:HIS:CD2 | 2.22 | 0.53 |
| 1:R:144:THR:HG23 | 1:R:302:MET:O | 2.09 | 0.53 |
| 1:D:45:LYS:HB3 | 1:D:275:MET:HE3 | 1.91 | 0.53 |
| 1:D:490:PRO:CB | 1:D:569:MET:HE1 | 2.38 | 0.53 |
| 1:E:627:HIS:HB2 | 1:E:640:GLN:HB2 | 1.90 | 0.53 |
| 1:J:264:ILE:HD12 | 1:J:312:LYS:HG3 | 1.90 | 0.53 |
| 1:L:280:THR:HG23 | 1:L:281:THR:CG2 | 2.38 | 0.53 |
| 1:L:258:ALA:CB | 1:L:314:VAL:HG13 | 2.39 | 0.53 |
| 1:A:109:ASN:N | 1:A:109:ASN:ND2 | 2.57 | 0.53 |
| 1:F:216:VAL:O | 1:F:302:MET:HG2 | 2.09 | 0.53 |
| 1:G:190:ASN:HD21 | 1:G:209:GLY:HA3 | 1.73 | 0.53 |
| 1:I:168:ARG:HG2 | 1:I:168:ARG:HH11 | 1.72 | 0.53 |
| 1:L:553:ILE:HD11 | 1:L:581:TRP:HZ3 | 1.73 | 0.53 |
| 1:M:84:ARG:O | 1:M:85:GLU:HB2 | 2.09 | 0.53 |
| 1:O:387:GLY:HA2 | 1:O:450:TYR:CE1 | 2.43 | 0.53 |
| 1:P:496:LEU:O | 1:P:499:ILE:HG12 | 2.09 | 0.53 |
| 1:Q:259:HIS:CD2 | 1:Q:259:HIS:C | 2.82 | 0.53 |
| 1:Q:392:LEU:CD1 | 1:Q:445:LEU:HB3 | 2.38 | 0.53 |
| 1:B:84:ARG:HB3 | 1:B:112:TRP:CH2 | 2.44 | 0.53 |
| 1:E:278:ASN:O | 1:E:280:THR:N | 2.40 | 0.53 |
| 1:J:128:GLN:OE1 | 1:J:129:ILE:O | 2.27 | 0.53 |
| 1:J:378:SER:HB3 | 1:J:400:ALA:HB2 | 1.91 | 0.53 |
| 1:K:126:VAL:HG12 | 1:K:162:LEU:HD11 | 1.90 | 0.53 |
| 1:K:143:ASP:O | 1:K:146:LEU:N | 2.32 | 0.53 |
| 1:L:490:PRO:HB3 | 1:L:569:MET:HE2 | 1.76 | 0.53 |
| 1:M:409:ASN:OD1 | 1:M:411:ARG:HG2 | 2.09 | 0.53 |
| 1:M:615:ILE:HG13 | 1:M:618:LEU:HD22 | 1.90 | 0.53 |
| 1:N:87:ALA:CB | 1:N:88:ASP:HB2 | 2.38 | 0.53 |
| 1:Q:410:GLU:HG3 | 1:Q:413:ARG:NH2 | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:184:HIS:HA | 1:R:187:LYS:HD3 | 1.90 | 0.53 |
| 1:R:178:ILE:HG13 | 1:R:267:LEU:HD22 | 1.90 | 0.53 |
| 1:R:49:GLY:O | 1:R:53:THR:OG1 | 2.27 | 0.53 |
| 1:J:410:GLU:OE2 | 1:K:19:GLU:HB3 | 2.09 | 0.52 |
| 1:K:485:VAL:O | 1:K:579:MET:HG3 | 2.09 | 0.52 |
| 1:M:516:GLU:HG2 | 1:M:520:LYS:HE3 | 1.90 | 0.52 |
| 1:Q:218:LEU:HD22 | 1:Q:221:MET:HE2 | 1.92 | 0.52 |
| 1:R:157:GLU:O | 1:R:160:GLU:HG2 | 2.09 | 0.52 |
| 1:B:567:ASP:O | 1:B:568:ASN:HB2 | 2.09 | 0.52 |
| 1:D:269:MET:HG2 | 1:D:306:TYR:HE1 | 1.73 | 0.52 |
| 1:D:445:LEU:HD12 | 1:D:480:GLU:HB2 | 1.91 | 0.52 |
| 1:E:35:ASP:O | 1:E:36:MET:C | 2.46 | 0.52 |
| 1:F:239:ASP:OD2 | 1:F:242:HIS:HD2 | 1.92 | 0.52 |
| 1:I:570:SER:HB3 | 1:I:622:LYS:HA | 1.92 | 0.52 |
| 1:J:561:LYS:O | 1:J:562:CYS:HB3 | 2.09 | 0.52 |
| 1:K:45:LYS:NZ | 1:K:294:ASN:HD22 | 2.07 | 0.52 |
| 1:O:280:THR:HG22 | 1:O:281:THR:HG22 | 1.90 | 0.52 |
| 1:R:597:SER:HA | 1:R:599:GLY:N | 2.23 | 0.52 |
| 1:E:595:ILE:HG22 | 1:E:599:GLY:HA2 | 1.90 | 0.52 |
| 1:M:457:TRP:CD1 | 1:M:457:TRP:O | 2.62 | 0.52 |
| 1:N:39:ASP:OD1 | 1:N:39:ASP:C | 2.47 | 0.52 |
| 1:O:291:ASN:OD1 | 1:O:294:ASN:HB2 | 2.10 | 0.52 |
| 1:R:502:ASP:OD2 | 1:R:616:THR:HG21 | 2.08 | 0.52 |
| 1:B:163:ALA:CB | 1:B:167:CYS:SG | 2.95 | 0.52 |
| 1:G:540:ILE:HD11 | 1:G:542:LYS:HE2 | 1.91 | 0.52 |
| 1:J:548:ILE:HD12 | 1:J:626:LEU:HD13 | 1.92 | 0.52 |
| 1:K:185:LEU:O | 1:K:188:MET:HB2 | 2.10 | 0.52 |
| 1:K:379:LYS:CA | 1:K:399:THR:HG23 | 2.38 | 0.52 |
| 1:L:57:LYS:HG2 | 1:L:135:ASP:HB3 | 1.91 | 0.52 |
| 1:R:593:LEU:O | 1:R:594:SER:HB3 | 2.10 | 0.52 |
| 1:A:273:ILE:HG13 | 1:A:275:MET:HE1 | 1.91 | 0.52 |
| 1:C:489:ILE:HG12 | 1:C:541:VAL:CG2 | 2.39 | 0.52 |
| 1:D:626:LEU:HD21 | 1:D:628:ALA:HB2 | 1.90 | 0.52 |
| 1:E:218:LEU:H | 1:E:303:GLN:HE21 | 1.55 | 0.52 |
| 1:E:506:VAL:N | 1:E:509:PHE:O | 2.37 | 0.52 |
| 1:F:147:ILE:HD11 | 1:F:331:LEU:HD13 | 1.91 | 0.52 |
| 1:F:478:ARG:CG | 1:F:478:ARG:HH21 | 2.22 | 0.52 |
| 1:I:275:MET:HA | 1:I:275:MET:CE | 2.39 | 0.52 |
| 1:J:478:ARG:HH21 | 1:J:478:ARG:HG2 | 1.74 | 0.52 |
| 1:L:297:TRP:CE3 | 1:L:495:ASP:HB3 | 2.45 | 0.52 |
| 1:N:169:VAL:HG13 | 1:N:241:GLU:HG2 | 1.89 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:506:VAL:HG12 | 1:O:507:ASN:HD22 | 1.74 | 0.52 |
| 1:A:541:VAL:HG11 | 1:A:595:ILE:HD13 | 1.91 | 0.52 |
| 1:D:630:PHE:CE1 | 1:D:635:GLY:HA2 | 2.44 | 0.52 |
| 1:G:379:LYS:CA | 1:G:399:THR:CG2 | 2.83 | 0.52 |
| 1:G:73:THR:OG1 | 1:G:76:GLY:HA2 | 2.09 | 0.52 |
| 1:K:497:GLN:H | 1:K:497:GLN:NE2 | 2.08 | 0.52 |
| 1:M:5:LYS:HD3 | 1:O:417:PHE:HE1 | 1.75 | 0.52 |
| 1:N:141:VAL:HG12 | 1:N:141:VAL:O | 2.09 | 0.52 |
| 1:R:478:ARG:HG2 | 1:R:478:ARG:NH2 | 2.21 | 0.52 |
| 1:D:114:ASP:HB3 | 1:B:65:LYS:HZ1 | 1.73 | 0.52 |
| 1:G:104:ARG:HB3 | 1:G:118:VAL:HB | 1.91 | 0.52 |
| 1:I:643:LYS:O | 1:I:644:SER:HB2 | 2.10 | 0.52 |
| 1:J:169:VAL:HG23 | 1:J:171:PRO:O | 2.10 | 0.52 |
| 1:J:144:THR:O | 1:J:269:MET:HE1 | 2.10 | 0.52 |
| 1:J:91:THR:HG21 | 1:J:129:ILE:HG21 | 1.92 | 0.52 |
| 1:P:7:ASN:HD21 | 1:P:640:GLN:NE2 | 2.08 | 0.52 |
| 1:I:616:THR:O | 1:I:619:ARG:HG2 | 2.10 | 0.52 |
| 1:J:406:ILE:HG12 | 1:J:431:ILE:HD11 | 1.91 | 0.52 |
| 1:J:71:ILE:HG12 | 1:J:93:LEU:HD12 | 1.91 | 0.52 |
| 1:K:177:TYR:HA | 1:K:233:ILE:O | 2.09 | 0.52 |
| 1:K:529:VAL:HG12 | 1:K:530:ASP:O | 2.10 | 0.52 |
| 1:R:291:ASN:CB | 1:R:295:TYR:HB2 | 2.32 | 0.52 |
| 1:R:35:ASP:OD2 | 1:R:300:HIS:HD2 | 1.93 | 0.52 |
| 1:R:433:LYS:HE3 | 1:R:436:SER:OG | 2.10 | 0.52 |
| 1:B:218:LEU:HD12 | 1:B:303:GLN:HB3 | 1.92 | 0.52 |
| 1:C:432:GLU:HG2 | 1:C:433:LYS:HG3 | 1.92 | 0.52 |
| 1:C:73:THR:OG1 | 1:C:76:GLY:HA2 | 2.10 | 0.52 |
| 1:D:547:GLU:OE2 | 1:D:550:ARG:NH1 | 2.37 | 0.52 |
| 1:M:39:ASP:OD2 | 1:M:298:ARG:CD | 2.57 | 0.52 |
| 1:Q:216:VAL:C | 1:Q:302:MET:HG2 | 2.29 | 0.52 |
| 1:R:280:THR:HG23 | 1:R:281:THR:N | 2.24 | 0.52 |
| 1:R:292:LYS:HA | 1:R:293:ASN:HD22 | 1.75 | 0.52 |
| 1:B:460:LEU:HB3 | 1:B:463:LEU:HD22 | 1.91 | 0.52 |
| 1:D:135:ASP:OD1 | 1:D:164:LYS:HD2 | 2.09 | 0.52 |
| 1:F:259:HIS:C | 1:F:259:HIS:CD2 | 2.83 | 0.52 |
| 1:G:27:GLU:HG2 | 1:G:96:PHE:CZ | 2.45 | 0.52 |
| 1:J:483:MET:HG2 | 1:J:550:ARG:HH21 | 1.75 | 0.52 |
| 1:M:542:LYS:HG3 | 1:M:571:SER:HB2 | 1.91 | 0.52 |
| 1:N:154:THR:O | 1:N:158:ALA:HB2 | 2.09 | 0.52 |
| 1:P:94:GLU:O | 1:P:120:SER:HA | 2.10 | 0.52 |
| 1:I:145:GLU:OE2 | 1:I:331:LEU:HB2 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:398:LYS:NZ | 1:I:398:LYS:HB3 | 2.25 | 0.51 |
| 1:J:217:GLN:HB2 | 1:J:536:GLU:HB3 | 1.93 | 0.51 |
| 1:M:269:MET:HG2 | 1:M:306:TYR:HE2 | 1.75 | 0.51 |
| 1:M:73:THR:HB | 1:M:92:ALA:HB1 | 1.92 | 0.51 |
| 1:B:43:ASN:O | 1:B:81:MET:CE | 2.58 | 0.51 |
| 1:C:67:HIS:HE1 | 1:C:91:THR:CG2 | 2.23 | 0.51 |
| 1:I:3:LEU:HB2 | 1:I:16:VAL:HG12 | 1.93 | 0.51 |
| 1:I:138:VAL:HG23 | 1:I:170:VAL:HB | 1.92 | 0.51 |
| 1:K:139:ALA:HB3 | 1:K:155:PHE:CZ | 2.45 | 0.51 |
| 1:I:337:GLY:HA2 | 1:K:245:LYS:HD3 | 1.92 | 0.51 |
| 1:M:178:ILE:HG13 | 1:M:233:ILE:HG23 | 1.93 | 0.51 |
| 1:M:550:ARG:H | 1:M:560:GLN:HE22 | 1.58 | 0.51 |
| 1:N:171:PRO:O | 1:N:240:PHE:HD2 | 1.93 | 0.51 |
| 1:P:450:TYR:N | 1:P:459:HIS:HD2 | 1.92 | 0.51 |
| 1:B:41:ASP:O | 1:B:43:ASN:N | 2.43 | 0.51 |
| 1:F:164:LYS:O | 1:F:167:CYS:HB2 | 2.11 | 0.51 |
| 1:G:619:ARG:HG2 | 1:G:619:ARG:HH11 | 1.75 | 0.51 |
| 1:K:522:ARG:O | 1:K:526:ASP:HB2 | 2.10 | 0.51 |
| 1:K:57:LYS:HA | 1:K:60:GLU:HB2 | 1.93 | 0.51 |
| 1:M:447:GLU:N | 1:M:448:PRO:HA | 2.26 | 0.51 |
| 1:M:492:LYS:O | 1:M:540:ILE:N | 2.38 | 0.51 |
| 1:N:595:ILE:CG2 | 1:N:599:GLY:HA2 | 2.40 | 0.51 |
| 1:O:229:LEU:HD13 | 1:O:314:VAL:CG1 | 2.40 | 0.51 |
| 1:C:111:PRO:HA | 1:O:47:LEU:HD13 | 1.92 | 0.51 |
| 1:O:535:TRP:CD2 | 1:O:605:LYS:HG2 | 2.45 | 0.51 |
| 1:O:632:LYS:HG3 | 1:O:633:SER:N | 2.25 | 0.51 |
| 1:Q:275:MET:HE1 | 1:Q:283:ILE:H | 1.75 | 0.51 |
| 1:B:216:VAL:C | 1:B:302:MET:HG2 | 2.30 | 0.51 |
| 1:F:181:VAL:HG11 | 1:F:226:PHE:HB2 | 1.92 | 0.51 |
| 1:G:626:LEU:HG | 1:G:641:PHE:CE2 | 2.45 | 0.51 |
| 1:L:129:ILE:O | 1:L:129:ILE:HG23 | 2.09 | 0.51 |
| 1:M:190:ASN:ND2 | 1:M:209:GLY:HA3 | 2.26 | 0.51 |
| 1:M:449:PHE:HA | 1:M:459:HIS:CD2 | 2.46 | 0.51 |
| 1:N:217:GLN:NE2 | 1:N:298:ARG:O | 2.31 | 0.51 |
| 1:N:517:ILE:HG13 | 1:N:518:SER:N | 2.25 | 0.51 |
| 1:A:556:ARG:HG2 | 1:A:556:ARG:HH11 | 1.75 | 0.51 |
| 1:C:567:ASP:C | 1:C:568:ASN:HD22 | 2.14 | 0.51 |
| 1:H:51:LYS:HG2 | 1:H:85:GLU:HG3 | 1.92 | 0.51 |
| 1:J:483:MET:HG2 | 1:J:550:ARG:NH2 | 2.26 | 0.51 |
| 1:K:68:VAL:O | 1:K:90:VAL:HA | 2.10 | 0.51 |
| 1:L:550:ARG:H | 1:L:560:GLN:HE22 | 1.57 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:238:PHE:HB3 | 1:M:240:PHE:CE1 | 2.45 | 0.51 |
| 1:M:258:ALA:HB3 | 1:M:315:GLU:O | 2.10 | 0.51 |
| 1:M:482:HIS:HA | 1:M:553:ILE:HG12 | 1.92 | 0.51 |
| 1:N:63:ASP:N | 1:N:64:GLY:HA2 | 2.25 | 0.51 |
| 1:O:450:TYR:H | 1:O:459:HIS:CD2 | 2.18 | 0.51 |
| 1:Q:232:PRO:HG3 | 1:Q:290:LYS:HE2 | 1.89 | 0.51 |
| 1:D:145:GLU:HA | 1:D:269:MET:CE | 2.41 | 0.51 |
| 1:D:271:TRP:CZ3 | 1:D:273:ILE:HG12 | 2.46 | 0.51 |
| 1:G:95:VAL:HB | 1:G:122:ARG:HG3 | 1.92 | 0.51 |
| 1:M:203:PRO:HA | 1:M:422:TYR:CG | 2.45 | 0.51 |
| 1:M:379:LYS:HA | 1:M:399:THR:HG22 | 1.90 | 0.51 |
| 1:M:356:GLN:NE2 | 1:M:608:LYS:HE3 | 2.25 | 0.51 |
| 1:M:83:ALA:HB2 | 1:M:116:ILE:HD11 | 1.92 | 0.51 |
| 1:O:2:PHE:CD2 | 1:O:520:LYS:HB3 | 2.46 | 0.51 |
| 1:Q:302:MET:HG2 | 1:Q:303:GLN:H | 1.75 | 0.51 |
| 1:R:638:ASN:N | 1:R:638:ASN:HD22 | 2.09 | 0.51 |
| 1:A:379:LYS:O | 1:A:381:LEU:HG | 2.11 | 0.51 |
| 1:B:3:LEU:O | 1:B:15:TRP:HA | 2.11 | 0.51 |
| 1:D:269:MET:HG2 | 1:D:306:TYR:CE1 | 2.45 | 0.51 |
| 1:H:626:LEU:HD23 | 1:H:627:HIS:N | 2.25 | 0.51 |
| 1:M:385:THR:CG2 | 4:M:802:HOH:O | 2.59 | 0.51 |
| 1:M:616:THR:O | 1:M:619:ARG:HB2 | 2.11 | 0.51 |
| 1:O:194:ARG:HG2 | 1:O:201:GLU:HB3 | 1.93 | 0.51 |
| 1:O:441:PRO:O | 1:O:477:LEU:HD11 | 2.11 | 0.51 |
| 1:Q:464:TYR:O | 1:Q:468:VAL:HG23 | 2.11 | 0.51 |
| 1:B:94:GLU:O | 1:B:120:SER:HA | 2.10 | 0.51 |
| 1:D:478:ARG:NH2 | 1:D:478:ARG:HG2 | 2.13 | 0.51 |
| 1:E:547:GLU:OE1 | 1:E:550:ARG:NH1 | 2.44 | 0.51 |
| 1:F:1:MET:N | 4:F:801:HOH:O | 2.43 | 0.51 |
| 1:N:326:HIS:HB2 | 1:N:331:LEU:HD12 | 1.92 | 0.51 |
| 1:P:379:LYS:CA | 1:P:399:THR:HG23 | 2.37 | 0.51 |
| 1:R:146:LEU:HD23 | 1:R:147:ILE:HG23 | 1.93 | 0.51 |
| 1:C:196:ASN:HB2 | 1:C:201:GLU:OE2 | 2.11 | 0.51 |
| 1:F:497:GLN:HE21 | 1:F:497:GLN:N | 1.98 | 0.51 |
| 1:J:103:ALA:O | 1:J:107:THR:HB | 2.11 | 0.51 |
| 1:L:412:PHE:HE2 | 1:L:451:MET:HG2 | 1.74 | 0.51 |
| 1:Q:243:GLU:HA | 1:Q:246:ILE:HD12 | 1.92 | 0.51 |
| 1:Q:553:ILE:O | 1:Q:553:ILE:CG2 | 2.59 | 0.51 |
| 1:A:58:LYS:HD3 | 1:A:64:GLY:O | 2.10 | 0.51 |
| 1:C:502:ASP:OD2 | 1:C:616:THR:HG21 | 2.11 | 0.51 |
| 1:E:157:GLU:O | 1:E:160:GLU:HG3 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:114:ASP:N | 1:I:114:ASP:OD1 | 2.38 | 0.51 |
| 1:L:73:THR:HB | 1:L:92:ALA:HB1 | 1.91 | 0.51 |
| 1:M:447:GLU:H | 1:M:448:PRO:HA | 1.75 | 0.51 |
| 1:O:173:THR:HG22 | 1:O:174:GLY:N | 2.25 | 0.51 |
| 1:Q:231:GLU:C | 1:Q:232:PRO:O | 2.49 | 0.51 |
| 1:R:220:GLU:HG3 | 1:R:536:GLU:O | 2.11 | 0.51 |
| 1:B:173:THR:HG22 | 1:B:274:ASP:HB3 | 1.93 | 0.50 |
| 1:C:233:ILE:HG12 | 1:C:256:ALA:HB2 | 1.94 | 0.50 |
| 1:C:569:MET:HA | 1:C:572:SER:HB2 | 1.93 | 0.50 |
| 1:F:446:ALA:O | 1:F:481:PRO:HD3 | 2.12 | 0.50 |
| 1:K:273:ILE:HD12 | 1:K:275:MET:CE | 2.40 | 0.50 |
| 1:L:39:ASP:OD2 | 1:L:298:ARG:CD | 2.60 | 0.50 |
| 1:M:142:PHE:HD2 | 1:M:146:LEU:HD12 | 1.76 | 0.50 |
| 1:P:486:LEU:HD11 | 1:P:577:MET:HE2 | 1.92 | 0.50 |
| 1:A:447:GLU:N | 1:A:448:PRO:HA | 2.26 | 0.50 |
| 1:E:107:THR:O | 1:E:110:SER:OG | 2.28 | 0.50 |
| 1:G:522:ARG:O | 1:G:526:ASP:HB2 | 2.10 | 0.50 |
| 1:J:269:MET:HG2 | 1:J:306:TYR:HE1 | 1.76 | 0.50 |
| 1:O:91:THR:HG22 | 1:O:117:THR:HG23 | 1.93 | 0.50 |
| 1:O:194:ARG:HG2 | 1:O:201:GLU:HB2 | 1.93 | 0.50 |
| 1:O:73:THR:HG23 | 1:O:74:GLY:N | 2.26 | 0.50 |
| 1:P:26:GLN:O | 1:P:30:ARG:CD | 2.59 | 0.50 |
| 1:Q:550:ARG:H | 1:Q:560:GLN:NE2 | 2.08 | 0.50 |
| 1:Q:82:ALA:O | 1:Q:87:ALA:HB3 | 2.11 | 0.50 |
| 1:A:101:ASP:O | 1:A:105:HIS:HB2 | 2.11 | 0.50 |
| 1:C:35:ASP:O | 1:C:38:LEU:N | 2.44 | 0.50 |
| 1:C:42:ARG:NH2 | 1:C:43:ASN:HD21 | 2.09 | 0.50 |
| 1:F:289:TRP:O | 1:F:290:LYS:HG2 | 2.11 | 0.50 |
| 1:I:627:HIS:HB2 | 1:I:640:GLN:HB2 | 1.94 | 0.50 |
| 1:J:300:HIS:CE1 | 1:J:301:TRP:CD2 | 2.99 | 0.50 |
| 1:K:556:ARG:H | 1:K:556:ARG:NH1 | 2.09 | 0.50 |
| 1:K:65:LYS:HA | 1:K:65:LYS:CE | 2.41 | 0.50 |
| 1:L:84:ARG:HG3 | 1:L:112:TRP:CZ2 | 2.46 | 0.50 |
| 1:M:541:VAL:HG22 | 1:M:601:PRO:HG3 | 1.92 | 0.50 |
| 1:N:203:PRO:HA | 1:N:422:TYR:CD2 | 2.46 | 0.50 |
| 1:N:578:TRP:CB | 1:N:591:GLY:HA3 | 2.41 | 0.50 |
| 1:D:434:VAL:HG12 | 1:D:469:LEU:CD1 | 2.36 | 0.50 |
| 1:K:217:GLN:HG3 | 1:K:537:TYR:CE1 | 2.46 | 0.50 |
| 1:K:356:GLN:HG2 | 1:K:357:THR:H | 1.75 | 0.50 |
| 1:N:153:ARG:HB2 | 1:N:328:GLU:OE2 | 2.12 | 0.50 |
| 1:O:27:GLU:HB3 | 1:O:96:PHE:CZ | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:269:MET:HG2 | 1:P:306:TYR:CE1 | 2.40 | 0.50 |
| 1:R:218:LEU:HD13 | 1:R:268:LEU:HD13 | 1.93 | 0.50 |
| 1:B:78:LEU:O | 1:B:81:MET:HB2 | 2.12 | 0.50 |
| 1:E:42:ARG:HH11 | 1:E:140:GLU:HG2 | 1.72 | 0.50 |
| 1:G:457:TRP:HA | 4:G:811:HOH:O | 2.09 | 0.50 |
| 1:I:566:ILE:CG2 | 1:I:569:MET:HE3 | 2.42 | 0.50 |
| 1:K:103:ALA:O | 1:K:107:THR:HB | 2.11 | 0.50 |
| 1:K:143:ASP:O | 1:K:144:THR:C | 2.50 | 0.50 |
| 1:M:269:MET:HG3 | 1:M:269:MET:O | 2.11 | 0.50 |
| 1:O:397:ALA:HA | 1:O:403:VAL:HG21 | 1.93 | 0.50 |
| 1:O:39:ASP:OD2 | 1:O:298:ARG:CD | 2.54 | 0.50 |
| 1:B:392:LEU:C | 1:B:392:LEU:CD2 | 2.79 | 0.50 |
| 1:D:528:ILE:HD12 | 1:D:528:ILE:H | 1.76 | 0.50 |
| 1:E:161:ARG:HB3 | 1:E:162:LEU:HD13 | 1.94 | 0.50 |
| 1:K:616:THR:C | 1:K:618:LEU:H | 2.15 | 0.50 |
| 1:M:142:PHE:CD2 | 1:M:146:LEU:HD12 | 2.46 | 0.50 |
| 1:O:353:LEU:HB3 | 1:O:357:THR:HB | 1.94 | 0.50 |
| 1:O:73:THR:CB | 1:O:92:ALA:HB1 | 2.32 | 0.50 |
| 1:Q:14:GLU:HG2 | 1:Q:523:THR:HG21 | 1.93 | 0.50 |
| 1:Q:629:LEU:O | 1:Q:637:ILE:HA | 2.12 | 0.50 |
| 1:R:421:HIS:O | 1:R:424:LYS:HE3 | 2.12 | 0.50 |
| 1:R:359:TYR:CZ | 1:R:605:LYS:HB2 | 2.46 | 0.50 |
| 1:B:486:LEU:HD12 | 1:B:548:ILE:HB | 1.94 | 0.50 |
| 1:D:379:LYS:CA | 1:D:399:THR:HG23 | 2.37 | 0.50 |
| 1:E:222:LYS:O | 1:E:225:GLU:HG2 | 2.12 | 0.50 |
| 1:F:489:ILE:O | 1:F:576:PRO:HD2 | 2.12 | 0.50 |
| 1:I:168:ARG:NH1 | 1:I:168:ARG:HG2 | 2.24 | 0.50 |
| 1:I:375:ASP:O | 1:I:399:THR:HG21 | 2.12 | 0.50 |
| 1:L:65:LYS:HA | 1:L:88:ASP:OD2 | 2.12 | 0.50 |
| 1:O:477:LEU:O | 1:O:479:VAL:HG12 | 2.12 | 0.50 |
| 1:P:143:ASP:O | 1:P:146:LEU:HA | 2.12 | 0.50 |
| 1:B:339:ASP:OD1 | 1:B:341:SER:HB2 | 2.12 | 0.50 |
| 1:D:230:SER:OG | 1:D:231:GLU:O | 2.28 | 0.50 |
| 1:G:273:ILE:O | 1:G:273:ILE:HG13 | 2.10 | 0.50 |
| 1:J:168:ARG:NH2 | 1:J:276:ASP:O | 2.43 | 0.50 |
| 1:J:625:CYS:SG | 1:J:627:HIS:CD2 | 3.05 | 0.50 |
| 1:K:84:ARG:HB2 | 1:K:112:TRP:NE1 | 2.27 | 0.50 |
| 1:K:487:LYS:HE3 | 1:K:547:GLU:HG2 | 1.94 | 0.50 |
| 1:N:359:TYR:C | 1:N:359:TYR:CD1 | 2.85 | 0.50 |
| 1:P:503:VAL:H | 1:P:515:ASP:CG | 2.15 | 0.50 |
| 1:C:244:GLU:OE2 | 1:C:244:GLU:CA | 2.60 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:168:ARG:HH22 | 1:E:276:ASP:C | 2.15 | 0.50 |
| 1:E:56:GLU:HG3 | 1:E:57:LYS:N | 2.25 | 0.50 |
| 1:J:26:GLN:O | 1:J:30:ARG:HD2 | 2.12 | 0.50 |
| 1:N:4:GLU:OE2 | 1:N:13:ARG:HD3 | 2.11 | 0.50 |
| 1:O:77:LEU:O | 1:O:81:MET:HG3 | 2.11 | 0.50 |
| 1:Q:367:ASN:HD21 | 1:Q:369:LYS:HG2 | 1.77 | 0.50 |
| 1:R:41:ASP:O | 1:R:45:LYS:HB2 | 2.12 | 0.50 |
| 1:R:556:ARG:HG3 | 1:R:556:ARG:NH1 | 2.09 | 0.50 |
| 1:R:612:TYR:OH | 1:R:615:ILE:HD12 | 2.11 | 0.50 |
| 1:A:273:ILE:HD11 | 1:A:283:ILE:HD12 | 1.93 | 0.49 |
| 1:B:452:SER:O | 1:B:453:ALA:C | 2.51 | 0.49 |
| 1:B:67:HIS:C | 1:B:67:HIS:ND1 | 2.64 | 0.49 |
| 1:C:485:VAL:CG2 | 1:C:547:GLU:HG3 | 2.42 | 0.49 |
| 1:D:489:ILE:CG1 | 1:D:490:PRO:HD2 | 2.40 | 0.49 |
| 1:F:299:ASP:OD1 | 1:F:537:TYR:OH | 2.15 | 0.49 |
| 1:H:222:LYS:NZ | 1:H:602:GLU:OE2 | 2.44 | 0.49 |
| 1:I:278:ASN:O | 1:I:280:THR:CG2 | 2.58 | 0.49 |
| 1:J:406:ILE:HG21 | 1:J:434:VAL:HG22 | 1.94 | 0.49 |
| 1:L:253:VAL:O | 1:L:253:VAL:HG22 | 2.10 | 0.49 |
| 1:N:87:ALA:HB1 | 1:N:88:ASP:HB2 | 1.94 | 0.49 |
| 1:O:356:GLN:O | 1:O:359:TYR:HB3 | 2.12 | 0.49 |
| 1:Q:141:VAL:O | 1:Q:141:VAL:HG12 | 2.12 | 0.49 |
| 1:R:218:LEU:O | 1:R:220:GLU:N | 2.44 | 0.49 |
| 1:R:7:ASN:O | 1:R:11:GLY:N | 2.40 | 0.49 |
| 1:A:221:MET:HE3 | 1:A:226:PHE:CD1 | 2.47 | 0.49 |
| 1:A:550:ARG:H | 1:A:560:GLN:NE2 | 2.10 | 0.49 |
| 1:B:141:VAL:O | 1:B:141:VAL:HG12 | 2.12 | 0.49 |
| 1:E:403:VAL:HB | 1:E:428:VAL:HB | 1.94 | 0.49 |
| 1:J:563:VAL:CG1 | 1:J:625:CYS:SG | 3.00 | 0.49 |
| 1:J:69:LEU:HD12 | 1:J:91:THR:O | 2.12 | 0.49 |
| 1:L:557:VAL:HG23 | 1:L:632:LYS:HB2 | 1.95 | 0.49 |
| 1:R:626:LEU:HD21 | 1:R:639:PHE:HD2 | 1.77 | 0.49 |
| 1:B:37:ILE:O | 1:B:37:ILE:HG22 | 2.13 | 0.49 |
| 1:B:629:LEU:O | 1:B:629:LEU:HG | 2.12 | 0.49 |
| 1:C:612:TYR:CE2 | 1:C:614:PRO:HA | 2.47 | 0.49 |
| 1:C:67:HIS:CE1 | 1:C:91:THR:HG22 | 2.42 | 0.49 |
| 1:E:315:GLU:HB3 | 1:E:318:GLN:HG3 | 1.93 | 0.49 |
| 1:F:144:THR:HG21 | 1:F:215:ASP:HB3 | 1.93 | 0.49 |
| 1:F:218:LEU:HD12 | 1:F:303:GLN:HB2 | 1.90 | 0.49 |
| 1:H:618:LEU:HD21 | 1:H:642:GLY:HA2 | 1.95 | 0.49 |
| 1:I:256:ALA:O | 1:I:319:THR:HA | 2.10 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:67:HIS:CE1 | 1:J:91:THR:HG22 | 2.43 | 0.49 |
| 1:K:137:ILE:O | 1:K:169:VAL:HA | 2.12 | 0.49 |
| 1:L:218:LEU:H | 1:L:303:GLN:HE21 | 1.60 | 0.49 |
| 1:M:136:ILE:HA | 1:M:168:ARG:O | 2.11 | 0.49 |
| 1:O:196:ASN:HB2 | 1:O:201:GLU:OE2 | 2.12 | 0.49 |
| 1:P:146:LEU:HB3 | 1:P:271:TRP:NE1 | 2.26 | 0.49 |
| 1:P:354:SER:O | 1:P:358:VAL:HG23 | 2.12 | 0.49 |
| 1:Q:114:ASP:N | 1:Q:114:ASP:OD1 | 2.44 | 0.49 |
| 1:Q:186:LEU:O | 1:Q:307:TYR:OH | 2.17 | 0.49 |
| 1:Q:269:MET:SD | 1:Q:270:TRP:N | 2.85 | 0.49 |
| 1:R:261:SER:OG | 1:R:316:MET:N | 2.43 | 0.49 |
| 1:R:51:LYS:NZ | 1:R:51:LYS:CB | 2.74 | 0.49 |
| 1:E:39:ASP:OD2 | 1:E:298:ARG:CD | 2.60 | 0.49 |
| 1:H:138:VAL:HG23 | 1:H:170:VAL:HB | 1.94 | 0.49 |
| 1:H:379:LYS:HA | 1:H:399:THR:HG23 | 1.94 | 0.49 |
| 1:J:42:ARG:HH11 | 1:J:140:GLU:HG2 | 1.76 | 0.49 |
| 1:O:194:ARG:HD2 | 1:O:198:GLU:O | 2.13 | 0.49 |
| 1:Q:153:ARG:NH1 | 1:Q:248:PHE:CZ | 2.80 | 0.49 |
| 1:R:143:ASP:OD2 | 1:R:148:GLY:HA3 | 2.13 | 0.49 |
| 1:R:297:TRP:CD2 | 1:R:495:ASP:HB3 | 2.48 | 0.49 |
| 1:F:626:LEU:HD23 | 1:F:626:LEU:C | 2.32 | 0.49 |
| 1:G:239:ASP:OD2 | 1:G:277:ARG:NH2 | 2.45 | 0.49 |
| 1:K:326:HIS:HB3 | 1:K:331:LEU:HD12 | 1.93 | 0.49 |
| 1:L:218:LEU:H | 1:L:303:GLN:NE2 | 2.09 | 0.49 |
| 1:M:434:VAL:HG12 | 1:M:469:LEU:CD1 | 2.42 | 0.49 |
| 1:A:375:ASP:O | 1:A:399:THR:HG21 | 2.13 | 0.49 |
| 1:F:67:HIS:ND1 | 1:F:89:LYS:HB3 | 2.27 | 0.49 |
| 1:G:405:ILE:HB | 1:G:430:ILE:HG12 | 1.93 | 0.49 |
| 1:I:634:THR:OG1 | 1:I:636:ASP:HB2 | 2.12 | 0.49 |
| 1:O:190:ASN:ND2 | 1:O:209:GLY:HA3 | 2.26 | 0.49 |
| 1:P:451:MET:HG3 | 1:P:452:SER:N | 2.28 | 0.49 |
| 1:C:480:GLU:HA | 1:C:481:PRO:C | 2.33 | 0.49 |
| 1:D:406:ILE:HG12 | 1:D:431:ILE:HD11 | 1.95 | 0.49 |
| 1:G:272:ASP:HA | 1:G:283:ILE:O | 2.12 | 0.49 |
| 1:H:42:ARG:NH2 | 1:H:43:ASN:HD21 | 2.09 | 0.49 |
| 1:I:35:ASP:OD1 | 1:I:300:HIS:CD2 | 2.65 | 0.49 |
| 1:K:493:PHE:HA | 1:K:539:GLY:HA2 | 1.94 | 0.49 |
| 1:L:241:GLU:HB2 | 1:L:277:ARG:NH2 | 2.27 | 0.49 |
| 1:O:624:LEU:HB2 | 1:O:642:GLY:O | 2.11 | 0.49 |
| 1:P:292:LYS:HB3 | 1:P:293:ASN:OD1 | 2.12 | 0.49 |
| 1:P:349:LEU:HD11 | 1:P:353:LEU:HD12 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:553:ILE:H | 1:R:553:ILE:HD12 | 1.77 | 0.49 |
| 1:R:567:ASP:HA | 1:R:623:SER:CB | 2.37 | 0.49 |
| 1:F:45:LYS:HE2 | 1:F:282:PHE:O | 2.12 | 0.49 |
| 1:H:273:ILE:HG13 | 1:H:275:MET:HE1 | 1.90 | 0.49 |
| 1:I:69:LEU:HD23 | 1:I:137:ILE:HG12 | 1.95 | 0.49 |
| 1:L:39:ASP:OD2 | 1:L:298:ARG:HD3 | 2.13 | 0.49 |
| 1:M:569:MET:HG3 | 1:M:624:LEU:HD13 | 1.83 | 0.49 |
| 1:N:255:GLU:HA | 1:N:320:PHE:O | 2.13 | 0.49 |
| 1:O:460:LEU:C | 1:O:462:PHE:N | 2.65 | 0.49 |
| 1:Q:139:ALA:O | 1:Q:142:PHE:CE1 | 2.65 | 0.49 |
| 1:R:109:ASN:HD22 | 1:R:109:ASN:N | 2.10 | 0.49 |
| 1:R:172:SER:HB3 | 1:R:241:GLU:OE2 | 2.12 | 0.49 |
| 1:R:87:ALA:O | 1:R:88:ASP:C | 2.51 | 0.49 |
| 1:F:171:PRO:CB | 1:F:273:ILE:HD12 | 2.43 | 0.49 |
| 1:F:353:LEU:HD22 | 1:F:357:THR:HG21 | 1.95 | 0.49 |
| 1:H:273:ILE:CG1 | 1:H:275:MET:HE3 | 2.28 | 0.49 |
| 1:I:497:GLN:NE2 | 1:I:497:GLN:N | 2.38 | 0.49 |
| 1:M:35:ASP:O | 1:M:37:ILE:N | 2.45 | 0.49 |
| 1:N:28:LEU:O | 1:N:31:SER:HB2 | 2.13 | 0.49 |
| 1:Q:443:ILE:HG13 | 1:Q:478:ARG:O | 2.13 | 0.49 |
| 1:R:42:ARG:HH11 | 1:R:140:GLU:HG2 | 1.78 | 0.49 |
| 1:R:218:LEU:HD22 | 1:R:221:MET:HE2 | 1.94 | 0.49 |
| 1:B:447:GLU:N | 1:B:448:PRO:CA | 2.76 | 0.49 |
| 1:C:168:ARG:NH1 | 1:C:241:GLU:OE2 | 2.46 | 0.49 |
| 1:C:378:SER:HB3 | 1:C:400:ALA:HB2 | 1.95 | 0.49 |
| 1:C:15:TRP:CD2 | 1:C:520:LYS:HG2 | 2.48 | 0.49 |
| 1:D:355:ARG:HD3 | 4:D:806:HOH:O | 2.11 | 0.49 |
| 1:G:470:LYS:O | 1:G:473:HIS:O | 2.30 | 0.49 |
| 1:H:42:ARG:HH11 | 1:H:140:GLU:CG | 2.22 | 0.49 |
| 1:J:443:ILE:HG12 | 1:J:445:LEU:HD13 | 1.95 | 0.49 |
| 1:M:214:PHE:HD2 | 1:M:305:VAL:HG22 | 1.75 | 0.49 |
| 1:M:569:MET:CG | 1:M:624:LEU:HD12 | 2.22 | 0.49 |
| 1:P:168:ARG:HH22 | 1:P:276:ASP:C | 2.16 | 0.49 |
| 1:Q:643:LYS:O | 1:Q:644:SER:CB | 2.61 | 0.49 |
| 1:F:145:GLU:CG | 1:F:331:LEU:HD22 | 2.42 | 0.48 |
| 1:G:353:LEU:HD22 | 1:G:357:THR:HG21 | 1.94 | 0.48 |
| 1:I:175:ASN:O | 1:I:271:TRP:HA | 2.13 | 0.48 |
| 1:K:90:VAL:HB | 1:K:116:ILE:HG12 | 1.94 | 0.48 |
| 1:K:299:ASP:O | 1:K:301:TRP:N | 2.46 | 0.48 |
| 1:M:278:ASN:O | 1:M:280:THR:N | 2.44 | 0.48 |
| 1:O:467:GLU:HA | 1:O:467:GLU:OE1 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:535:TRP:CD1 | 1:O:605:LYS:HA | 2.48 | 0.48 |
| 1:Q:275:MET:HE1 | 1:Q:283:ILE:N | 2.28 | 0.48 |
| 1:R:169:VAL:HG23 | 1:R:171:PRO:O | 2.13 | 0.48 |
| 1:R:284:ASP:HB3 | 1:R:291:ASN:HD21 | 1.78 | 0.48 |
| 1:A:218:LEU:HD12 | 1:A:303:GLN:CB | 2.42 | 0.48 |
| 1:C:218:LEU:HD13 | 1:C:268:LEU:HD13 | 1.95 | 0.48 |
| 1:D:80:LEU:HD13 | 1:D:509:PHE:CD1 | 2.48 | 0.48 |
| 1:I:273:ILE:CG1 | 1:I:275:MET:HE1 | 2.43 | 0.48 |
| 1:J:490:PRO:HB2 | 1:J:569:MET:HE2 | 1.90 | 0.48 |
| 1:K:316:MET:HG2 | 1:K:317:ASN:N | 2.27 | 0.48 |
| 1:L:193:PRO:HA | 1:L:362:ASN:ND2 | 2.28 | 0.48 |
| 1:R:175:ASN:ND2 | 1:R:237:LYS:HG2 | 2.28 | 0.48 |
| 1:B:66:VAL:CG1 | 1:B:67:HIS:N | 2.76 | 0.48 |
| 1:C:218:LEU:H | 1:C:303:GLN:HE21 | 1.61 | 0.48 |
| 1:E:41:ASP:O | 1:E:42:ARG:C | 2.51 | 0.48 |
| 1:K:444:VAL:HG13 | 1:K:479:VAL:HB | 1.95 | 0.48 |
| 1:N:188:MET:O | 1:N:362:ASN:OD1 | 2.31 | 0.48 |
| 1:P:141:VAL:O | 1:P:141:VAL:CG1 | 2.61 | 0.48 |
| 1:P:500:ALA:HB1 | 1:P:522:ARG:HH22 | 1.78 | 0.48 |
| 1:P:106:ILE:HD11 | 1:P:513:PHE:HB3 | 1.96 | 0.48 |
| 1:R:539:GLY:O | 1:R:601:PRO:HD2 | 2.13 | 0.48 |
| 1:B:218:LEU:HD12 | 1:B:303:GLN:CB | 2.43 | 0.48 |
| 1:C:57:LYS:HE2 | 1:C:135:ASP:HB3 | 1.95 | 0.48 |
| 1:C:62:THR:N | 1:C:63:ASP:HB3 | 2.29 | 0.48 |
| 1:I:291:ASN:ND2 | 1:I:295:TYR:HA | 2.29 | 0.48 |
| 1:I:45:LYS:NZ | 1:I:282:PHE:O | 2.45 | 0.48 |
| 1:J:242:HIS:O | 1:J:245:LYS:HB2 | 2.12 | 0.48 |
| 1:M:111:PRO:C | 1:M:113:SER:H | 2.17 | 0.48 |
| 1:M:89:LYS:HZ2 | 1:M:89:LYS:HB3 | 1.78 | 0.48 |
| 1:N:56:GLU:OE1 | 1:N:168:ARG:HD2 | 2.14 | 0.48 |
| 1:O:599:GLY:O | 1:O:601:PRO:HD3 | 2.13 | 0.48 |
| 1:Q:269:MET:HG2 | 1:Q:306:TYR:HE1 | 1.79 | 0.48 |
| 1:R:218:LEU:C | 1:R:220:GLU:H | 2.16 | 0.48 |
| 1:C:280:THR:HG23 | 1:C:281:THR:HG23 | 1.95 | 0.48 |
| 1:E:168:ARG:HA | 1:E:241:GLU:OE2 | 2.13 | 0.48 |
| 1:E:36:MET:SD | 2:E:701:SAH:HG1 | 2.54 | 0.48 |
| 1:M:550:ARG:O | 1:M:560:GLN:OE1 | 2.31 | 0.48 |
| 1:O:467:GLU:OE2 | 1:O:556:ARG:HA | 2.13 | 0.48 |
| 1:O:297:TRP:CD2 | 1:O:495:ASP:HB3 | 2.48 | 0.48 |
| 1:O:569:MET:HA | 1:O:572:SER:HB2 | 1.95 | 0.48 |
| 1:P:280:THR:HG23 | 1:P:281:THR:HG23 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:631:ASP:O | 1:P:635:GLY:N | 2.41 | 0.48 |
| 1:Q:570:SER:CB | 1:Q:622:LYS:HD3 | 2.40 | 0.48 |
| 1:H:51:LYS:HG3 | 1:H:85:GLU:CG | 2.43 | 0.48 |
| 1:I:136:ILE:HA | 1:I:168:ARG:O | 2.13 | 0.48 |
| 1:K:273:ILE:HD12 | 1:K:275:MET:HE3 | 1.95 | 0.48 |
| 1:L:253:VAL:O | 1:L:253:VAL:CG2 | 2.61 | 0.48 |
| 1:L:420:ILE:HD11 | 1:L:428:VAL:HG22 | 1.94 | 0.48 |
| 1:O:548:ILE:O | 1:O:562:CYS:SG | 2.67 | 0.48 |
| 1:Q:51:LYS:HA | 1:Q:85:GLU:CD | 2.33 | 0.48 |
| 1:R:36:MET:HA | 1:R:300:HIS:CD2 | 2.48 | 0.48 |
| 1:B:178:ILE:HA | 1:B:268:LEU:O | 2.14 | 0.48 |
| 1:C:484:GLY:HA3 | 1:C:581:TRP:CZ3 | 2.49 | 0.48 |
| 1:D:528:ILE:HD12 | 1:D:528:ILE:N | 2.28 | 0.48 |
| 1:E:226:PHE:CD1 | 1:E:226:PHE:N | 2.81 | 0.48 |
| 1:E:275:MET:HE1 | 1:E:283:ILE:H | 1.78 | 0.48 |
| 1:I:543:GLY:HA3 | 1:I:568:ASN:HD22 | 1.77 | 0.48 |
| 1:I:587:ASN:C | 1:I:587:ASN:ND2 | 2.67 | 0.48 |
| 1:J:169:VAL:CG2 | 1:J:171:PRO:O | 2.62 | 0.48 |
| 1:J:308:LEU:HD13 | 1:J:333:PHE:O | 2.13 | 0.48 |
| 1:L:290:LYS:HG2 | 1:L:290:LYS:O | 2.13 | 0.48 |
| 1:N:84:ARG:HD2 | 1:N:85:GLU:HG2 | 1.95 | 0.48 |
| 1:O:535:TRP:CE3 | 1:O:535:TRP:O | 2.67 | 0.48 |
| 1:A:467:GLU:CD | 1:A:557:VAL:HG12 | 2.34 | 0.48 |
| 1:D:489:ILE:O | 1:D:576:PRO:HD2 | 2.13 | 0.48 |
| 1:E:75:THR:O | 1:E:103:ALA:HA | 2.13 | 0.48 |
| 1:J:193:PRO:HA | 1:J:362:ASN:ND2 | 2.26 | 0.48 |
| 1:N:42:ARG:NH1 | 1:N:140:GLU:HG2 | 2.28 | 0.48 |
| 1:N:387:GLY:HA2 | 1:N:450:TYR:CE2 | 2.48 | 0.48 |
| 1:N:84:ARG:O | 1:N:85:GLU:HB2 | 2.14 | 0.48 |
| 1:O:553:ILE:HG13 | 1:O:554:ASP:H | 1.79 | 0.48 |
| 1:P:228:GLU:OE2 | 1:P:290:LYS:NZ | 2.47 | 0.48 |
| 1:P:455:ASN:HB2 | 1:P:458:ASN:HB2 | 1.96 | 0.48 |
| 1:R:338:LYS:HD3 | 1:R:338:LYS:HA | 1.52 | 0.48 |
| 1:B:218:LEU:HD13 | 1:B:268:LEU:HD13 | 1.96 | 0.48 |
| 1:B:460:LEU:HD21 | 1:B:579:MET:CE | 2.44 | 0.48 |
| 1:E:388:GLU:OE1 | 1:E:452:SER:HB2 | 2.13 | 0.48 |
| 1:H:38:LEU:HD21 | 1:H:503:VAL:HA | 1.96 | 0.48 |
| 1:I:273:ILE:HG13 | 1:I:283:ILE:HB | 1.96 | 0.48 |
| 1:K:220:GLU:HG3 | 1:K:536:GLU:O | 2.13 | 0.48 |
| 1:K:218:LEU:HD13 | 1:K:268:LEU:HD22 | 1.95 | 0.48 |
| 1:K:145:GLU:HG3 | 1:K:331:LEU:CD2 | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:159:LEU:HD13 | 1:M:243:GLU:N | 2.29 | 0.48 |
| 1:M:300:HIS:CE1 | 1:M:301:TRP:CE2 | 3.02 | 0.48 |
| 1:N:405:ILE:HB | 1:N:430:ILE:HG12 | 1.95 | 0.48 |
| 1:Q:143:ASP:C | 1:Q:145:GLU:H | 2.17 | 0.48 |
| 1:Q:356:GLN:O | 1:Q:359:TYR:HB3 | 2.13 | 0.48 |
| 1:R:548:ILE:HG22 | 1:R:549:LEU:HD22 | 1.95 | 0.48 |
| 1:C:293:ASN:N | 1:C:293:ASN:OD1 | 2.46 | 0.48 |
| 1:D:443:ILE:HG13 | 1:D:478:ARG:HB3 | 1.95 | 0.48 |
| 1:G:56:GLU:C | 1:G:58:LYS:H | 2.16 | 0.48 |
| 1:K:297:TRP:CE3 | 1:K:495:ASP:HB3 | 2.48 | 0.48 |
| 1:O:382:HIS:HD2 | 1:O:441:PRO:HA | 1.73 | 0.48 |
| 1:O:522:ARG:O | 1:O:526:ASP:HB2 | 2.14 | 0.48 |
| 1:A:612:TYR:CE2 | 1:A:614:PRO:HA | 2.49 | 0.47 |
| 1:C:323:VAL:HG12 | 1:C:325:ASN:HD21 | 1.79 | 0.47 |
| 1:D:578:TRP:CG | 1:D:591:GLY:HA3 | 2.49 | 0.47 |
| 1:F:497:GLN:NE2 | 1:F:497:GLN:N | 2.59 | 0.47 |
| 1:H:20:GLU:HG3 | 1:H:20:GLU:H | 1.52 | 0.47 |
| 1:I:615:ILE:O | 1:I:616:THR:C | 2.52 | 0.47 |
| 1:K:291:ASN:HB3 | 1:K:295:TYR:HB2 | 1.96 | 0.47 |
| 1:M:271:TRP:O | 1:M:285:MET:HB2 | 2.14 | 0.47 |
| 1:N:339:ASP:HA | 1:Q:244:GLU:HG3 | 1.96 | 0.47 |
| 1:N:67:HIS:HB3 | 1:N:135:ASP:H | 1.79 | 0.47 |
| 1:O:375:ASP:HB3 | 1:O:399:THR:OG1 | 2.14 | 0.47 |
| 1:P:531:GLU:HA | 1:P:609:GLN:O | 2.14 | 0.47 |
| 1:P:72:GLY:O | 2:P:701:SAH:N | 2.42 | 0.47 |
| 1:Q:489:ILE:HG22 | 1:Q:578:TRP:HZ3 | 1.79 | 0.47 |
| 1:D:202:GLU:HA | 4:D:852:HOH:O | 2.14 | 0.47 |
| 1:D:22:TYR:CE2 | 1:D:525:THR:HG22 | 2.50 | 0.47 |
| 1:D:239:ASP:OD2 | 1:D:242:HIS:HD2 | 1.96 | 0.47 |
| 1:D:435:THR:HA | 1:D:472:MET:SD | 2.54 | 0.47 |
| 1:D:67:HIS:HE1 | 1:D:91:THR:HG22 | 1.77 | 0.47 |
| 1:L:385:THR:HG22 | 4:L:825:HOH:O | 2.13 | 0.47 |
| 1:M:497:GLN:N | 1:M:497:GLN:HE21 | 1.99 | 0.47 |
| 1:N:84:ARG:CB | 1:N:112:TRP:CZ2 | 2.97 | 0.47 |
| 1:N:180:PRO:HB2 | 1:N:264:ILE:HG12 | 1.96 | 0.47 |
| 1:O:85:GLU:HA | 1:O:85:GLU:OE1 | 2.14 | 0.47 |
| 1:Q:236:PHE:CE2 | 1:Q:326:HIS:HD2 | 2.32 | 0.47 |
| 1:A:76:GLY:O | 1:A:77:LEU:C | 2.53 | 0.47 |
| 1:B:491:GLU:HG3 | 1:B:492:LYS:N | 2.29 | 0.47 |
| 1:C:480:GLU:OE2 | 1:C:482:HIS:CD2 | 2.55 | 0.47 |
| 1:C:28:LEU:HD23 | 1:C:521:ALA:HB2 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:140:GLU:HG3 | 1:F:140:GLU:O | 2.14 | 0.47 |
| 1:G:489:ILE:HG13 | 1:G:490:PRO:HD2 | 1.95 | 0.47 |
| 1:H:218:LEU:HD13 | 1:H:268:LEU:HD13 | 1.96 | 0.47 |
| 1:H:51:LYS:NZ | 1:H:51:LYS:CB | 2.78 | 0.47 |
| 1:J:270:TRP:CE2 | 1:J:286:GLY:HA2 | 2.49 | 0.47 |
| 1:J:356:GLN:O | 1:J:606:GLY:HA2 | 2.14 | 0.47 |
| 1:K:353:LEU:HD22 | 1:K:357:THR:HG21 | 1.95 | 0.47 |
| 1:K:532:GLN:HB2 | 1:K:532:GLN:HE21 | 1.45 | 0.47 |
| 1:L:317:ASN:ND2 | 1:L:317:ASN:N | 2.63 | 0.47 |
| 1:M:111:PRO:HG2 | 1:M:112:TRP:CE3 | 2.48 | 0.47 |
| 1:M:250:GLU:HB2 | 1:M:326:HIS:CD2 | 2.49 | 0.47 |
| 1:M:507:ASN:N | 1:M:507:ASN:HD22 | 2.11 | 0.47 |
| 1:O:218:LEU:H | 1:O:303:GLN:HE22 | 1.57 | 0.47 |
| 1:Q:357:THR:O | 1:Q:361:VAL:HG23 | 2.15 | 0.47 |
| 1:R:291:ASN:O | 1:R:292:LYS:HD2 | 2.12 | 0.47 |
| 1:A:243:GLU:HG2 | 1:A:244:GLU:OE1 | 2.14 | 0.47 |
| 1:B:535:TRP:CE3 | 1:B:605:LYS:HE3 | 2.49 | 0.47 |
| 1:E:157:GLU:HA | 1:E:160:GLU:CG | 2.45 | 0.47 |
| 1:E:284:ASP:HB3 | 1:E:294:ASN:HB2 | 1.96 | 0.47 |
| 1:F:42:ARG:HH21 | 1:F:43:ASN:ND2 | 2.11 | 0.47 |
| 1:G:478:ARG:NH2 | 1:G:480:GLU:OE1 | 2.47 | 0.47 |
| 1:J:450:TYR:H | 1:J:459:HIS:CD2 | 2.20 | 0.47 |
| 1:K:193:PRO:HA | 1:K:362:ASN:ND2 | 2.28 | 0.47 |
| 1:K:196:ASN:HB2 | 1:K:201:GLU:OE2 | 2.15 | 0.47 |
| 1:K:412:PHE:CE2 | 1:K:451:MET:HG2 | 2.44 | 0.47 |
| 1:K:489:ILE:HD12 | 1:K:545:ALA:HB2 | 1.95 | 0.47 |
| 1:O:168:ARG:HG2 | 1:O:241:GLU:OE2 | 2.14 | 0.47 |
| 1:O:146:LEU:HB2 | 1:O:271:TRP:CD1 | 2.49 | 0.47 |
| 1:R:643:LYS:O | 1:R:644:SER:HB3 | 2.15 | 0.47 |
| 1:B:507:ASN:N | 1:B:507:ASN:HD22 | 2.13 | 0.47 |
| 1:F:250:GLU:OE2 | 1:F:252:PHE:CE2 | 2.68 | 0.47 |
| 1:H:277:ARG:O | 1:H:277:ARG:HG2 | 2.13 | 0.47 |
| 1:J:490:PRO:HB2 | 1:J:572:SER:OG | 2.14 | 0.47 |
| 1:R:218:LEU:N | 1:R:303:GLN:HE21 | 2.11 | 0.47 |
| 1:A:623:SER:O | 1:A:624:LEU:HD23 | 2.15 | 0.47 |
| 1:B:470:LYS:NZ | 1:B:553:ILE:O | 2.47 | 0.47 |
| 1:E:567:ASP:OD1 | 1:E:623:SER:OG | 2.29 | 0.47 |
| 1:G:112:TRP:HD1 | 1:G:115:LYS:HD2 | 1.78 | 0.47 |
| 1:I:420:ILE:HD11 | 1:I:428:VAL:HG22 | 1.95 | 0.47 |
| 1:J:143:ASP:HB3 | 1:J:149:GLU:HG3 | 1.95 | 0.47 |
| 1:L:61:ASN:O | 1:L:63:ASP:O | 2.33 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:625:CYS:HB2 | 1:N:643:LYS:O | 2.13 | 0.47 |
| 1:O:556:ARG:O | 1:O:558:SER:OG | 2.30 | 0.47 |
| 1:R:243:GLU:CD | 1:R:243:GLU:H | 2.16 | 0.47 |
| 1:R:437:LEU:HD13 | 1:R:441:PRO:HD3 | 1.95 | 0.47 |
| 1:R:548:ILE:HD12 | 1:R:564:VAL:HG21 | 1.96 | 0.47 |
| 1:A:452:SER:O | 1:A:453:ALA:C | 2.53 | 0.47 |
| 1:C:261:SER:OG | 1:C:316:MET:N | 2.47 | 0.47 |
| 1:C:35:ASP:O | 1:C:36:MET:C | 2.53 | 0.47 |
| 1:D:379:LYS:HA | 1:D:399:THR:HG22 | 1.92 | 0.47 |
| 1:E:108:SER:O | 1:E:110:SER:N | 2.47 | 0.47 |
| 1:E:451:MET:HG3 | 1:E:452:SER:N | 2.28 | 0.47 |
| 1:E:71:ILE:HG23 | 1:E:93:LEU:HD12 | 1.96 | 0.47 |
| 1:F:316:MET:HA | 1:F:317:ASN:HA | 1.63 | 0.47 |
| 1:H:450:TYR:N | 1:H:459:HIS:HD2 | 2.02 | 0.47 |
| 1:I:137:ILE:O | 1:I:169:VAL:HA | 2.15 | 0.47 |
| 1:I:297:TRP:CD2 | 1:I:495:ASP:HB3 | 2.50 | 0.47 |
| 1:M:181:VAL:HG21 | 1:M:268:LEU:CD1 | 2.37 | 0.47 |
| 1:M:540:ILE:HD12 | 1:M:542:LYS:HE2 | 1.97 | 0.47 |
| 1:M:568:ASN:N | 1:M:568:ASN:ND2 | 2.62 | 0.47 |
| 1:P:387:GLY:HA2 | 1:P:450:TYR:CE1 | 2.50 | 0.47 |
| 1:Q:438:THR:HG21 | 1:R:629:LEU:HD21 | 1.97 | 0.47 |
| 1:A:480:GLU:HA | 1:A:481:PRO:C | 2.34 | 0.47 |
| 1:A:556:ARG:HG2 | 1:A:556:ARG:NH1 | 2.29 | 0.47 |
| 1:B:258:ALA:O | 1:B:316:MET:HA | 2.14 | 0.47 |
| 1:D:218:LEU:H | 1:D:303:GLN:HE21 | 1.62 | 0.47 |
| 1:H:497:GLN:N | 1:H:497:GLN:NE2 | 2.43 | 0.47 |
| 1:J:444:VAL:HG13 | 1:J:479:VAL:HB | 1.96 | 0.47 |
| 1:M:179:VAL:HG22 | 1:M:232:PRO:HA | 1.96 | 0.47 |
| 1:N:325:ASN:HB2 | 1:N:332:TRP:CE2 | 2.50 | 0.47 |
| 1:O:177:TYR:O | 1:O:269:MET:HA | 2.14 | 0.47 |
| 1:O:539:GLY:O | 1:O:601:PRO:HD2 | 2.14 | 0.47 |
| 1:O:587:ASN:C | 1:O:587:ASN:HD22 | 2.18 | 0.47 |
| 1:R:13:ARG:HB2 | 1:R:13:ARG:NH1 | 2.30 | 0.47 |
| 1:R:375:ASP:OD1 | 1:R:375:ASP:N | 2.48 | 0.47 |
| 1:R:69:LEU:HD11 | 1:R:71:ILE:HG12 | 1.97 | 0.47 |
| 1:B:78:LEU:HD22 | 2:B:701:SAH:HN2 | 1.80 | 0.47 |
| 1:D:278:ASN:HB2 | 1:D:280:THR:HG22 | 1.95 | 0.47 |
| 1:E:45:LYS:O | 1:E:275:MET:HG2 | 2.15 | 0.47 |
| 1:M:95:VAL:CB | 1:M:122:ARG:HG3 | 2.44 | 0.47 |
| 1:N:43:ASN:HD22 | 1:N:43:ASN:N | 2.12 | 0.47 |
| 1:P:367:ASN:HD21 | 1:P:369:LYS:HD3 | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:478:ARG:CG | 1:Q:478:ARG:HH21 | 2.20 | 0.47 |
| 1:R:604:ASN:OD1 | 1:R:606:GLY:N | 2.33 | 0.47 |
| 1:F:416:PHE:O | 1:F:420:ILE:HG13 | 2.15 | 0.47 |
| 1:G:375:ASP:O | 1:G:399:THR:HG21 | 2.14 | 0.47 |
| 1:I:177:TYR:HA | 1:I:233:ILE:O | 2.14 | 0.47 |
| 1:K:168:ARG:HH11 | 1:K:168:ARG:HG2 | 1.80 | 0.47 |
| 1:N:275:MET:HE2 | 1:N:275:MET:H | 1.79 | 0.47 |
| 1:N:57:LYS:HB3 | 1:N:66:VAL:HG11 | 1.97 | 0.47 |
| 1:R:354:SER:O | 1:R:358:VAL:HG23 | 2.14 | 0.47 |
| 1:R:578:TRP:HE1 | 1:R:580:GLU:HG3 | 1.80 | 0.47 |
| 1:R:84:ARG:O | 1:R:85:GLU:HB2 | 2.15 | 0.47 |
| 1:A:241:GLU:HG3 | 1:A:277:ARG:HH21 | 1.79 | 0.47 |
| 1:B:416:PHE:O | 1:B:420:ILE:HG13 | 2.15 | 0.47 |
| 1:D:292:LYS:HA | 1:D:293:ASN:HA | 1.53 | 0.47 |
| 1:F:57:LYS:HG2 | 1:F:135:ASP:HB3 | 1.97 | 0.47 |
| 1:G:179:VAL:HG22 | 1:G:232:PRO:HA | 1.96 | 0.47 |
| 1:I:298:ARG:HD2 | 1:I:301:TRP:HE3 | 1.80 | 0.47 |
| 1:I:566:ILE:HG22 | 1:I:569:MET:HE3 | 1.97 | 0.47 |
| 1:J:129:ILE:O | 1:J:131:GLY:N | 2.47 | 0.47 |
| 1:K:181:VAL:HG21 | 1:K:268:LEU:HD11 | 1.97 | 0.47 |
| 1:M:111:PRO:HG2 | 1:M:112:TRP:CZ3 | 2.50 | 0.47 |
| 1:M:615:ILE:O | 1:M:615:ILE:HG13 | 2.14 | 0.47 |
| 1:N:514:PHE:O | 1:N:518:SER:CB | 2.63 | 0.47 |
| 1:P:529:VAL:HG12 | 1:P:530:ASP:O | 2.15 | 0.47 |
| 1:Q:222:LYS:HB3 | 1:Q:224:HIS:HB3 | 1.96 | 0.47 |
| 1:R:35:ASP:O | 1:R:36:MET:C | 2.53 | 0.47 |
| 1:R:97:LYS:HB2 | 1:R:98:PRO:HD3 | 1.96 | 0.47 |
| 1:B:516:GLU:HG2 | 1:B:517:ILE:N | 2.30 | 0.46 |
| 1:B:59:HIS:O | 1:B:60:GLU:C | 2.52 | 0.46 |
| 1:C:73:THR:O | 2:C:701:SAH:HA | 2.15 | 0.46 |
| 1:E:216:VAL:O | 1:E:302:MET:HG2 | 2.16 | 0.46 |
| 1:E:84:ARG:HG3 | 1:E:85:GLU:N | 2.31 | 0.46 |
| 1:F:259:HIS:O | 1:F:259:HIS:CD2 | 2.68 | 0.46 |
| 1:F:449:PHE:CD1 | 1:F:449:PHE:C | 2.89 | 0.46 |
| 1:G:483:MET:SD | 1:G:550:ARG:HG3 | 2.55 | 0.46 |
| 1:G:492:LYS:HB2 | 1:G:571:SER:O | 2.14 | 0.46 |
| 1:G:57:LYS:NZ | 1:G:166:GLY:O | 2.48 | 0.46 |
| 1:H:137:ILE:O | 1:H:169:VAL:HA | 2.15 | 0.46 |
| 1:I:146:LEU:HB2 | 1:I:271:TRP:CD1 | 2.50 | 0.46 |
| 1:K:180:PRO:O | 1:K:181:VAL:HG23 | 2.16 | 0.46 |
| 1:L:412:PHE:CE2 | 1:L:451:MET:HG2 | 2.49 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:512:SER:O | 1:N:515:ASP:HB2 | 2.15 | 0.46 |
| 1:N:595:ILE:HG22 | 1:N:599:GLY:HA2 | 1.97 | 0.46 |
| 1:O:269:MET:HG3 | 1:O:304:ALA:HB3 | 1.97 | 0.46 |
| 1:P:285:MET:O | 1:P:303:GLN:OE1 | 2.33 | 0.46 |
| 1:P:407:ASP:O | 1:P:413:ARG:HD3 | 2.15 | 0.46 |
| 1:Q:179:VAL:HG21 | 1:Q:270:TRP:CH2 | 2.51 | 0.46 |
| 1:Q:460:LEU:HD22 | 1:Q:463:LEU:HD21 | 1.97 | 0.46 |
| 1:R:580:GLU:HA | 1:R:588:LEU:O | 2.15 | 0.46 |
| 1:B:297:TRP:CE3 | 1:B:298:ARG:HA | 2.50 | 0.46 |
| 1:B:434:VAL:HG12 | 1:B:469:LEU:HD13 | 1.97 | 0.46 |
| 1:E:179:VAL:HG11 | 1:E:228:GLU:HG2 | 1.97 | 0.46 |
| 1:E:258:ALA:HB2 | 1:E:314:VAL:HG13 | 1.98 | 0.46 |
| 1:E:406:ILE:HG12 | 1:E:431:ILE:HD11 | 1.97 | 0.46 |
| 1:F:198:GLU:O | 1:F:201:GLU:HG3 | 2.16 | 0.46 |
| 1:J:381:LEU:HD23 | 1:J:381:LEU:HA | 1.73 | 0.46 |
| 1:K:104:ARG:HA | 1:K:107:THR:HG22 | 1.98 | 0.46 |
| 1:N:27:GLU:HB3 | 1:N:96:PHE:CE1 | 2.50 | 0.46 |
| 1:N:56:GLU:O | 1:N:60:GLU:HG3 | 2.14 | 0.46 |
| 1:O:419:TYR:O | 1:O:422:TYR:N | 2.44 | 0.46 |
| 1:R:53:THR:HB | 1:R:136:ILE:HD13 | 1.96 | 0.46 |
| 1:C:168:ARG:CG | 1:C:168:ARG:NH1 | 2.52 | 0.46 |
| 1:C:70:ASP:HA | 1:C:138:VAL:O | 2.14 | 0.46 |
| 1:E:242:HIS:HB3 | 1:E:244:GLU:OE2 | 2.15 | 0.46 |
| 1:F:107:THR:HG21 | 1:F:116:ILE:HG21 | 1.97 | 0.46 |
| 1:F:360:HIS:NE2 | 1:F:447:GLU:OE2 | 2.40 | 0.46 |
| 1:G:550:ARG:H | 1:G:560:GLN:HE22 | 1.64 | 0.46 |
| 1:G:75:THR:O | 1:G:106:ILE:HD12 | 2.15 | 0.46 |
| 1:H:178:ILE:HA | 1:H:268:LEU:O | 2.15 | 0.46 |
| 1:I:271:TRP:HZ3 | 1:I:283:ILE:HG22 | 1.79 | 0.46 |
| 1:I:398:LYS:HZ3 | 1:I:398:LYS:HB3 | 1.81 | 0.46 |
| 1:J:51:LYS:HG3 | 1:J:85:GLU:CD | 2.34 | 0.46 |
| 1:K:218:LEU:HD11 | 1:K:268:LEU:HD22 | 1.98 | 0.46 |
| 1:M:381:LEU:HB3 | 1:M:442:ASP:HB2 | 1.97 | 0.46 |
| 1:M:94:GLU:OE2 | 2:M:701:SAH:H1' | 2.15 | 0.46 |
| 1:N:160:GLU:H | 1:N:160:GLU:HG2 | 1.55 | 0.46 |
| 1:N:553:ILE:HD12 | 1:N:553:ILE:HA | 1.72 | 0.46 |
| 1:N:549:LEU:HD12 | 1:N:560:GLN:NE2 | 2.30 | 0.46 |
| 1:O:84:ARG:HG3 | 1:O:112:TRP:CZ2 | 2.50 | 0.46 |
| 1:R:181:VAL:CG1 | 1:R:226:PHE:HB2 | 2.45 | 0.46 |
| 1:R:480:GLU:OE2 | 1:R:482:HIS:HD2 | 1.97 | 0.46 |
| 1:C:144:THR:O | 1:C:271:TRP:CD1 | 2.68 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:250:GLU:HB2 | 1:H:326:HIS:CD2 | 2.51 | 0.46 |
| 1:I:555:GLY:HA3 | 1:I:556:ARG:O | 2.14 | 0.46 |
| 1:J:175:ASN:ND2 | 1:J:237:LYS:HG2 | 2.31 | 0.46 |
| 1:K:28:LEU:HD11 | 1:K:517:ILE:HD12 | 1.98 | 0.46 |
| 1:M:175:ASN:HD21 | 1:M:237:LYS:NZ | 2.13 | 0.46 |
| 1:M:193:PRO:HA | 1:M:362:ASN:HD21 | 1.81 | 0.46 |
| 1:O:38:LEU:HD21 | 1:O:503:VAL:HA | 1.96 | 0.46 |
| 1:O:410:GLU:HG3 | 1:O:410:GLU:O | 2.14 | 0.46 |
| 1:O:498:ASN:HA | 1:O:501:SER:OG | 2.15 | 0.46 |
| 1:Q:254:ARG:O | 1:Q:321:GLU:CA | 2.59 | 0.46 |
| 1:Q:392:LEU:HD12 | 1:Q:445:LEU:HB3 | 1.97 | 0.46 |
| 1:Q:522:ARG:O | 1:Q:526:ASP:HB2 | 2.14 | 0.46 |
| 1:R:553:ILE:HD12 | 1:R:553:ILE:N | 2.29 | 0.46 |
| 1:A:244:GLU:CD | 1:A:244:GLU:H | 2.18 | 0.46 |
| 1:F:169:VAL:HG22 | 1:F:241:GLU:HG2 | 1.97 | 0.46 |
| 1:F:73:THR:O | 1:F:74:GLY:C | 2.54 | 0.46 |
| 1:G:258:ALA:HB3 | 1:G:315:GLU:O | 2.15 | 0.46 |
| 1:G:144:THR:HG23 | 1:G:302:MET:O | 2.16 | 0.46 |
| 1:H:218:LEU:H | 1:H:303:GLN:NE2 | 2.12 | 0.46 |
| 1:M:483:MET:HE3 | 1:M:550:ARG:HG2 | 1.96 | 0.46 |
| 1:N:349:LEU:HD23 | 1:N:350:HIS:N | 2.30 | 0.46 |
| 1:P:157:GLU:O | 1:P:161:ARG:HB2 | 2.15 | 0.46 |
| 1:P:45:LYS:HZ1 | 1:P:294:ASN:HD22 | 1.61 | 0.46 |
| 1:P:447:GLU:N | 1:P:448:PRO:HA | 2.30 | 0.46 |
| 1:Q:420:ILE:HD11 | 1:R:5:LYS:HA | 1.98 | 0.46 |
| 1:R:140:GLU:HG3 | 1:R:140:GLU:O | 2.16 | 0.46 |
| 1:R:258:ALA:C | 1:R:260:SER:H | 2.19 | 0.46 |
| 1:B:71:ILE:HG21 | 1:B:154:THR:HG23 | 1.98 | 0.46 |
| 1:C:56:GLU:OE1 | 1:C:168:ARG:HD2 | 2.16 | 0.46 |
| 1:E:67:HIS:CE1 | 1:E:91:THR:CG2 | 2.88 | 0.46 |
| 1:G:559:SER:HA | 1:G:630:PHE:O | 2.16 | 0.46 |
| 1:H:258:ALA:HB2 | 1:H:314:VAL:CG2 | 2.46 | 0.46 |
| 1:J:323:VAL:HG23 | 1:J:335:ASN:HA | 1.96 | 0.46 |
| 1:K:335:ASN:O | 1:K:338:LYS:HB2 | 2.16 | 0.46 |
| 1:K:34:GLY:C | 1:K:499:ILE:HA | 2.36 | 0.46 |
| 1:J:421:HIS:HB2 | 1:K:3:LEU:HB3 | 1.97 | 0.46 |
| 1:L:145:GLU:HG3 | 1:L:213:VAL:HG21 | 1.96 | 0.46 |
| 1:L:179:VAL:HG21 | 1:L:270:TRP:CH2 | 2.50 | 0.46 |
| 1:L:190:ASN:HD21 | 1:L:209:GLY:HA3 | 1.81 | 0.46 |
| 1:L:146:LEU:HB2 | 1:L:271:TRP:CD1 | 2.49 | 0.46 |
| 1:M:218:LEU:H | 1:M:303:GLN:HE21 | 1.62 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:379:LYS:CA | 1:N:399:THR:CG2 | 2.86 | 0.46 |
| 1:N:627:HIS:HB2 | 1:N:640:GLN:HB2 | 1.98 | 0.46 |
| 1:O:621:ASP:OD1 | 1:O:621:ASP:N | 2.46 | 0.46 |
| 1:Q:339:ASP:C | 1:Q:341:SER:H | 2.19 | 0.46 |
| 1:A:169:VAL:HG22 | 1:A:171:PRO:O | 2.15 | 0.46 |
| 1:A:175:ASN:ND2 | 1:A:237:LYS:HG2 | 2.30 | 0.46 |
| 1:A:168:ARG:NH1 | 1:A:241:GLU:OE2 | 2.49 | 0.46 |
| 1:B:156:LYS:HE2 | 1:B:246:ILE:O | 2.16 | 0.46 |
| 1:C:190:ASN:ND2 | 1:C:209:GLY:HA3 | 2.31 | 0.46 |
| 1:C:631:ASP:C | 1:C:631:ASP:OD1 | 2.54 | 0.46 |
| 1:D:452:SER:O | 1:D:453:ALA:C | 2.54 | 0.46 |
| 1:D:506:VAL:O | 1:D:507:ASN:C | 2.53 | 0.46 |
| 1:E:143:ASP:O | 1:E:146:LEU:HA | 2.16 | 0.46 |
| 1:F:480:GLU:HA | 1:F:481:PRO:C | 2.35 | 0.46 |
| 1:G:502:ASP:OD2 | 1:G:616:THR:HG21 | 2.16 | 0.46 |
| 1:H:478:ARG:NH2 | 1:H:478:ARG:CG | 2.70 | 0.46 |
| 1:I:478:ARG:NH2 | 1:I:478:ARG:HG2 | 2.30 | 0.46 |
| 1:J:502:ASP:OD2 | 1:J:616:THR:HG21 | 2.16 | 0.46 |
| 1:K:123:SER:CB | 2:K:701:SAH:HN62 | 2.17 | 0.46 |
| 1:N:385:THR:HA | 1:N:445:LEU:O | 2.15 | 0.46 |
| 1:P:216:VAL:HG22 | 1:P:218:LEU:HD23 | 1.98 | 0.46 |
| 1:P:253:VAL:HG23 | 1:P:253:VAL:O | 2.15 | 0.46 |
| 1:Q:139:ALA:O | 1:Q:142:PHE:HE1 | 1.99 | 0.46 |
| 1:A:145:GLU:O | 1:A:146:LEU:HB3 | 2.16 | 0.46 |
| 1:A:272:ASP:C | 1:A:272:ASP:OD1 | 2.54 | 0.46 |
| 1:C:16:VAL:HG22 | 4:C:811:HOH:O | 2.16 | 0.46 |
| 1:C:314:VAL:HG23 | 1:C:320:PHE:CD2 | 2.50 | 0.46 |
| 1:F:7:ASN:ND2 | 1:F:640:GLN:OE1 | 2.45 | 0.46 |
| 1:G:151:ALA:O | 1:G:155:PHE:HD2 | 1.99 | 0.46 |
| 1:G:93:LEU:CD2 | 1:G:119:ILE:HB | 2.46 | 0.46 |
| 1:I:379:LYS:CA | 1:I:399:THR:HG23 | 2.36 | 0.46 |
| 1:J:274:ASP:OD2 | 1:J:277:ARG:CA | 2.63 | 0.46 |
| 1:M:280:THR:CG2 | 1:M:281:THR:N | 2.79 | 0.46 |
| 1:M:218:LEU:N | 1:M:303:GLN:NE2 | 2.64 | 0.46 |
| 1:M:67:HIS:HD2 | 1:M:133:ARG:O | 1.98 | 0.46 |
| 1:N:327:ASP:OD1 | 1:N:328:GLU:N | 2.49 | 0.46 |
| 1:P:73:THR:O | 2:P:701:SAH:HA | 2.15 | 0.46 |
| 1:Q:42:ARG:HE | 1:Q:43:ASN:ND2 | 2.14 | 0.46 |
| 1:A:554:ASP:O | 1:A:555:GLY:O | 2.34 | 0.46 |
| 1:D:626:LEU:CD2 | 1:D:628:ALA:HB2 | 2.45 | 0.46 |
| 1:E:385:THR:HA | 1:E:445:LEU:O | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:42:ARG:HE | 1:E:43:ASN:HD21 | 1.64 | 0.46 |
| 1:F:203:PRO:HA | 1:F:422:TYR:CG | 2.51 | 0.46 |
| 1:G:156:LYS:HA | 1:G:243:GLU:HB3 | 1.97 | 0.46 |
| 1:G:190:ASN:ND2 | 1:G:209:GLY:HA3 | 2.31 | 0.46 |
| 1:H:242:HIS:O | 1:H:245:LYS:HB2 | 2.16 | 0.46 |
| 1:H:67:HIS:CE1 | 1:H:89:LYS:HE3 | 2.51 | 0.46 |
| 1:I:298:ARG:O | 1:I:301:TRP:O | 2.34 | 0.46 |
| 1:I:492:LYS:HA | 1:I:573:ASN:OD1 | 2.16 | 0.46 |
| 1:K:257:VAL:O | 1:K:257:VAL:HG12 | 2.14 | 0.46 |
| 1:M:364:MET:HG3 | 1:M:370:PHE:CE2 | 2.51 | 0.46 |
| 1:P:406:ILE:HD13 | 1:P:434:VAL:HA | 1.97 | 0.46 |
| 1:C:140:GLU:CG | 1:C:140:GLU:O | 2.61 | 0.46 |
| 1:D:138:VAL:HG23 | 1:D:170:VAL:HB | 1.97 | 0.46 |
| 1:F:48:ALA:O | 1:F:51:LYS:N | 2.48 | 0.46 |
| 1:F:73:THR:O | 1:F:76:GLY:N | 2.49 | 0.46 |
| 1:G:35:ASP:OD1 | 1:G:35:ASP:N | 2.48 | 0.46 |
| 1:H:133:ARG:HG3 | 1:H:164:LYS:HG2 | 1.98 | 0.46 |
| 1:H:239:ASP:OD1 | 1:H:242:HIS:HB2 | 2.16 | 0.46 |
| 1:H:460:LEU:HD21 | 1:H:579:MET:CE | 2.46 | 0.46 |
| 1:J:216:VAL:O | 1:J:302:MET:HG2 | 2.16 | 0.46 |
| 1:K:367:ASN:OD1 | 1:K:370:PHE:N | 2.48 | 0.46 |
| 1:M:289:TRP:O | 1:M:290:LYS:HG2 | 2.16 | 0.46 |
| 1:M:418:LYS:HB2 | 1:M:418:LYS:HE3 | 1.79 | 0.46 |
| 1:P:502:ASP:OD2 | 1:P:616:THR:HB | 2.15 | 0.46 |
| 1:C:247:ILE:HB | 1:C:250:GLU:OE2 | 2.16 | 0.45 |
| 1:C:61:ASN:HD22 | 1:C:61:ASN:N | 2.14 | 0.45 |
| 1:D:45:LYS:O | 1:D:275:MET:HG2 | 2.15 | 0.45 |
| 1:G:217:GLN:HB2 | 1:G:536:GLU:HB3 | 1.98 | 0.45 |
| 1:J:291:ASN:HB3 | 1:J:295:TYR:HB2 | 1.98 | 0.45 |
| 1:K:404:THR:HG23 | 1:K:429:GLU:HG3 | 1.99 | 0.45 |
| 1:K:360:HIS:HB2 | 1:K:606:GLY:HA3 | 1.98 | 0.45 |
| 1:L:353:LEU:HD22 | 1:L:357:THR:HG21 | 1.97 | 0.45 |
| 1:M:483:MET:CE | 1:M:550:ARG:HG2 | 2.46 | 0.45 |
| 1:O:412:PHE:HE2 | 1:O:451:MET:HG2 | 1.81 | 0.45 |
| 1:P:164:LYS:O | 1:P:167:CYS:HB2 | 2.16 | 0.45 |
| 1:Q:99:MET:O | 1:Q:102:CYS:HB3 | 2.16 | 0.45 |
| 1:R:243:GLU:N | 1:R:243:GLU:OE1 | 2.43 | 0.45 |
| 1:R:316:MET:HA | 1:R:317:ASN:HA | 1.69 | 0.45 |
| 1:R:353:LEU:HD22 | 1:R:357:THR:CG2 | 2.46 | 0.45 |
| 1:A:385:THR:HA | 1:A:445:LEU:O | 2.16 | 0.45 |
| 1:A:84:ARG:HG3 | 1:A:112:TRP:CZ2 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:466:VAL:HG11 | 1:B:553:ILE:CG2 | 2.46 | 0.45 |
| 1:B:569:MET:HA | 1:B:572:SER:HB2 | 1.97 | 0.45 |
| 1:E:48:ALA:HA | 1:E:51:LYS:HB2 | 1.98 | 0.45 |
| 1:E:490:PRO:CB | 1:E:569:MET:HE1 | 2.46 | 0.45 |
| 1:F:502:ASP:OD2 | 1:F:616:THR:HG21 | 2.17 | 0.45 |
| 1:G:478:ARG:HH21 | 1:G:478:ARG:CG | 2.29 | 0.45 |
| 1:G:489:ILE:HG12 | 1:G:541:VAL:HG22 | 1.99 | 0.45 |
| 1:J:144:THR:CG2 | 1:J:144:THR:O | 2.64 | 0.45 |
| 1:J:218:LEU:N | 1:J:303:GLN:NE2 | 2.62 | 0.45 |
| 1:K:179:VAL:CG2 | 1:K:270:TRP:CH2 | 2.99 | 0.45 |
| 1:K:193:PRO:HA | 1:K:362:ASN:HD21 | 1.82 | 0.45 |
| 1:L:447:GLU:N | 1:L:448:PRO:HA | 2.32 | 0.45 |
| 1:N:566:ILE:HG21 | 1:N:569:MET:CE | 2.42 | 0.45 |
| 1:O:143:ASP:HB3 | 1:O:149:GLU:HG3 | 1.98 | 0.45 |
| 1:O:427:ASN:OD1 | 1:O:427:ASN:N | 2.49 | 0.45 |
| 1:P:39:ASP:OD2 | 1:P:298:ARG:HD3 | 2.16 | 0.45 |
| 1:Q:218:LEU:HD23 | 1:Q:218:LEU:HA | 1.42 | 0.45 |
| 1:Q:287:PRO:HG2 | 1:Q:289:TRP:CZ2 | 2.50 | 0.45 |
| 1:Q:395:LEU:C | 1:Q:397:ALA:H | 2.18 | 0.45 |
| 1:Q:468:VAL:O | 1:Q:472:MET:HG3 | 2.16 | 0.45 |
| 1:A:447:GLU:H | 1:A:448:PRO:HA | 1.82 | 0.45 |
| 1:B:119:ILE:HG22 | 1:B:121:GLU:HG2 | 1.99 | 0.45 |
| 1:B:190:ASN:O | 1:B:190:ASN:ND2 | 2.50 | 0.45 |
| 1:B:357:THR:O | 1:B:361:VAL:HG23 | 2.16 | 0.45 |
| 1:B:297:TRP:CE3 | 1:B:495:ASP:HB3 | 2.51 | 0.45 |
| 1:C:456:PRO:HD2 | 1:C:457:TRP:CE3 | 2.51 | 0.45 |
| 1:C:592:LEU:HD21 | 1:C:595:ILE:HD11 | 1.97 | 0.45 |
| 1:F:72:GLY:CA | 2:F:701:SAH:O4' | 2.65 | 0.45 |
| 1:G:540:ILE:HB | 1:G:599:GLY:O | 2.15 | 0.45 |
| 1:H:269:MET:CG | 1:H:306:TYR:HE1 | 2.27 | 0.45 |
| 1:H:47:LEU:HD22 | 1:H:51:LYS:CD | 2.46 | 0.45 |
| 1:K:292:LYS:HA | 1:K:293:ASN:HB3 | 1.98 | 0.45 |
| 1:L:157:GLU:HA | 1:L:160:GLU:HG2 | 1.97 | 0.45 |
| 1:M:174:GLY:HA2 | 1:M:273:ILE:HA | 1.98 | 0.45 |
| 1:M:35:ASP:HB3 | 1:M:300:HIS:H | 1.80 | 0.45 |
| 1:N:315:GLU:CB | 1:N:318:GLN:HG2 | 2.44 | 0.45 |
| 1:O:460:LEU:HD11 | 1:O:637:ILE:HD11 | 1.98 | 0.45 |
| 1:P:110:SER:HB2 | 1:P:112:TRP:CZ3 | 2.51 | 0.45 |
| 1:A:4:GLU:OE2 | 1:A:13:ARG:NH1 | 2.50 | 0.45 |
| 1:A:480:GLU:HG2 | 1:A:584:GLY:H | 1.79 | 0.45 |
| 1:B:287:PRO:O | 1:B:289:TRP:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:534:LEU:HD11 | 1:B:611:VAL:CG1 | 2.46 | 0.45 |
| 1:B:535:TRP:CG | 1:B:605:LYS:HG2 | 2.51 | 0.45 |
| 1:B:43:ASN:O | 1:B:81:MET:HE1 | 2.16 | 0.45 |
| 1:F:214:PHE:O | 1:F:304:ALA:HA | 2.17 | 0.45 |
| 1:F:179:VAL:HG22 | 1:F:232:PRO:HA | 1.98 | 0.45 |
| 1:G:258:ALA:CB | 1:G:314:VAL:HG13 | 2.47 | 0.45 |
| 1:I:420:ILE:HD11 | 1:I:428:VAL:CG2 | 2.46 | 0.45 |
| 1:I:72:GLY:O | 2:I:701:SAH:N | 2.50 | 0.45 |
| 1:K:181:VAL:O | 1:K:265:ASP:N | 2.49 | 0.45 |
| 1:L:137:ILE:HB | 1:L:169:VAL:HB | 1.97 | 0.45 |
| 1:M:385:THR:HG22 | 4:M:802:HOH:O | 2.15 | 0.45 |
| 1:N:287:PRO:O | 1:N:291:ASN:HB3 | 2.16 | 0.45 |
| 1:A:488:ALA:HA | 1:A:576:PRO:O | 2.16 | 0.45 |
| 1:B:193:PRO:HA | 1:B:362:ASN:ND2 | 2.32 | 0.45 |
| 1:B:56:GLU:O | 1:B:59:HIS:HB2 | 2.17 | 0.45 |
| 1:C:349:LEU:HD11 | 1:C:391:PHE:HZ | 1.82 | 0.45 |
| 1:E:83:ALA:O | 1:E:84:ARG:C | 2.55 | 0.45 |
| 1:I:111:PRO:HB2 | 1:I:112:TRP:CE3 | 2.52 | 0.45 |
| 1:I:612:TYR:CZ | 1:I:614:PRO:HA | 2.51 | 0.45 |
| 1:J:45:LYS:O | 1:J:275:MET:HG3 | 2.17 | 0.45 |
| 1:M:67:HIS:N | 1:M:135:ASP:OD2 | 2.36 | 0.45 |
| 1:M:42:ARG:HH11 | 1:M:140:GLU:CG | 2.20 | 0.45 |
| 1:N:577:MET:CE | 1:N:626:LEU:HD11 | 2.47 | 0.45 |
| 1:O:567:ASP:O | 1:O:568:ASN:CB | 2.62 | 0.45 |
| 1:P:258:ALA:O | 1:P:317:ASN:HA | 2.17 | 0.45 |
| 1:Q:480:GLU:HA | 1:Q:481:PRO:C | 2.36 | 0.45 |
| 1:B:567:ASP:O | 1:B:568:ASN:CB | 2.64 | 0.45 |
| 1:C:349:LEU:HD12 | 1:C:415:ILE:HD13 | 1.99 | 0.45 |
| 1:D:550:ARG:H | 1:D:560:GLN:NE2 | 2.11 | 0.45 |
| 1:E:161:ARG:HB3 | 1:E:162:LEU:CD1 | 2.46 | 0.45 |
| 1:E:241:GLU:HG3 | 1:E:277:ARG:NH2 | 2.31 | 0.45 |
| 1:E:275:MET:CE | 1:E:283:ILE:HG13 | 2.46 | 0.45 |
| 1:E:443:ILE:HG12 | 1:E:445:LEU:HD13 | 1.99 | 0.45 |
| 1:E:452:SER:O | 1:E:453:ALA:C | 2.54 | 0.45 |
| 1:F:95:VAL:HG23 | 1:F:122:ARG:HB2 | 1.98 | 0.45 |
| 1:F:269:MET:HE3 | 1:F:304:ALA:HB3 | 1.99 | 0.45 |
| 1:J:597:SER:HB2 | 1:J:598:ALA:HB3 | 1.91 | 0.45 |
| 1:K:188:MET:O | 1:K:359:TYR:HA | 2.16 | 0.45 |
| 1:K:203:PRO:HA | 1:K:422:TYR:CG | 2.52 | 0.45 |
| 1:L:216:VAL:O | 1:L:302:MET:HG2 | 2.17 | 0.45 |
| 1:M:432:GLU:HG2 | 1:M:433:LYS:HG3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:63:ASP:OD2 | 1:M:65:LYS:HB2 | 2.16 | 0.45 |
| 1:O:470:LYS:HE3 | 1:O:554:ASP:HA | 1.98 | 0.45 |
| 1:Q:35:ASP:O | 1:Q:36:MET:C | 2.53 | 0.45 |
| 1:A:84:ARG:O | 1:A:85:GLU:HB2 | 2.17 | 0.45 |
| 1:B:292:LYS:HA | 1:B:293:ASN:HA | 1.75 | 0.45 |
| 1:C:323:VAL:HG12 | 1:C:325:ASN:ND2 | 2.31 | 0.45 |
| 1:E:258:ALA:CB | 1:E:314:VAL:HG13 | 2.47 | 0.45 |
| 1:H:258:ALA:HB2 | 1:H:314:VAL:HG22 | 1.97 | 0.45 |
| 1:H:56:GLU:O | 1:H:60:GLU:HG2 | 2.17 | 0.45 |
| 1:J:199:LYS:HA | 1:J:200:ASP:HA | 1.71 | 0.45 |
| 1:K:491:GLU:OE1 | 1:K:539:GLY:HA3 | 2.16 | 0.45 |
| 1:M:169:VAL:HG22 | 1:M:171:PRO:O | 2.16 | 0.45 |
| 1:M:485:VAL:HG12 | 1:M:580:GLU:HB2 | 1.98 | 0.45 |
| 1:N:146:LEU:HB2 | 1:N:271:TRP:CD1 | 2.52 | 0.45 |
| 1:N:268:LEU:HD12 | 1:N:289:TRP:HH2 | 1.82 | 0.45 |
| 1:O:277:ARG:HG2 | 1:O:277:ARG:O | 2.17 | 0.45 |
| 1:P:168:ARG:HB3 | 1:P:168:ARG:HE | 1.67 | 0.45 |
| 1:P:368:GLN:O | 1:P:369:LYS:C | 2.55 | 0.45 |
| 1:Q:68:VAL:HG23 | 1:Q:136:ILE:HB | 1.99 | 0.45 |
| 1:Q:437:LEU:HA | 1:Q:437:LEU:HD23 | 1.87 | 0.45 |
| 1:Q:68:VAL:HG13 | 1:Q:90:VAL:HG12 | 1.90 | 0.45 |
| 1:A:104:ARG:HA | 1:A:107:THR:HG22 | 1.99 | 0.45 |
| 1:A:178:ILE:HA | 1:A:268:LEU:O | 2.17 | 0.45 |
| 1:B:412:PHE:CE2 | 1:B:451:MET:HG2 | 2.44 | 0.45 |
| 1:F:158:ALA:HA | 1:F:162:LEU:HB2 | 1.98 | 0.45 |
| 1:F:275:MET:HE1 | 1:F:283:ILE:CG1 | 2.39 | 0.45 |
| 1:H:61:ASN:O | 1:H:62:THR:C | 2.55 | 0.45 |
| 1:K:373:GLU:O | 1:K:377:LEU:HD12 | 2.17 | 0.45 |
| 1:L:16:VAL:CG1 | 1:L:17:VAL:N | 2.79 | 0.45 |
| 1:L:629:LEU:O | 1:L:637:ILE:HA | 2.17 | 0.45 |
| 1:M:379:LYS:CA | 1:M:399:THR:HG23 | 2.38 | 0.45 |
| 1:M:447:GLU:HB2 | 1:M:449:PHE:N | 2.32 | 0.45 |
| 1:N:297:TRP:CD2 | 1:N:495:ASP:HB3 | 2.52 | 0.45 |
| 1:N:549:LEU:HD21 | 1:N:628:ALA:HB1 | 1.98 | 0.45 |
| 1:P:241:GLU:HG3 | 1:P:277:ARG:NH2 | 2.10 | 0.45 |
| 1:Q:316:MET:HA | 1:Q:317:ASN:HA | 1.70 | 0.45 |
| 1:Q:321:GLU:O | 1:Q:322:ILE:HD12 | 2.17 | 0.45 |
| 1:Q:381:LEU:O | 1:Q:400:ALA:HB1 | 2.17 | 0.45 |
| 1:Q:466:VAL:CG1 | 1:Q:470:LYS:HE2 | 2.46 | 0.45 |
| 1:Q:95:VAL:CB | 1:Q:122:ARG:HG3 | 2.46 | 0.45 |
| 1:R:344:TYR:O | 1:R:346:VAL:HG13 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:84:ARG:NH1 | 1:E:509:PHE:CE2 | 2.85 | 0.45 |
| 1:F:20:GLU:H | 1:F:20:GLU:HG3 | 1.62 | 0.45 |
| 1:I:200:ASP:N | 1:I:200:ASP:OD1 | 2.39 | 0.45 |
| 1:J:534:LEU:HG | 1:J:609:GLN:HB2 | 1.98 | 0.45 |
| 1:K:168:ARG:NH1 | 1:K:168:ARG:HG2 | 2.32 | 0.45 |
| 1:K:176:VAL:HG22 | 1:K:235:ALA:HB3 | 1.99 | 0.45 |
| 1:M:141:VAL:CG1 | 1:M:141:VAL:O | 2.65 | 0.45 |
| 1:M:382:HIS:HD2 | 1:M:402:ARG:HG3 | 1.80 | 0.45 |
| 1:M:450:TYR:HE1 | 1:M:462:PHE:HB2 | 1.82 | 0.45 |
| 1:M:542:LYS:CG | 1:M:571:SER:HB2 | 2.46 | 0.45 |
| 1:N:178:ILE:HG13 | 1:N:233:ILE:HB | 1.99 | 0.45 |
| 1:N:414:ASP:O | 1:N:418:LYS:HG3 | 2.17 | 0.45 |
| 1:O:19:GLU:HG2 | 1:O:19:GLU:O | 2.14 | 0.45 |
| 1:O:292:LYS:HD2 | 1:O:292:LYS:HA | 1.54 | 0.45 |
| 1:P:317:ASN:HD22 | 1:P:317:ASN:C | 2.16 | 0.45 |
| 1:A:225:GLU:HA | 1:A:225:GLU:OE1 | 2.17 | 0.45 |
| 1:B:157:GLU:HA | 1:B:160:GLU:HG2 | 1.98 | 0.45 |
| 1:F:325:ASN:HB3 | 1:F:332:TRP:CE2 | 2.52 | 0.45 |
| 1:K:143:ASP:O | 1:K:145:GLU:N | 2.50 | 0.45 |
| 1:J:414:ASP:OD2 | 1:K:19:GLU:HG2 | 2.17 | 0.45 |
| 1:M:493:PHE:HA | 1:M:539:GLY:CA | 2.47 | 0.45 |
| 1:M:632:LYS:HG3 | 1:M:633:SER:N | 2.32 | 0.45 |
| 1:M:95:VAL:HG13 | 1:M:96:PHE:H | 1.80 | 0.45 |
| 1:O:72:GLY:N | 1:O:93:LEU:O | 2.48 | 0.45 |
| 1:Q:431:ILE:HD12 | 1:Q:436:SER:HB2 | 1.99 | 0.45 |
| 1:Q:631:ASP:HB3 | 1:Q:634:THR:OG1 | 2.16 | 0.45 |
| 1:B:123:SER:C | 1:B:125:ASP:H | 2.18 | 0.44 |
| 1:B:427:ASN:HA | 1:C:8:GLN:HE22 | 1.81 | 0.44 |
| 1:E:432:GLU:HG2 | 1:E:433:LYS:HG2 | 1.99 | 0.44 |
| 1:G:420:ILE:HD11 | 1:G:428:VAL:HG22 | 1.99 | 0.44 |
| 1:I:181:VAL:HG21 | 1:I:226:PHE:HB2 | 1.98 | 0.44 |
| 1:J:600:VAL:HA | 1:J:601:PRO:HD3 | 1.86 | 0.44 |
| 1:M:569:MET:CG | 1:M:624:LEU:HD11 | 2.39 | 0.44 |
| 1:N:54:ILE:HG13 | 1:N:58:LYS:HD3 | 1.99 | 0.44 |
| 1:O:480:GLU:HG3 | 1:O:481:PRO:HA | 1.99 | 0.44 |
| 1:O:512:SER:O | 1:O:515:ASP:HB2 | 2.17 | 0.44 |
| 1:P:136:ILE:HA | 1:P:168:ARG:O | 2.16 | 0.44 |
| 1:P:26:GLN:O | 1:P:30:ARG:HD2 | 2.17 | 0.44 |
| 1:P:365:PHE:O | 1:P:371:LYS:NZ | 2.50 | 0.44 |
| 1:Q:480:GLU:CG | 1:Q:584:GLY:N | 2.78 | 0.44 |
| 1:R:476:GLU:H | 1:R:476:GLU:CD | 2.20 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:505:THR:HA | 1:R:509:PHE:O | 2.17 | 0.44 |
| 1:D:218:LEU:H | 1:D:303:GLN:NE2 | 2.15 | 0.44 |
| 1:F:319:THR:O | 1:F:320:PHE:HB3 | 2.17 | 0.44 |
| 1:H:632:LYS:HG2 | 1:H:633:SER:N | 2.31 | 0.44 |
| 1:L:228:GLU:OE2 | 1:L:290:LYS:HE2 | 2.17 | 0.44 |
| 1:L:631:ASP:OD1 | 1:L:633:SER:N | 2.47 | 0.44 |
| 1:M:231:GLU:H | 1:M:231:GLU:HG2 | 1.58 | 0.44 |
| 1:M:276:ASP:OD1 | 1:M:278:ASN:HB2 | 2.16 | 0.44 |
| 1:M:316:MET:HA | 1:M:317:ASN:HA | 1.78 | 0.44 |
| 1:O:353:LEU:HD22 | 1:O:357:THR:HG21 | 1.98 | 0.44 |
| 1:O:483:MET:CG | 1:O:550:ARG:HH21 | 2.30 | 0.44 |
| 1:O:541:VAL:N | 1:O:599:GLY:O | 2.41 | 0.44 |
| 1:O:623:SER:O | 1:O:624:LEU:HB3 | 2.17 | 0.44 |
| 1:A:67:HIS:CE1 | 1:A:91:THR:HG23 | 2.47 | 0.44 |
| 1:C:447:GLU:N | 1:C:448:PRO:HA | 2.33 | 0.44 |
| 1:E:492:LYS:HB2 | 1:E:542:LYS:HE2 | 1.99 | 0.44 |
| 1:G:450:TYR:H | 1:G:459:HIS:CD2 | 2.22 | 0.44 |
| 1:J:300:HIS:HE1 | 1:J:301:TRP:CE3 | 2.35 | 0.44 |
| 1:K:378:SER:HB2 | 1:K:399:THR:HG22 | 1.99 | 0.44 |
| 1:M:287:PRO:O | 1:M:288:LYS:C | 2.56 | 0.44 |
| 1:N:460:LEU:HB3 | 1:N:463:LEU:HD22 | 1.99 | 0.44 |
| 1:P:48:ALA:HA | 1:P:51:LYS:HD2 | 1.99 | 0.44 |
| 1:Q:569:MET:CE | 1:Q:575:ILE:HG12 | 2.47 | 0.44 |
| 1:B:519:THR:O | 1:B:520:LYS:C | 2.54 | 0.44 |
| 1:E:20:GLU:HG3 | 1:E:20:GLU:H | 1.21 | 0.44 |
| 1:E:488:ALA:HB2 | 1:E:577:MET:HE3 | 1.98 | 0.44 |
| 1:F:159:LEU:HB3 | 1:F:243:GLU:HG2 | 1.98 | 0.44 |
| 1:G:385:THR:CG2 | 1:G:405:ILE:HG23 | 2.47 | 0.44 |
| 1:G:67:HIS:HE1 | 1:G:91:THR:HG23 | 1.81 | 0.44 |
| 1:H:190:ASN:ND2 | 1:H:209:GLY:HA3 | 2.31 | 0.44 |
| 1:I:190:ASN:CG | 1:I:190:ASN:O | 2.56 | 0.44 |
| 1:I:452:SER:O | 1:I:453:ALA:C | 2.56 | 0.44 |
| 1:I:507:ASN:N | 1:I:507:ASN:ND2 | 2.65 | 0.44 |
| 1:J:178:ILE:HB | 1:J:267:LEU:HD22 | 1.99 | 0.44 |
| 1:J:300:HIS:CE1 | 1:J:301:TRP:CE3 | 3.05 | 0.44 |
| 1:K:169:VAL:CG1 | 1:K:241:GLU:HG2 | 2.39 | 0.44 |
| 1:K:375:ASP:O | 1:K:399:THR:HG21 | 2.17 | 0.44 |
| 1:L:516:GLU:O | 1:L:520:LYS:HG3 | 2.18 | 0.44 |
| 1:M:68:VAL:HA | 1:M:136:ILE:O | 2.17 | 0.44 |
| 1:N:353:LEU:HB3 | 1:N:357:THR:HB | 1.99 | 0.44 |
| 1:O:145:GLU:HA | 1:O:269:MET:HE1 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:395:LEU:HA | 1:O:395:LEU:HD23 | 1.75 | 0.44 |
| 1:P:26:GLN:O | 1:P:30:ARG:HD3 | 2.16 | 0.44 |
| 1:P:42:ARG:NH2 | 1:P:43:ASN:HD21 | 2.09 | 0.44 |
| 1:Q:583:PHE:CB | 1:Q:588:LEU:CD1 | 2.96 | 0.44 |
| 1:R:192:ILE:HG23 | 1:R:204:LEU:HD12 | 1.99 | 0.44 |
| 1:R:379:LYS:CA | 1:R:399:THR:HG21 | 2.42 | 0.44 |
| 1:F:51:LYS:HG3 | 1:F:85:GLU:HG3 | 1.98 | 0.44 |
| 1:G:28:LEU:HG | 1:G:28:LEU:O | 2.17 | 0.44 |
| 1:I:156:LYS:NZ | 1:I:243:GLU:O | 2.51 | 0.44 |
| 1:I:31:SER:O | 1:I:33:PHE:CD2 | 2.71 | 0.44 |
| 1:L:143:ASP:O | 1:L:146:LEU:N | 2.43 | 0.44 |
| 1:M:80:LEU:HD21 | 1:M:107:THR:HG22 | 2.00 | 0.44 |
| 1:M:269:MET:HG2 | 1:M:306:TYR:CE2 | 2.51 | 0.44 |
| 1:M:502:ASP:OD1 | 1:M:616:THR:HG21 | 2.17 | 0.44 |
| 1:N:218:LEU:HD12 | 1:N:303:GLN:CB | 2.47 | 0.44 |
| 1:N:387:GLY:HA2 | 1:N:450:TYR:CZ | 2.53 | 0.44 |
| 1:N:460:LEU:C | 1:N:462:PHE:N | 2.70 | 0.44 |
| 1:O:550:ARG:HD2 | 1:O:550:ARG:HA | 1.80 | 0.44 |
| 1:Q:216:VAL:HG13 | 1:Q:218:LEU:HG | 2.00 | 0.44 |
| 1:Q:460:LEU:C | 1:Q:462:PHE:N | 2.71 | 0.44 |
| 1:B:43:ASN:N | 1:B:43:ASN:HD22 | 2.07 | 0.44 |
| 1:D:50:LEU:O | 1:D:54:ILE:CG1 | 2.65 | 0.44 |
| 1:E:362:ASN:O | 1:E:366:GLU:HG2 | 2.18 | 0.44 |
| 1:F:392:LEU:HD22 | 1:F:392:LEU:O | 2.17 | 0.44 |
| 1:G:403:VAL:HB | 1:G:428:VAL:HB | 1.99 | 0.44 |
| 1:M:269:MET:HG3 | 1:M:304:ALA:HB3 | 2.00 | 0.44 |
| 1:M:316:MET:O | 1:M:316:MET:HG3 | 2.17 | 0.44 |
| 1:N:168:ARG:NH1 | 1:N:241:GLU:OE2 | 2.51 | 0.44 |
| 1:Q:108:SER:HA | 1:Q:113:SER:HB2 | 1.99 | 0.44 |
| 1:Q:375:ASP:CA | 1:Q:399:THR:HG21 | 2.21 | 0.44 |
| 1:Q:404:THR:HG23 | 1:Q:429:GLU:HG3 | 2.00 | 0.44 |
| 1:Q:490:PRO:HB2 | 1:Q:572:SER:OG | 2.18 | 0.44 |
| 1:A:412:PHE:HE2 | 1:A:451:MET:HG2 | 1.82 | 0.44 |
| 1:B:489:ILE:HD13 | 1:B:541:VAL:HG22 | 1.99 | 0.44 |
| 1:D:140:GLU:OE1 | 1:D:140:GLU:C | 2.56 | 0.44 |
| 1:F:277:ARG:O | 1:F:279:GLY:N | 2.51 | 0.44 |
| 1:H:211:ALA:HB2 | 1:H:343:SER:O | 2.17 | 0.44 |
| 1:I:185:LEU:O | 1:I:185:LEU:HD22 | 2.18 | 0.44 |
| 1:I:51:LYS:HG3 | 1:I:85:GLU:HG2 | 2.00 | 0.44 |
| 1:J:395:LEU:O | 1:J:398:LYS:HB2 | 2.18 | 0.44 |
| 1:J:449:PHE:C | 1:J:449:PHE:CD1 | 2.91 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:56:GLU:OE1 | 1:J:168:ARG:HD2 | 2.18 | 0.44 |
| 1:L:359:TYR:C | 1:L:359:TYR:CD1 | 2.90 | 0.44 |
| 1:N:201:GLU:HA | 1:N:422:TYR:OH | 2.17 | 0.44 |
| 1:P:497:GLN:HE21 | 1:P:497:GLN:H | 1.65 | 0.44 |
| 1:Q:235:ALA:HB1 | 1:Q:324:CYS:SG | 2.58 | 0.44 |
| 1:Q:383:VAL:HG23 | 1:Q:384:ALA:N | 2.33 | 0.44 |
| 1:Q:52:THR:O | 1:Q:55:ALA:HB3 | 2.17 | 0.44 |
| 1:Q:566:ILE:HG22 | 1:Q:569:MET:HE2 | 2.00 | 0.44 |
| 1:R:94:GLU:OE2 | 2:R:701:SAH:H1' | 2.18 | 0.44 |
| 1:A:434:VAL:HG13 | 1:A:469:LEU:CD1 | 2.47 | 0.44 |
| 1:C:57:LYS:HG2 | 1:C:135:ASP:HB3 | 1.99 | 0.44 |
| 1:F:186:LEU:O | 1:F:307:TYR:OH | 2.21 | 0.44 |
| 1:F:264:ILE:HB | 1:F:312:LYS:HB3 | 2.00 | 0.44 |
| 1:I:145:GLU:HG3 | 1:I:331:LEU:HD22 | 2.00 | 0.44 |
| 1:J:490:PRO:HB3 | 1:J:569:MET:HE2 | 1.81 | 0.44 |
| 1:J:593:LEU:HD12 | 1:J:593:LEU:HA | 1.91 | 0.44 |
| 1:K:244:GLU:CD | 1:K:244:GLU:H | 2.19 | 0.44 |
| 1:M:383:VAL:HG13 | 1:M:403:VAL:HG22 | 2.00 | 0.44 |
| 1:O:233:ILE:CD1 | 1:O:254:ARG:HB3 | 2.42 | 0.44 |
| 1:O:145:GLU:HA | 1:O:269:MET:CE | 2.48 | 0.44 |
| 1:P:110:SER:O | 1:P:113:SER:HB3 | 2.18 | 0.44 |
| 1:P:84:ARG:O | 1:P:85:GLU:HB2 | 2.18 | 0.44 |
| 1:Q:168:ARG:NH1 | 1:Q:168:ARG:CG | 2.65 | 0.44 |
| 1:Q:146:LEU:HD13 | 1:Q:271:TRP:CD2 | 2.53 | 0.44 |
| 1:R:201:GLU:C | 1:R:203:PRO:HD3 | 2.37 | 0.44 |
| 1:R:69:LEU:HD13 | 1:R:91:THR:HG23 | 1.99 | 0.44 |
| 1:A:103:ALA:O | 1:A:107:THR:CB | 2.47 | 0.44 |
| 1:B:231:GLU:O | 1:B:233:ILE:HG22 | 2.18 | 0.44 |
| 1:D:297:TRP:CE3 | 1:D:495:ASP:HB3 | 2.53 | 0.44 |
| 1:F:292:LYS:HA | 1:F:292:LYS:HD2 | 1.74 | 0.44 |
| 1:G:107:THR:O | 1:G:110:SER:OG | 2.35 | 0.44 |
| 1:G:42:ARG:HG3 | 1:G:301:TRP:CH2 | 2.53 | 0.44 |
| 1:K:147:ILE:HD11 | 1:K:331:LEU:HD13 | 2.00 | 0.44 |
| 1:L:80:LEU:HB3 | 1:L:509:PHE:CE1 | 2.53 | 0.44 |
| 1:M:235:ALA:HA | 1:M:254:ARG:HG3 | 2.00 | 0.44 |
| 1:M:269:MET:CG | 1:M:304:ALA:HB3 | 2.48 | 0.44 |
| 1:M:68:VAL:HB | 1:M:90:VAL:HG22 | 2.00 | 0.44 |
| 1:O:297:TRP:CE3 | 1:O:495:ASP:HB3 | 2.52 | 0.44 |
| 1:Q:169:VAL:HG22 | 1:Q:241:GLU:HG2 | 2.00 | 0.44 |
| 1:R:168:ARG:HG2 | 1:R:241:GLU:OE1 | 2.18 | 0.44 |
| 1:R:550:ARG:CZ | 1:R:550:ARG:HB2 | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:67:HIS:CE1 | 1:R:89:LYS:HG2 | 2.53 | 0.44 |
| 1:B:169:VAL:HG22 | 1:B:171:PRO:O | 2.17 | 0.43 |
| 1:C:275:MET:HE1 | 1:C:283:ILE:H | 1.82 | 0.43 |
| 1:C:338:LYS:N | 1:F:244:GLU:HG3 | 2.32 | 0.43 |
| 1:E:480:GLU:OE2 | 1:E:482:HIS:CD2 | 2.69 | 0.43 |
| 1:E:63:ASP:CG | 1:E:64:GLY:H | 2.21 | 0.43 |
| 1:F:625:CYS:HB2 | 1:F:644:SER:HA | 2.00 | 0.43 |
| 1:G:497:GLN:N | 1:G:497:GLN:NE2 | 2.60 | 0.43 |
| 1:I:63:ASP:N | 1:I:63:ASP:OD1 | 2.48 | 0.43 |
| 1:J:191:ASP:OD2 | 1:J:194:ARG:NH1 | 2.51 | 0.43 |
| 1:K:510:ASP:C | 1:K:512:SER:H | 2.22 | 0.43 |
| 1:O:219:SER:HB3 | 1:O:288:LYS:HB2 | 2.00 | 0.43 |
| 1:O:404:THR:HG21 | 1:O:437:LEU:HD23 | 2.00 | 0.43 |
| 1:O:442:ASP:O | 1:O:478:ARG:CB | 2.62 | 0.43 |
| 1:O:451:MET:HG3 | 1:O:452:SER:N | 2.32 | 0.43 |
| 1:Q:274:ASP:OD2 | 1:Q:277:ARG:N | 2.50 | 0.43 |
| 1:Q:513:PHE:O | 1:Q:516:GLU:HB3 | 2.18 | 0.43 |
| 1:R:35:ASP:OD1 | 1:R:300:HIS:N | 2.47 | 0.43 |
| 1:B:168:ARG:HG2 | 1:B:168:ARG:NH1 | 2.31 | 0.43 |
| 1:C:146:LEU:HD13 | 1:C:271:TRP:CG | 2.53 | 0.43 |
| 1:C:230:SER:OG | 1:C:231:GLU:O | 2.36 | 0.43 |
| 1:C:288:LYS:HG3 | 1:C:295:TYR:CE2 | 2.53 | 0.43 |
| 1:C:403:VAL:HB | 1:C:428:VAL:HB | 2.00 | 0.43 |
| 1:C:578:TRP:CB | 1:C:591:GLY:HA3 | 2.48 | 0.43 |
| 1:D:518:SER:O | 1:D:522:ARG:HG3 | 2.18 | 0.43 |
| 1:J:54:ILE:HD13 | 1:J:85:GLU:HB3 | 1.99 | 0.43 |
| 1:K:171:PRO:HB3 | 1:K:275:MET:HE1 | 1.99 | 0.43 |
| 1:K:348:GLY:CA | 1:K:411:ARG:HH22 | 2.31 | 0.43 |
| 1:L:190:ASN:ND2 | 1:L:209:GLY:HA3 | 2.33 | 0.43 |
| 1:N:251:SER:OG | 1:N:340:LYS:HD3 | 2.18 | 0.43 |
| 1:N:258:ALA:HB3 | 1:N:315:GLU:O | 2.18 | 0.43 |
| 1:O:414:ASP:O | 1:O:418:LYS:HG3 | 2.17 | 0.43 |
| 1:Q:67:HIS:O | 1:Q:135:ASP:N | 2.47 | 0.43 |
| 1:R:178:ILE:HA | 1:R:268:LEU:O | 2.18 | 0.43 |
| 1:B:218:LEU:HD22 | 1:B:221:MET:CE | 2.48 | 0.43 |
| 1:B:514:PHE:HA | 1:B:517:ILE:HG12 | 1.99 | 0.43 |
| 1:E:623:SER:O | 1:E:624:LEU:HD23 | 2.18 | 0.43 |
| 1:F:178:ILE:HB | 1:F:267:LEU:HD22 | 1.99 | 0.43 |
| 1:H:70:ASP:HA | 1:H:138:VAL:O | 2.18 | 0.43 |
| 1:H:455:ASN:HB3 | 1:H:457:TRP:CE2 | 2.53 | 0.43 |
| 1:I:451:MET:HE2 | 1:I:452:SER:HA | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:593:LEU:HD12 | 1:I:593:LEU:HA | 1.73 | 0.43 |
| 1:J:124:THR:O | 1:J:161:ARG:NH2 | 2.51 | 0.43 |
| 1:J:194:ARG:HG2 | 1:J:201:GLU:CB | 2.37 | 0.43 |
| 1:K:229:LEU:CD1 | 1:K:314:VAL:HG12 | 2.48 | 0.43 |
| 1:K:641:PHE:CD1 | 1:K:641:PHE:N | 2.85 | 0.43 |
| 1:L:141:VAL:CG1 | 1:L:141:VAL:O | 2.66 | 0.43 |
| 1:L:84:ARG:HG3 | 1:L:112:TRP:HZ2 | 1.83 | 0.43 |
| 1:M:349:LEU:HD11 | 1:M:353:LEU:HD12 | 1.99 | 0.43 |
| 1:N:339:ASP:OD1 | 1:N:340:LYS:N | 2.51 | 0.43 |
| 1:N:447:GLU:N | 1:N:448:PRO:HA | 2.32 | 0.43 |
| 1:N:474:GLY:HA3 | 1:N:476:GLU:OE2 | 2.18 | 0.43 |
| 1:O:198:GLU:O | 1:O:201:GLU:HB2 | 2.17 | 0.43 |
| 1:O:548:ILE:HD12 | 1:O:626:LEU:HD13 | 2.01 | 0.43 |
| 1:P:156:LYS:O | 1:P:160:GLU:CG | 2.65 | 0.43 |
| 1:P:83:ALA:HB1 | 1:P:112:TRP:CG | 2.53 | 0.43 |
| 1:Q:67:HIS:HA | 1:Q:89:LYS:O | 2.17 | 0.43 |
| 1:R:218:LEU:HA | 1:R:218:LEU:HD23 | 1.72 | 0.43 |
| 1:R:512:SER:O | 1:R:515:ASP:HB2 | 2.18 | 0.43 |
| 1:R:485:VAL:HA | 1:R:549:LEU:O | 2.19 | 0.43 |
| 1:A:297:TRP:CE3 | 1:A:495:ASP:HB3 | 2.53 | 0.43 |
| 1:B:111:PRO:HG2 | 1:B:112:TRP:CH2 | 2.53 | 0.43 |
| 1:D:622:LYS:CD | 1:D:622:LYS:N | 2.79 | 0.43 |
| 1:E:643:LYS:O | 1:E:644:SER:OG | 2.27 | 0.43 |
| 1:J:93:LEU:HD23 | 1:J:119:ILE:HB | 2.01 | 0.43 |
| 1:J:226:PHE:CZ | 1:J:289:TRP:CZ2 | 3.06 | 0.43 |
| 1:J:261:SER:OG | 1:J:316:MET:N | 2.52 | 0.43 |
| 1:J:68:VAL:O | 1:J:90:VAL:HA | 2.18 | 0.43 |
| 1:N:190:ASN:HD21 | 1:N:209:GLY:HA3 | 1.83 | 0.43 |
| 1:O:178:ILE:HG21 | 1:O:333:PHE:CZ | 2.53 | 0.43 |
| 1:O:367:ASN:O | 1:O:371:LYS:HD3 | 2.18 | 0.43 |
| 1:O:466:VAL:HA | 1:O:469:LEU:HB2 | 1.99 | 0.43 |
| 1:O:483:MET:HB3 | 1:O:582:GLU:HG2 | 1.99 | 0.43 |
| 1:Q:140:GLU:O | 1:Q:140:GLU:HG3 | 2.17 | 0.43 |
| 1:R:52:THR:HG21 | 1:R:276:ASP:CB | 2.46 | 0.43 |
| 1:R:466:VAL:HG11 | 1:R:553:ILE:HG21 | 2.00 | 0.43 |
| 1:R:69:LEU:HD12 | 1:R:69:LEU:C | 2.39 | 0.43 |
| 1:A:144:THR:O | 1:A:269:MET:HE1 | 2.17 | 0.43 |
| 1:A:359:TYR:C | 1:A:359:TYR:CD1 | 2.92 | 0.43 |
| 1:B:388:GLU:OE1 | 1:B:452:SER:HB2 | 2.19 | 0.43 |
| 1:F:143:ASP:O | 1:F:146:LEU:N | 2.34 | 0.43 |
| 1:F:368:GLN:NE2 | 1:F:371:LYS:CE | 2.80 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:378:SER:O | 1:G:400:ALA:HA | 2.18 | 0.43 |
| 1:G:42:ARG:HG3 | 1:G:301:TRP:CZ3 | 2.53 | 0.43 |
| 1:H:375:ASP:O | 1:H:399:THR:HG21 | 2.19 | 0.43 |
| 1:J:290:LYS:HD3 | 1:J:290:LYS:HA | 1.92 | 0.43 |
| 1:K:534:LEU:C | 1:K:536:GLU:H | 2.22 | 0.43 |
| 1:K:492:LYS:HD3 | 1:K:542:LYS:NZ | 2.33 | 0.43 |
| 1:M:111:PRO:C | 1:M:113:SER:N | 2.72 | 0.43 |
| 1:M:480:GLU:CG | 1:M:584:GLY:H | 2.32 | 0.43 |
| 1:N:55:ALA:CA | 1:N:58:LYS:HD2 | 2.47 | 0.43 |
| 1:N:612:TYR:CE2 | 1:N:614:PRO:HA | 2.53 | 0.43 |
| 1:P:600:VAL:HA | 1:P:601:PRO:HD3 | 1.86 | 0.43 |
| 1:Q:143:ASP:C | 1:Q:145:GLU:N | 2.71 | 0.43 |
| 1:Q:1:MET:O | 1:Q:17:VAL:HG12 | 2.19 | 0.43 |
| 1:R:136:ILE:HG23 | 1:R:168:ARG:O | 2.18 | 0.43 |
| 1:R:487:LYS:HE3 | 1:R:547:GLU:HG2 | 2.00 | 0.43 |
| 1:A:216:VAL:O | 1:A:302:MET:HG2 | 2.18 | 0.43 |
| 1:C:176:VAL:HG13 | 1:C:236:PHE:HB2 | 1.99 | 0.43 |
| 1:E:269:MET:HG2 | 1:E:306:TYR:CE1 | 2.54 | 0.43 |
| 1:E:384:ALA:O | 1:E:444:VAL:HA | 2.18 | 0.43 |
| 1:H:449:PHE:HA | 1:H:459:HIS:CD2 | 2.54 | 0.43 |
| 1:I:264:ILE:HD12 | 1:I:312:LYS:HG2 | 2.00 | 0.43 |
| 1:I:550:ARG:HH11 | 1:I:550:ARG:CG | 2.30 | 0.43 |
| 1:K:253:VAL:CG2 | 1:K:253:VAL:O | 2.66 | 0.43 |
| 1:K:264:ILE:HD12 | 1:K:312:LYS:HG3 | 2.01 | 0.43 |
| 1:K:550:ARG:O | 1:K:560:GLN:OE1 | 2.36 | 0.43 |
| 1:K:616:THR:O | 1:K:618:LEU:N | 2.52 | 0.43 |
| 1:L:569:MET:HA | 1:L:572:SER:HB2 | 2.00 | 0.43 |
| 1:M:4:GLU:O | 1:O:420:ILE:HD11 | 2.19 | 0.43 |
| 1:M:515:ASP:O | 1:M:519:THR:HB | 2.18 | 0.43 |
| 1:N:437:LEU:HD11 | 1:N:441:PRO:HD3 | 2.00 | 0.43 |
| 1:P:480:GLU:OE2 | 1:P:482:HIS:HD2 | 2.01 | 0.43 |
| 1:R:297:TRP:CZ3 | 1:R:495:ASP:HB3 | 2.54 | 0.43 |
| 1:A:460:LEU:HD22 | 1:A:463:LEU:HD22 | 2.00 | 0.43 |
| 1:A:480:GLU:HG2 | 1:A:584:GLY:N | 2.34 | 0.43 |
| 1:B:476:GLU:CD | 1:B:476:GLU:N | 2.72 | 0.43 |
| 1:C:489:ILE:HG12 | 1:C:541:VAL:HG22 | 1.99 | 0.43 |
| 1:D:190:ASN:ND2 | 1:D:209:GLY:HA3 | 2.33 | 0.43 |
| 1:D:47:LEU:HD22 | 1:D:51:LYS:HE2 | 2.01 | 0.43 |
| 1:D:84:ARG:HG3 | 1:D:112:TRP:CZ2 | 2.54 | 0.43 |
| 1:G:489:ILE:CD1 | 1:G:541:VAL:HG21 | 2.48 | 0.43 |
| 1:H:480:GLU:HG3 | 1:H:584:GLY:H | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:427:ASN:HA | 1:H:8:GLN:OE1 | 2.18 | 0.43 |
| 1:I:570:SER:CB | 1:I:622:LYS:HG2 | 2.38 | 0.43 |
| 1:M:151:ALA:O | 1:M:154:THR:HG22 | 2.18 | 0.43 |
| 1:M:615:ILE:CG1 | 1:M:618:LEU:HD22 | 2.48 | 0.43 |
| 1:N:214:PHE:C | 1:N:214:PHE:CD1 | 2.91 | 0.43 |
| 1:N:169:VAL:HG12 | 1:N:241:GLU:HG2 | 2.00 | 0.43 |
| 1:O:269:MET:HG2 | 1:O:306:TYR:CE1 | 2.54 | 0.43 |
| 1:O:7:ASN:HD21 | 1:O:640:GLN:NE2 | 2.14 | 0.43 |
| 1:P:161:ARG:HB3 | 1:P:162:LEU:HD13 | 2.01 | 0.43 |
| 1:P:218:LEU:H | 1:P:303:GLN:HE21 | 1.66 | 0.43 |
| 1:A:203:PRO:HA | 1:A:422:TYR:CG | 2.54 | 0.43 |
| 1:B:111:PRO:HG2 | 1:B:112:TRP:CZ3 | 2.54 | 0.43 |
| 1:C:315:GLU:HB3 | 1:C:318:GLN:HG3 | 1.99 | 0.43 |
| 1:C:403:VAL:O | 1:C:428:VAL:HA | 2.19 | 0.43 |
| 1:D:78:LEU:HD12 | 1:D:78:LEU:HA | 1.82 | 0.43 |
| 1:E:176:VAL:CG1 | 1:E:236:PHE:HB2 | 2.49 | 0.43 |
| 1:E:54:ILE:HD13 | 1:E:87:ALA:H | 1.83 | 0.43 |
| 1:F:534:LEU:HD23 | 1:F:534:LEU:HA | 1.88 | 0.43 |
| 1:G:269:MET:HG2 | 1:G:306:TYR:CE1 | 2.53 | 0.43 |
| 1:G:35:ASP:O | 1:G:36:MET:C | 2.56 | 0.43 |
| 1:I:291:ASN:HD21 | 1:I:295:TYR:HA | 1.84 | 0.43 |
| 1:J:138:VAL:HG23 | 1:J:170:VAL:HB | 2.00 | 0.43 |
| 1:J:423:TYR:O | 1:J:424:LYS:C | 2.57 | 0.43 |
| 1:L:163:ALA:HB1 | 1:L:167:CYS:SG | 2.58 | 0.43 |
| 1:L:258:ALA:O | 1:L:317:ASN:HA | 2.18 | 0.43 |
| 1:L:69:LEU:HD12 | 1:L:91:THR:O | 2.18 | 0.43 |
| 1:O:534:LEU:C | 1:O:536:GLU:H | 2.22 | 0.43 |
| 1:R:385:THR:HG21 | 1:R:405:ILE:HG23 | 2.01 | 0.43 |
| 1:R:569:MET:HG3 | 1:R:624:LEU:HG | 2.00 | 0.43 |
| 1:B:103:ALA:O | 1:B:107:THR:HB | 2.19 | 0.43 |
| 1:B:170:VAL:HA | 1:B:171:PRO:HA | 1.85 | 0.43 |
| 1:B:367:ASN:O | 1:B:371:LYS:HD3 | 2.18 | 0.43 |
| 1:D:569:MET:HA | 1:D:572:SER:HB2 | 2.01 | 0.43 |
| 1:E:170:VAL:HA | 1:E:171:PRO:HA | 1.92 | 0.43 |
| 1:H:67:HIS:CE1 | 1:H:91:THR:HG22 | 2.53 | 0.43 |
| 1:H:92:ALA:HB3 | 1:H:118:VAL:HG22 | 2.00 | 0.43 |
| 1:I:502:ASP:OD2 | 1:I:616:THR:CG2 | 2.65 | 0.43 |
| 1:M:176:VAL:CG2 | 1:M:236:PHE:HD2 | 2.31 | 0.43 |
| 1:M:43:ASN:ND2 | 1:M:43:ASN:N | 2.64 | 0.43 |
| 1:M:96:PHE:CD2 | 1:M:98:PRO:HD2 | 2.54 | 0.43 |
| 1:N:327:ASP:OD1 | 1:N:327:ASP:C | 2.58 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:63:ASP:CB | 1:N:65:LYS:N | 2.72 | 0.43 |
| 1:O:35:ASP:CG | 1:O:299:ASP:H | 2.22 | 0.43 |
| 1:Q:215:ASP:HA | 1:Q:304:ALA:HA | 2.00 | 0.43 |
| 1:R:359:TYR:CD1 | 1:R:359:TYR:C | 2.91 | 0.43 |
| 1:C:20:GLU:HG3 | 1:C:20:GLU:H | 1.40 | 0.43 |
| 1:G:118:VAL:C | 1:G:119:ILE:HD12 | 2.39 | 0.43 |
| 1:G:339:ASP:OD1 | 1:G:341:SER:HB2 | 2.18 | 0.43 |
| 1:G:357:THR:O | 1:G:360:HIS:HB3 | 2.19 | 0.43 |
| 1:H:178:ILE:HG21 | 1:H:333:PHE:CZ | 2.54 | 0.43 |
| 1:H:97:LYS:N | 1:H:98:PRO:CD | 2.82 | 0.43 |
| 1:J:274:ASP:HB2 | 1:J:282:PHE:CE1 | 2.54 | 0.43 |
| 1:J:547:GLU:OE2 | 1:J:550:ARG:CG | 2.66 | 0.43 |
| 1:N:254:ARG:O | 1:N:321:GLU:HB3 | 2.19 | 0.43 |
| 1:N:535:TRP:CE2 | 1:N:536:GLU:HG3 | 2.54 | 0.43 |
| 1:O:71:ILE:HG21 | 1:O:154:THR:CG2 | 2.49 | 0.43 |
| 1:Q:566:ILE:CG2 | 1:Q:569:MET:CE | 2.97 | 0.43 |
| 1:R:110:SER:C | 1:R:112:TRP:H | 2.23 | 0.43 |
| 1:A:550:ARG:HB2 | 1:A:550:ARG:NH1 | 2.33 | 0.42 |
| 1:A:577:MET:HE2 | 1:A:639:PHE:CE1 | 2.54 | 0.42 |
| 1:B:502:ASP:OD2 | 1:B:616:THR:HG21 | 2.19 | 0.42 |
| 1:D:506:VAL:HG21 | 1:D:511:LEU:HD12 | 2.00 | 0.42 |
| 1:D:490:PRO:HB2 | 1:D:569:MET:CE | 2.45 | 0.42 |
| 1:E:169:VAL:HG13 | 1:E:172:SER:HA | 2.01 | 0.42 |
| 1:E:621:ASP:OD1 | 1:E:621:ASP:N | 2.52 | 0.42 |
| 1:G:159:LEU:HB2 | 1:G:243:GLU:HG3 | 2.01 | 0.42 |
| 1:G:291:ASN:HB3 | 1:G:295:TYR:HB2 | 2.01 | 0.42 |
| 1:H:578:TRP:CG | 1:H:591:GLY:HA3 | 2.54 | 0.42 |
| 1:H:563:VAL:HG22 | 1:H:627:HIS:CG | 2.54 | 0.42 |
| 1:I:162:LEU:N | 1:I:162:LEU:HD13 | 2.34 | 0.42 |
| 1:I:77:LEU:HD11 | 1:I:506:VAL:HG12 | 2.00 | 0.42 |
| 1:J:146:LEU:HD22 | 1:J:176:VAL:HG12 | 2.01 | 0.42 |
| 1:J:51:LYS:HG3 | 1:J:85:GLU:OE2 | 2.19 | 0.42 |
| 1:M:627:HIS:HB2 | 1:M:640:GLN:HB2 | 2.01 | 0.42 |
| 1:N:65:LYS:HA | 1:N:88:ASP:OD2 | 2.19 | 0.42 |
| 1:O:275:MET:CE | 1:O:283:ILE:H | 2.31 | 0.42 |
| 1:O:379:LYS:O | 1:O:381:LEU:N | 2.52 | 0.42 |
| 1:Q:547:GLU:CD | 1:Q:550:ARG:HH11 | 2.23 | 0.42 |
| 1:C:138:VAL:HG23 | 1:C:170:VAL:HB | 2.01 | 0.42 |
| 1:D:180:PRO:CB | 1:D:264:ILE:HD13 | 2.50 | 0.42 |
| 1:E:548:ILE:HD12 | 1:E:564:VAL:HG21 | 2.00 | 0.42 |
| 1:F:142:PHE:HD1 | 1:F:146:LEU:HD12 | 1.80 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:615:ILE:CG1 | 1:F:618:LEU:HD22 | 2.49 | 0.42 |
| 1:H:496:LEU:O | 1:H:499:ILE:HG12 | 2.19 | 0.42 |
| 1:I:416:PHE:O | 1:I:420:ILE:HG13 | 2.18 | 0.42 |
| 1:I:615:ILE:HG12 | 1:I:618:LEU:HD22 | 2.01 | 0.42 |
| 1:K:253:VAL:HG23 | 1:K:253:VAL:O | 2.19 | 0.42 |
| 1:K:534:LEU:C | 1:K:536:GLU:N | 2.72 | 0.42 |
| 1:K:490:PRO:HG3 | 1:K:566:ILE:HG22 | 2.01 | 0.42 |
| 1:L:42:ARG:HH12 | 1:L:140:GLU:HG2 | 1.75 | 0.42 |
| 1:L:470:LYS:HG2 | 1:L:475:ASP:HA | 1.99 | 0.42 |
| 1:M:10:THR:C | 1:M:12:GLU:H | 2.22 | 0.42 |
| 1:M:95:VAL:HB | 1:M:122:ARG:HG3 | 2.02 | 0.42 |
| 1:M:599:GLY:O | 1:M:601:PRO:HD3 | 2.19 | 0.42 |
| 1:N:245:LYS:HE3 | 1:Q:337:GLY:O | 2.18 | 0.42 |
| 1:N:308:LEU:HD12 | 1:N:308:LEU:HA | 1.91 | 0.42 |
| 1:O:490:PRO:HG2 | 1:O:543:GLY:HA3 | 2.01 | 0.42 |
| 1:P:239:ASP:OD1 | 1:P:277:ARG:NH2 | 2.52 | 0.42 |
| 1:Q:553:ILE:O | 1:Q:553:ILE:HG23 | 2.19 | 0.42 |
| 1:R:231:GLU:O | 1:R:232:PRO:C | 2.57 | 0.42 |
| 1:A:470:LYS:NZ | 1:A:554:ASP:HA | 2.34 | 0.42 |
| 1:A:503:VAL:HB | 1:A:515:ASP:OD1 | 2.19 | 0.42 |
| 1:G:46:PHE:CZ | 1:G:140:GLU:HB3 | 2.54 | 0.42 |
| 1:H:563:VAL:HA | 1:H:626:LEU:O | 2.19 | 0.42 |
| 1:H:69:LEU:CD1 | 1:H:91:THR:HG23 | 2.49 | 0.42 |
| 1:H:72:GLY:O | 2:H:701:SAH:N | 2.53 | 0.42 |
| 1:K:53:THR:HG22 | 1:K:168:ARG:NE | 2.34 | 0.42 |
| 1:L:210:THR:HG21 | 4:L:809:HOH:O | 2.18 | 0.42 |
| 1:M:51:LYS:HD3 | 1:M:85:GLU:OE2 | 2.19 | 0.42 |
| 1:N:391:PHE:O | 1:N:394:LEU:HB2 | 2.19 | 0.42 |
| 1:N:38:LEU:HD21 | 1:N:503:VAL:HA | 2.00 | 0.42 |
| 1:N:550:ARG:O | 1:N:560:GLN:OE1 | 2.37 | 0.42 |
| 1:O:423:TYR:HB2 | 1:O:425:LEU:HG | 2.01 | 0.42 |
| 1:O:440:SER:HA | 1:O:441:PRO:HD3 | 1.86 | 0.42 |
| 1:O:483:MET:HB3 | 1:O:582:GLU:CG | 2.49 | 0.42 |
| 1:P:323:VAL:HB | 1:P:334:SER:OG | 2.19 | 0.42 |
| 1:Q:273:ILE:O | 1:Q:282:PHE:HA | 2.19 | 0.42 |
| 1:R:578:TRP:NE1 | 1:R:580:GLU:HG3 | 2.34 | 0.42 |
| 1:C:463:LEU:HD22 | 1:C:463:LEU:H | 1.83 | 0.42 |
| 1:D:190:ASN:HD21 | 1:D:209:GLY:HA3 | 1.84 | 0.42 |
| 1:D:217:GLN:HB2 | 1:D:536:GLU:HB3 | 2.00 | 0.42 |
| 1:D:550:ARG:O | 1:D:560:GLN:OE1 | 2.37 | 0.42 |
| 1:G:627:HIS:HB2 | 1:G:640:GLN:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:491:GLU:HG3 | 1:H:492:LYS:N | 2.34 | 0.42 |
| 1:H:82:ALA:O | 1:H:84:ARG:O | 2.37 | 0.42 |
| 1:I:145:GLU:CG | 1:I:331:LEU:HD22 | 2.49 | 0.42 |
| 1:J:107:THR:HG22 | 1:J:108:SER:N | 2.35 | 0.42 |
| 1:J:480:GLU:HA | 1:J:481:PRO:C | 2.39 | 0.42 |
| 1:L:178:ILE:HA | 1:L:268:LEU:O | 2.18 | 0.42 |
| 1:L:241:GLU:HB2 | 1:L:277:ARG:HH21 | 1.85 | 0.42 |
| 1:N:516:GLU:O | 1:N:520:LYS:HG3 | 2.20 | 0.42 |
| 1:O:491:GLU:HG3 | 1:O:492:LYS:N | 2.34 | 0.42 |
| 1:P:56:GLU:O | 1:P:56:GLU:HG2 | 2.19 | 0.42 |
| 1:P:84:ARG:C | 1:P:86:GLY:N | 2.73 | 0.42 |
| 1:R:613:PHE:HA | 1:R:614:PRO:HD2 | 1.93 | 0.42 |
| 1:A:577:MET:HE2 | 1:A:639:PHE:CZ | 2.54 | 0.42 |
| 1:C:288:LYS:HG3 | 1:C:295:TYR:CZ | 2.54 | 0.42 |
| 1:G:514:PHE:O | 1:G:515:ASP:C | 2.57 | 0.42 |
| 1:G:67:HIS:CE1 | 1:G:91:THR:HG23 | 2.54 | 0.42 |
| 1:H:123:SER:C | 1:H:125:ASP:H | 2.22 | 0.42 |
| 1:H:75:THR:HG22 | 1:H:514:PHE:CD1 | 2.55 | 0.42 |
| 1:K:325:ASN:O | 1:K:331:LEU:HA | 2.19 | 0.42 |
| 1:L:485:VAL:HG22 | 1:L:487:LYS:HG3 | 2.01 | 0.42 |
| 1:M:217:GLN:C | 1:M:219:SER:H | 2.22 | 0.42 |
| 1:N:420:ILE:CD1 | 1:N:428:VAL:HG22 | 2.50 | 0.42 |
| 1:N:477:LEU:O | 1:N:479:VAL:HG12 | 2.20 | 0.42 |
| 1:N:55:ALA:H | 1:N:58:LYS:NZ | 2.05 | 0.42 |
| 1:O:618:LEU:HB3 | 1:O:624:LEU:HD11 | 2.01 | 0.42 |
| 1:P:292:LYS:HA | 1:P:292:LYS:NZ | 2.34 | 0.42 |
| 1:Q:182:GLU:HG3 | 1:Q:263:THR:O | 2.20 | 0.42 |
| 1:Q:182:GLU:HB2 | 1:Q:229:LEU:HD11 | 2.02 | 0.42 |
| 1:R:326:HIS:HA | 1:R:330:SER:O | 2.20 | 0.42 |
| 1:R:627:HIS:HB2 | 1:R:640:GLN:HB2 | 2.00 | 0.42 |
| 1:B:541:VAL:HG11 | 1:B:595:ILE:HD13 | 2.02 | 0.42 |
| 1:C:169:VAL:HG23 | 1:C:172:SER:HA | 2.01 | 0.42 |
| 1:C:272:ASP:OD1 | 1:C:272:ASP:C | 2.58 | 0.42 |
| 1:C:542:LYS:HA | 1:C:542:LYS:HD3 | 1.78 | 0.42 |
| 1:E:434:VAL:HG13 | 1:E:469:LEU:CD1 | 2.49 | 0.42 |
| 1:E:77:LEU:O | 1:E:81:MET:HG3 | 2.20 | 0.42 |
| 1:F:133:ARG:HB2 | 1:F:164:LYS:HG3 | 2.02 | 0.42 |
| 1:F:399:THR:HG22 | 1:F:399:THR:O | 2.19 | 0.42 |
| 1:G:112:TRP:O | 1:G:113:SER:C | 2.58 | 0.42 |
| 1:G:416:PHE:O | 1:G:420:ILE:HG13 | 2.19 | 0.42 |
| 1:H:22:TYR:CE1 | 1:H:525:THR:HG22 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:158:ALA:HA | 1:I:162:LEU:HD22 | 2.00 | 0.42 |
| 1:I:379:LYS:N | 1:I:399:THR:CG2 | 2.83 | 0.42 |
| 1:K:195:LEU:HB3 | 1:K:423:TYR:CZ | 2.54 | 0.42 |
| 1:K:423:TYR:O | 1:K:424:LYS:C | 2.58 | 0.42 |
| 1:L:269:MET:HG3 | 1:L:306:TYR:HE1 | 1.85 | 0.42 |
| 1:M:91:THR:CG2 | 1:M:117:THR:CG2 | 2.86 | 0.42 |
| 1:M:194:ARG:O | 1:M:195:LEU:C | 2.58 | 0.42 |
| 1:Q:177:TYR:CD1 | 1:Q:177:TYR:N | 2.88 | 0.42 |
| 1:R:497:GLN:NE2 | 1:R:497:GLN:H | 2.11 | 0.42 |
| 1:B:182:GLU:OE2 | 1:B:227:ARG:NH1 | 2.52 | 0.42 |
| 1:C:534:LEU:HD21 | 1:C:611:VAL:HG11 | 2.02 | 0.42 |
| 1:D:218:LEU:HD13 | 1:D:268:LEU:HD13 | 2.02 | 0.42 |
| 1:E:445:LEU:HD12 | 1:E:480:GLU:HB2 | 2.01 | 0.42 |
| 1:E:44:ASP:O | 1:E:47:LEU:HB3 | 2.20 | 0.42 |
| 1:F:158:ALA:O | 1:F:162:LEU:N | 2.52 | 0.42 |
| 1:F:397:ALA:O | 1:F:399:THR:N | 2.52 | 0.42 |
| 1:F:93:LEU:HD13 | 1:F:123:SER:HA | 2.02 | 0.42 |
| 1:G:619:ARG:HG2 | 1:G:619:ARG:NH1 | 2.34 | 0.42 |
| 1:G:96:PHE:HD2 | 1:G:99:MET:HG2 | 1.84 | 0.42 |
| 1:H:35:ASP:O | 1:H:36:MET:C | 2.57 | 0.42 |
| 1:I:592:LEU:HD21 | 1:I:595:ILE:HD11 | 2.02 | 0.42 |
| 1:I:616:THR:C | 1:I:618:LEU:H | 2.22 | 0.42 |
| 1:K:45:LYS:HE2 | 1:K:282:PHE:O | 2.19 | 0.42 |
| 1:L:269:MET:CG | 1:L:306:TYR:HE1 | 2.32 | 0.42 |
| 1:M:181:VAL:HG12 | 1:M:183:SER:HB3 | 2.02 | 0.42 |
| 1:N:27:GLU:HB3 | 1:N:96:PHE:CZ | 2.55 | 0.42 |
| 1:N:316:MET:HA | 1:N:317:ASN:HA | 1.65 | 0.42 |
| 1:N:96:PHE:CD2 | 1:N:98:PRO:HD2 | 2.54 | 0.42 |
| 1:Q:323:VAL:HG23 | 1:Q:334:SER:O | 2.20 | 0.42 |
| 1:Q:395:LEU:C | 1:Q:397:ALA:N | 2.72 | 0.42 |
| 1:R:391:PHE:O | 1:R:394:LEU:HB2 | 2.20 | 0.42 |
| 1:A:57:LYS:HA | 1:A:57:LYS:HD2 | 1.82 | 0.42 |
| 1:A:612:TYR:CZ | 1:A:614:PRO:HA | 2.55 | 0.42 |
| 1:C:190:ASN:HD21 | 1:C:209:GLY:HA3 | 1.85 | 0.42 |
| 1:C:490:PRO:CB | 1:C:569:MET:HE1 | 2.47 | 0.42 |
| 1:E:269:MET:HG2 | 1:E:306:TYR:HE1 | 1.84 | 0.42 |
| 1:E:491:GLU:HG3 | 1:E:540:ILE:O | 2.19 | 0.42 |
| 1:F:184:HIS:O | 1:F:185:LEU:C | 2.58 | 0.42 |
| 1:F:229:LEU:HA | 1:F:229:LEU:HD23 | 1.63 | 0.42 |
| 1:F:354:SER:O | 1:F:358:VAL:HG23 | 2.19 | 0.42 |
| 1:F:73:THR:HG22 | 1:F:94:GLU:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:119:ILE:N | 1:G:119:ILE:HD12 | 2.35 | 0.42 |
| 1:G:447:GLU:N | 1:G:448:PRO:HA | 2.35 | 0.42 |
| 1:H:169:VAL:HG11 | 1:H:240:PHE:O | 2.20 | 0.42 |
| 1:H:119:ILE:HG23 | 1:J:128:GLN:HG2 | 2.02 | 0.42 |
| 1:J:141:VAL:O | 1:J:141:VAL:CG1 | 2.68 | 0.42 |
| 1:J:168:ARG:HH22 | 1:J:277:ARG:HB2 | 1.84 | 0.42 |
| 1:K:532:GLN:HG2 | 1:K:537:TYR:HE2 | 1.85 | 0.42 |
| 1:O:481:PRO:HB3 | 1:O:583:PHE:HD1 | 1.85 | 0.42 |
| 1:O:58:LYS:NZ | 1:O:86:GLY:O | 2.45 | 0.42 |
| 1:P:379:LYS:O | 1:P:381:LEU:HG | 2.20 | 0.42 |
| 1:Q:55:ALA:O | 1:Q:56:GLU:C | 2.58 | 0.42 |
| 1:A:566:ILE:O | 1:A:623:SER:HA | 2.20 | 0.42 |
| 1:C:320:PHE:CD1 | 1:C:320:PHE:C | 2.93 | 0.42 |
| 1:C:349:LEU:O | 1:C:350:HIS:C | 2.58 | 0.42 |
| 1:F:91:THR:HG22 | 1:F:117:THR:CG2 | 2.50 | 0.42 |
| 1:G:269:MET:HG2 | 1:G:306:TYR:HE1 | 1.84 | 0.42 |
| 1:H:53:THR:HG22 | 1:H:168:ARG:HE | 1.85 | 0.42 |
| 1:H:51:LYS:HB3 | 1:H:51:LYS:NZ | 2.35 | 0.42 |
| 1:H:574:ALA:C | 1:H:575:ILE:HG13 | 2.40 | 0.42 |
| 1:H:6:ILE:O | 1:H:8:GLN:NE2 | 2.50 | 0.42 |
| 1:I:403:VAL:HB | 1:I:428:VAL:HB | 2.00 | 0.42 |
| 1:I:577:MET:HA | 1:I:578:TRP:CE3 | 2.55 | 0.42 |
| 1:J:51:LYS:HA | 1:J:85:GLU:HG2 | 2.02 | 0.42 |
| 1:L:631:ASP:CG | 1:L:633:SER:HB2 | 2.40 | 0.42 |
| 1:M:301:TRP:O | 1:M:302:MET:HB3 | 2.20 | 0.42 |
| 1:M:384:ALA:O | 1:M:444:VAL:HA | 2.19 | 0.42 |
| 1:M:451:MET:HB2 | 1:M:451:MET:HE2 | 1.93 | 0.42 |
| 1:N:467:GLU:OE1 | 1:N:557:VAL:HG13 | 2.20 | 0.42 |
| 1:P:144:THR:O | 1:P:269:MET:HE1 | 2.20 | 0.42 |
| 1:Q:190:ASN:ND2 | 1:Q:209:GLY:HA3 | 2.29 | 0.42 |
| 1:R:3:LEU:O | 1:R:15:TRP:HA | 2.20 | 0.42 |
| 1:B:339:ASP:OD1 | 1:B:341:SER:N | 2.45 | 0.42 |
| 1:C:412:PHE:HE2 | 1:C:451:MET:HG2 | 1.85 | 0.42 |
| 1:C:569:MET:SD | 1:C:575:ILE:HD11 | 2.60 | 0.42 |
| 1:E:146:LEU:HD23 | 1:E:146:LEU:H | 1.85 | 0.42 |
| 1:I:550:ARG:HB2 | 1:I:550:ARG:HH11 | 1.85 | 0.42 |
| 1:J:434:VAL:HG12 | 1:J:469:LEU:HD13 | 2.01 | 0.42 |
| 1:J:563:VAL:HG22 | 1:J:627:HIS:CD2 | 2.55 | 0.42 |
| 1:K:310:GLU:OE2 | 1:K:338:LYS:HG2 | 2.20 | 0.42 |
| 1:K:403:VAL:HB | 1:K:428:VAL:HB | 2.02 | 0.42 |
| 1:M:275:MET:HB2 | 1:M:275:MET:HE3 | 1.74 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:455:ASN:HA | 1:M:456:PRO:HD3 | 1.87 | 0.42 |
| 1:M:66:VAL:HA | 1:M:135:ASP:OD2 | 2.20 | 0.42 |
| 1:N:227:ARG:NH2 | 1:N:261:SER:O | 2.53 | 0.42 |
| 1:Q:186:LEU:HD11 | 1:Q:268:LEU:HD21 | 2.02 | 0.42 |
| 1:Q:193:PRO:HA | 1:Q:362:ASN:HD21 | 1.84 | 0.42 |
| 1:Q:618:LEU:HG | 1:Q:624:LEU:HD22 | 2.01 | 0.42 |
| 1:R:323:VAL:HG12 | 1:R:325:ASN:HD21 | 1.85 | 0.42 |
| 1:R:550:ARG:O | 1:R:560:GLN:NE2 | 2.48 | 0.42 |
| 1:R:57:LYS:O | 1:R:61:ASN:ND2 | 2.52 | 0.42 |
| 1:A:505:THR:HA | 1:A:509:PHE:O | 2.20 | 0.41 |
| 1:B:134:ALA:HB3 | 1:B:163:ALA:HA | 2.01 | 0.41 |
| 1:B:522:ARG:O | 1:B:526:ASP:HB2 | 2.19 | 0.41 |
| 1:B:59:HIS:O | 1:B:61:ASN:N | 2.52 | 0.41 |
| 1:C:295:TYR:CD2 | 1:C:295:TYR:C | 2.93 | 0.41 |
| 1:F:535:TRP:CG | 1:F:605:LYS:HG2 | 2.54 | 0.41 |
| 1:G:191:ASP:OD2 | 1:G:194:ARG:NH1 | 2.42 | 0.41 |
| 1:G:369:LYS:HB3 | 1:G:369:LYS:HE3 | 1.93 | 0.41 |
| 1:G:490:PRO:CB | 1:G:569:MET:HE3 | 2.23 | 0.41 |
| 1:H:374:VAL:O | 1:H:378:SER:OG | 2.37 | 0.41 |
| 1:H:84:ARG:O | 1:H:85:GLU:CB | 2.62 | 0.41 |
| 1:H:97:LYS:HB2 | 1:H:98:PRO:HD3 | 2.02 | 0.41 |
| 1:J:447:GLU:N | 1:J:448:PRO:HA | 2.35 | 0.41 |
| 1:K:178:ILE:HA | 1:K:268:LEU:O | 2.20 | 0.41 |
| 1:K:359:TYR:CZ | 1:K:605:LYS:HB2 | 2.55 | 0.41 |
| 1:L:39:ASP:OD2 | 1:L:298:ARG:HD2 | 2.20 | 0.41 |
| 1:M:416:PHE:HB2 | 1:M:430:ILE:HD13 | 2.00 | 0.41 |
| 1:M:612:TYR:CE2 | 1:M:614:PRO:HA | 2.55 | 0.41 |
| 1:O:179:VAL:HG11 | 1:O:228:GLU:HG2 | 2.00 | 0.41 |
| 1:O:216:VAL:C | 1:O:302:MET:HG2 | 2.40 | 0.41 |
| 1:Q:169:VAL:HG21 | 1:Q:240:PHE:C | 2.41 | 0.41 |
| 1:Q:191:ASP:O | 1:Q:192:ILE:C | 2.58 | 0.41 |
| 1:R:267:LEU:C | 1:R:268:LEU:HD23 | 2.41 | 0.41 |
| 1:A:570:SER:HB3 | 1:A:622:LYS:HG3 | 2.02 | 0.41 |
| 1:B:403:VAL:HB | 1:B:428:VAL:HB | 2.01 | 0.41 |
| 1:B:437:LEU:HD22 | 1:B:439:ASP:O | 2.19 | 0.41 |
| 1:B:66:VAL:CG1 | 1:B:67:HIS:H | 2.32 | 0.41 |
| 1:E:550:ARG:H | 1:E:560:GLN:NE2 | 2.13 | 0.41 |
| 1:E:96:PHE:CZ | 1:E:98:PRO:HG2 | 2.55 | 0.41 |
| 1:G:169:VAL:HG11 | 1:G:240:PHE:C | 2.41 | 0.41 |
| 1:H:178:ILE:HG21 | 1:H:333:PHE:CE2 | 2.55 | 0.41 |
| 1:H:179:VAL:HG22 | 1:H:232:PRO:HA | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:387:GLY:HA2 | 1:H:450:TYR:CE2 | 2.55 | 0.41 |
| 1:I:478:ARG:NH2 | 1:I:478:ARG:CG | 2.83 | 0.41 |
| 1:J:391:PHE:O | 1:J:392:LEU:C | 2.58 | 0.41 |
| 1:J:478:ARG:HH21 | 1:J:478:ARG:CG | 2.33 | 0.41 |
| 1:K:198:GLU:O | 1:K:201:GLU:HG3 | 2.19 | 0.41 |
| 1:L:280:THR:HG23 | 1:L:281:THR:N | 2.35 | 0.41 |
| 1:M:52:THR:HG21 | 1:M:278:ASN:HD21 | 1.85 | 0.41 |
| 1:Q:231:GLU:HG2 | 1:Q:231:GLU:H | 1.68 | 0.41 |
| 1:Q:269:MET:HG2 | 1:Q:306:TYR:CE1 | 2.54 | 0.41 |
| 1:R:385:THR:CG2 | 1:R:405:ILE:HG23 | 2.49 | 0.41 |
| 1:R:54:ILE:HD13 | 1:R:54:ILE:HA | 1.90 | 0.41 |
| 1:A:502:ASP:CG | 1:A:616:THR:HG21 | 2.34 | 0.41 |
| 1:B:182:GLU:HG3 | 1:B:263:THR:O | 2.19 | 0.41 |
| 1:C:228:GLU:OE2 | 1:C:290:LYS:NZ | 2.51 | 0.41 |
| 1:C:47:LEU:HD23 | 1:C:47:LEU:HA | 1.83 | 0.41 |
| 1:D:291:ASN:H | 1:D:292:LYS:HZ1 | 1.64 | 0.41 |
| 1:D:357:THR:HG21 | 1:D:449:PHE:CZ | 2.54 | 0.41 |
| 1:H:348:GLY:O | 1:H:352:MET:HG2 | 2.20 | 0.41 |
| 1:H:449:PHE:C | 1:H:449:PHE:CD1 | 2.94 | 0.41 |
| 1:I:495:ASP:C | 1:I:497:GLN:NE2 | 2.74 | 0.41 |
| 1:I:576:PRO:HA | 1:I:611:VAL:HA | 2.02 | 0.41 |
| 1:K:136:ILE:HA | 1:K:168:ARG:O | 2.20 | 0.41 |
| 1:K:6:ILE:O | 1:K:8:GLN:NE2 | 2.53 | 0.41 |
| 1:M:631:ASP:O | 1:M:635:GLY:N | 2.50 | 0.41 |
| 1:N:133:ARG:HH21 | 1:N:133:ARG:CB | 2.25 | 0.41 |
| 1:N:275:MET:HE1 | 1:N:283:ILE:HG13 | 2.01 | 0.41 |
| 1:N:27:GLU:OE2 | 1:N:96:PHE:HE1 | 1.96 | 0.41 |
| 1:N:514:PHE:O | 1:N:518:SER:HB3 | 2.20 | 0.41 |
| 1:N:548:ILE:O | 1:N:549:LEU:HD13 | 2.21 | 0.41 |
| 1:O:385:THR:HB | 1:O:405:ILE:HD13 | 2.01 | 0.41 |
| 1:O:597:SER:HB3 | 1:O:598:ALA:H | 1.73 | 0.41 |
| 1:Q:190:ASN:ND2 | 1:Q:190:ASN:O | 2.54 | 0.41 |
| 1:Q:216:VAL:N | 1:Q:302:MET:SD | 2.93 | 0.41 |
| 1:Q:70:ASP:HB3 | 1:Q:79:SER:OG | 2.20 | 0.41 |
| 1:R:84:ARG:O | 1:R:85:GLU:CB | 2.68 | 0.41 |
| 1:A:273:ILE:HG13 | 1:A:275:MET:CE | 2.49 | 0.41 |
| 1:B:427:ASN:HA | 1:C:8:GLN:NE2 | 2.35 | 0.41 |
| 1:E:143:ASP:OD2 | 1:E:148:GLY:HA3 | 2.19 | 0.41 |
| 1:E:379:LYS:HA | 1:E:399:THR:HG22 | 1.93 | 0.41 |
| 1:E:467:GLU:OE1 | 1:E:556:ARG:HG3 | 2.21 | 0.41 |
| 1:F:264:ILE:N | 1:F:312:LYS:O | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:42:ARG:HH11 | 1:F:140:GLU:CG | 2.30 | 0.41 |
| 1:F:569:MET:HA | 1:F:572:SER:HB2 | 2.01 | 0.41 |
| 1:G:562:CYS:SG | 1:G:564:VAL:HG22 | 2.60 | 0.41 |
| 1:G:83:ALA:HA | 1:G:87:ALA:HB3 | 2.01 | 0.41 |
| 1:G:9:LYS:HD2 | 1:G:9:LYS:HA | 1.72 | 0.41 |
| 1:H:400:ALA:O | 1:H:427:ASN:ND2 | 2.50 | 0.41 |
| 1:H:535:TRP:CE3 | 1:H:605:LYS:HE3 | 2.55 | 0.41 |
| 1:J:104:ARG:HA | 1:J:118:VAL:HG21 | 2.02 | 0.41 |
| 1:J:613:PHE:HA | 1:J:614:PRO:HD2 | 1.89 | 0.41 |
| 1:K:417:PHE:CZ | 1:K:430:ILE:HB | 2.55 | 0.41 |
| 1:K:443:ILE:HG13 | 1:K:478:ARG:HB3 | 2.03 | 0.41 |
| 1:M:153:ARG:HB2 | 1:M:248:PHE:CZ | 2.54 | 0.41 |
| 1:M:173:THR:HG23 | 1:M:174:GLY:N | 2.35 | 0.41 |
| 1:M:173:THR:CG2 | 1:M:174:GLY:N | 2.83 | 0.41 |
| 1:M:199:LYS:HA | 1:M:200:ASP:HA | 1.34 | 0.41 |
| 1:M:235:ALA:HB1 | 1:M:324:CYS:HB3 | 2.03 | 0.41 |
| 1:M:382:HIS:ND1 | 1:M:441:PRO:HA | 2.35 | 0.41 |
| 1:N:54:ILE:CA | 1:N:58:LYS:NZ | 2.51 | 0.41 |
| 1:O:53:THR:HG22 | 1:O:168:ARG:HE | 1.84 | 0.41 |
| 1:O:513:PHE:O | 1:O:516:GLU:HB3 | 2.21 | 0.41 |
| 1:P:107:THR:C | 1:P:109:ASN:N | 2.74 | 0.41 |
| 1:P:39:ASP:OD2 | 1:P:298:ARG:CD | 2.68 | 0.41 |
| 1:P:540:ILE:HG22 | 1:P:542:LYS:HE3 | 2.03 | 0.41 |
| 1:B:164:LYS:O | 1:B:167:CYS:HB2 | 2.20 | 0.41 |
| 1:B:549:LEU:HA | 1:B:549:LEU:HD12 | 1.93 | 0.41 |
| 1:E:84:ARG:HD3 | 1:O:620:ASN:HD21 | 1.84 | 0.41 |
| 1:F:180:PRO:HB2 | 1:F:229:LEU:HB2 | 2.03 | 0.41 |
| 1:H:109:ASN:HD22 | 1:H:109:ASN:N | 2.18 | 0.41 |
| 1:H:141:VAL:O | 1:H:141:VAL:CG1 | 2.69 | 0.41 |
| 1:I:129:ILE:HG22 | 1:I:130:GLY:N | 2.36 | 0.41 |
| 1:J:643:LYS:HG3 | 1:J:644:SER:H | 1.86 | 0.41 |
| 1:K:104:ARG:NH1 | 1:K:118:VAL:HG12 | 2.34 | 0.41 |
| 1:K:218:LEU:HB2 | 1:K:303:GLN:NE2 | 2.31 | 0.41 |
| 1:K:616:THR:C | 1:K:618:LEU:N | 2.73 | 0.41 |
| 1:L:290:LYS:HZ2 | 1:L:290:LYS:HG3 | 1.76 | 0.41 |
| 1:M:176:VAL:HG22 | 1:M:236:PHE:HB2 | 2.01 | 0.41 |
| 1:M:297:TRP:CE3 | 1:M:298:ARG:HA | 2.55 | 0.41 |
| 1:M:68:VAL:HG22 | 1:M:136:ILE:CB | 2.40 | 0.41 |
| 1:N:42:ARG:HH11 | 1:N:140:GLU:HG2 | 1.85 | 0.41 |
| 1:N:216:VAL:HG13 | 1:N:218:LEU:HG | 2.03 | 0.41 |
| 1:P:111:PRO:HD2 | 1:P:112:TRP:CZ3 | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:639:PHE:HB3 | 1:R:641:PHE:CE1 | 2.55 | 0.41 |
| 1:B:444:VAL:O | 1:B:445:LEU:HD12 | 2.21 | 0.41 |
| 1:C:84:ARG:HG3 | 1:C:112:TRP:CZ2 | 2.55 | 0.41 |
| 1:A:16:VAL:HG11 | 1:C:417:PHE:CG | 2.55 | 0.41 |
| 1:I:616:THR:C | 1:I:618:LEU:N | 2.74 | 0.41 |
| 1:J:618:LEU:O | 1:J:620:ASN:N | 2.53 | 0.41 |
| 1:K:143:ASP:C | 1:K:145:GLU:N | 2.73 | 0.41 |
| 1:K:312:LYS:HD3 | 1:K:312:LYS:HA | 1.87 | 0.41 |
| 1:L:93:LEU:CD1 | 1:L:123:SER:HA | 2.50 | 0.41 |
| 1:N:36:MET:HA | 1:N:300:HIS:NE2 | 2.35 | 0.41 |
| 1:N:85:GLU:N | 1:N:86:GLY:HA2 | 2.36 | 0.41 |
| 1:O:386:VAL:HG23 | 1:O:446:ALA:HB2 | 2.02 | 0.41 |
| 1:O:390:SER:OG | 1:O:447:GLU:OE1 | 2.33 | 0.41 |
| 1:O:632:LYS:HG3 | 1:O:633:SER:H | 1.86 | 0.41 |
| 1:P:259:HIS:CD2 | 1:P:260:SER:OG | 2.54 | 0.41 |
| 1:P:316:MET:HA | 1:P:317:ASN:HA | 1.71 | 0.41 |
| 1:Q:110:SER:HB2 | 1:Q:111:PRO:HD2 | 2.01 | 0.41 |
| 1:B:314:VAL:HG22 | 1:B:315:GLU:N | 2.30 | 0.41 |
| 1:E:437:LEU:HD11 | 1:E:441:PRO:HG3 | 2.01 | 0.41 |
| 1:G:108:SER:O | 1:G:109:ASN:CB | 2.67 | 0.41 |
| 1:G:163:ALA:HB1 | 1:G:167:CYS:SG | 2.61 | 0.41 |
| 1:G:239:ASP:OD1 | 1:G:277:ARG:NH2 | 2.54 | 0.41 |
| 1:I:553:ILE:H | 1:I:553:ILE:HD12 | 1.86 | 0.41 |
| 1:I:355:ARG:NE | 3:I:702:PO4:O1 | 2.45 | 0.41 |
| 1:J:263:THR:HA | 1:J:313:LYS:HA | 2.02 | 0.41 |
| 1:J:84:ARG:HG3 | 1:J:112:TRP:CZ2 | 2.56 | 0.41 |
| 1:K:156:LYS:HG3 | 1:K:246:ILE:HB | 2.02 | 0.41 |
| 1:K:381:LEU:O | 1:K:400:ALA:HB1 | 2.20 | 0.41 |
| 1:K:535:TRP:O | 1:K:535:TRP:CE3 | 2.74 | 0.41 |
| 1:L:180:PRO:HA | 1:L:267:LEU:HD23 | 2.01 | 0.41 |
| 1:M:222:LYS:O | 1:M:225:GLU:CG | 2.64 | 0.41 |
| 1:M:218:LEU:HB2 | 1:M:303:GLN:HE21 | 1.86 | 0.41 |
| 1:N:378:SER:O | 1:N:379:LYS:C | 2.59 | 0.41 |
| 1:P:27:GLU:HB3 | 1:P:96:PHE:CZ | 2.56 | 0.41 |
| 1:P:369:LYS:CG | 1:P:370:PHE:N | 2.82 | 0.41 |
| 1:P:45:LYS:O | 1:P:275:MET:HG2 | 2.21 | 0.41 |
| 1:P:297:TRP:CD2 | 1:P:495:ASP:HB3 | 2.55 | 0.41 |
| 1:P:67:HIS:HE1 | 1:P:91:THR:HG23 | 1.85 | 0.41 |
| 1:Q:137:ILE:O | 1:Q:169:VAL:HA | 2.21 | 0.41 |
| 1:Q:378:SER:HB2 | 1:Q:399:THR:CG2 | 2.41 | 0.41 |
| 1:Q:556:ARG:HB2 | 1:Q:556:ARG:HE | 1.67 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:150:GLY:O | 1:C:151:ALA:C | 2.59 | 0.41 |
| 1:E:216:VAL:CG2 | 1:E:217:GLN:N | 2.83 | 0.41 |
| 1:D:629:LEU:CD2 | 1:E:438:THR:HG21 | 2.48 | 0.41 |
| 1:E:57:LYS:O | 1:E:66:VAL:CG2 | 2.58 | 0.41 |
| 1:E:595:ILE:HG23 | 1:E:599:GLY:HA2 | 2.02 | 0.41 |
| 1:G:168:ARG:NH2 | 1:G:276:ASP:O | 2.54 | 0.41 |
| 1:I:71:ILE:HG21 | 1:I:154:THR:HG23 | 2.02 | 0.41 |
| 1:I:446:ALA:HB3 | 1:I:462:PHE:CE1 | 2.56 | 0.41 |
| 1:I:445:LEU:HD12 | 1:I:480:GLU:HB2 | 2.02 | 0.41 |
| 1:J:493:PHE:HA | 1:J:539:GLY:HA3 | 2.03 | 0.41 |
| 1:K:112:TRP:O | 1:K:114:ASP:N | 2.54 | 0.41 |
| 1:K:164:LYS:O | 1:K:165:PRO:C | 2.59 | 0.41 |
| 1:L:255:GLU:HG2 | 1:L:321:GLU:HG2 | 2.03 | 0.41 |
| 1:L:288:LYS:HE2 | 1:L:288:LYS:HB3 | 1.63 | 0.41 |
| 1:M:177:TYR:HA | 1:M:233:ILE:O | 2.21 | 0.41 |
| 1:M:534:LEU:C | 1:M:536:GLU:N | 2.72 | 0.41 |
| 1:N:186:LEU:HD23 | 1:N:186:LEU:HA | 1.95 | 0.41 |
| 1:N:58:LYS:N | 1:N:58:LYS:CE | 2.84 | 0.41 |
| 1:O:182:GLU:HB2 | 1:O:229:LEU:HD21 | 2.03 | 0.41 |
| 1:O:185:LEU:C | 1:O:185:LEU:HD23 | 2.41 | 0.41 |
| 1:O:410:GLU:HB2 | 1:O:413:ARG:NH2 | 2.35 | 0.41 |
| 1:O:443:ILE:HA | 1:O:478:ARG:O | 2.20 | 0.41 |
| 1:O:447:GLU:H | 1:O:448:PRO:HA | 1.85 | 0.41 |
| 1:O:7:ASN:HB2 | 1:O:14:GLU:OE1 | 2.21 | 0.41 |
| 1:P:45:LYS:HZ1 | 1:P:294:ASN:ND2 | 2.19 | 0.41 |
| 1:P:554:ASP:C | 1:P:556:ARG:H | 2.24 | 0.41 |
| 1:Q:485:VAL:HG12 | 1:Q:487:LYS:HG3 | 2.02 | 0.41 |
| 1:R:471:MET:HG3 | 1:R:556:ARG:NH2 | 2.35 | 0.41 |
| 1:A:478:ARG:NH2 | 1:A:478:ARG:CG | 2.70 | 0.41 |
| 1:B:38:LEU:HD13 | 1:B:498:ASN:HD22 | 1.86 | 0.41 |
| 1:C:141:VAL:CG1 | 1:C:141:VAL:O | 2.65 | 0.41 |
| 1:C:616:THR:C | 1:C:618:LEU:H | 2.24 | 0.41 |
| 1:E:316:MET:HA | 1:E:317:ASN:HA | 1.86 | 0.41 |
| 1:E:353:LEU:HD22 | 1:E:357:THR:HG21 | 2.02 | 0.41 |
| 1:E:15:TRP:NE1 | 1:E:520:LYS:HE2 | 2.36 | 0.41 |
| 1:F:60:GLU:HG3 | 1:F:60:GLU:O | 2.21 | 0.41 |
| 1:G:169:VAL:HG11 | 1:G:240:PHE:O | 2.21 | 0.41 |
| 1:G:448:PRO:HG2 | 1:G:448:PRO:O | 2.21 | 0.41 |
| 1:I:243:GLU:HG2 | 1:I:244:GLU:N | 2.34 | 0.41 |
| 1:I:275:MET:HE2 | 1:I:275:MET:CA | 2.43 | 0.41 |
| 1:I:455:ASN:HA | 1:I:456:PRO:HD2 | 1.65 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:96:PHE:CZ | 1:I:98:PRO:HG2 | 2.56 | 0.41 |
| 1:J:446:ALA:O | 1:J:481:PRO:HD3 | 2.21 | 0.41 |
| 1:K:478:ARG:NH2 | 1:K:480:GLU:OE1 | 2.54 | 0.41 |
| 1:M:437:LEU:HA | 1:M:437:LEU:HD23 | 1.88 | 0.41 |
| 1:M:57:LYS:HD3 | 1:M:57:LYS:HA | 1.96 | 0.41 |
| 1:M:482:HIS:CE1 | 1:M:582:GLU:HB3 | 2.56 | 0.41 |
| 1:P:449:PHE:HA | 1:P:459:HIS:CD2 | 2.56 | 0.41 |
| 1:R:96:PHE:HD2 | 1:R:99:MET:HG2 | 1.85 | 0.41 |
| 1:A:186:LEU:O | 1:A:187:LYS:C | 2.59 | 0.41 |
| 1:D:437:LEU:C | 1:D:437:LEU:HD22 | 2.41 | 0.41 |
| 1:E:42:ARG:HE | 1:E:43:ASN:ND2 | 2.18 | 0.41 |
| 1:F:627:HIS:O | 1:F:639:PHE:HA | 2.21 | 0.41 |
| 1:F:70:ASP:HA | 1:F:138:VAL:O | 2.20 | 0.41 |
| 1:G:185:LEU:HD23 | 1:G:359:TYR:HE2 | 1.86 | 0.41 |
| 1:H:268:LEU:HD12 | 1:H:289:TRP:HH2 | 1.85 | 0.41 |
| 1:H:327:ASP:C | 1:H:327:ASP:OD1 | 2.60 | 0.41 |
| 1:H:46:PHE:CZ | 1:H:140:GLU:HB2 | 2.56 | 0.41 |
| 1:I:190:ASN:HD21 | 1:I:209:GLY:HA3 | 1.86 | 0.41 |
| 1:I:326:HIS:HA | 1:I:330:SER:O | 2.21 | 0.41 |
| 1:J:119:ILE:HG22 | 1:J:121:GLU:HG3 | 2.02 | 0.41 |
| 1:J:413:ARG:NH1 | 1:J:432:GLU:HG3 | 2.36 | 0.41 |
| 1:J:547:GLU:OE2 | 1:J:550:ARG:HD2 | 2.21 | 0.41 |
| 1:K:516:GLU:CG | 1:K:520:LYS:HE3 | 2.50 | 0.41 |
| 1:K:623:SER:O | 1:K:644:SER:OG | 2.30 | 0.41 |
| 1:L:105:HIS:O | 1:L:109:ASN:ND2 | 2.46 | 0.41 |
| 1:L:42:ARG:HH21 | 1:L:43:ASN:HD21 | 1.68 | 0.41 |
| 1:M:487:LYS:O | 1:M:577:MET:HA | 2.21 | 0.41 |
| 1:M:52:THR:HG21 | 1:M:278:ASN:ND2 | 2.36 | 0.41 |
| 1:N:302:MET:HG2 | 1:N:303:GLN:H | 1.86 | 0.41 |
| 1:N:427:ASN:N | 1:N:427:ASN:OD1 | 2.53 | 0.41 |
| 1:R:550:ARG:H | 1:R:560:GLN:NE2 | 2.18 | 0.41 |
| 1:A:119:ILE:HG22 | 1:A:121:GLU:HG2 | 2.02 | 0.41 |
| 1:B:164:LYS:O | 1:B:165:PRO:C | 2.58 | 0.41 |
| 1:B:460:LEU:HD21 | 1:B:579:MET:HE2 | 2.02 | 0.41 |
| 1:C:420:ILE:HD11 | 1:C:428:VAL:HG22 | 2.02 | 0.41 |
| 1:C:549:LEU:HD12 | 1:C:549:LEU:HA | 1.68 | 0.41 |
| 1:D:226:PHE:N | 1:D:226:PHE:CD1 | 2.89 | 0.41 |
| 1:D:447:GLU:N | 1:D:448:PRO:HA | 2.35 | 0.41 |
| 1:E:383:VAL:HB | 1:E:443:ILE:CG2 | 2.51 | 0.41 |
| 1:F:434:VAL:CG1 | 1:F:469:LEU:HD13 | 2.52 | 0.41 |
| 1:G:216:VAL:CG2 | 1:G:217:GLN:N | 2.83 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:292:LYS:HA | 1:H:293:ASN:HA | 1.93 | 0.41 |
| 1:H:505:THR:HA | 1:H:509:PHE:O | 2.20 | 0.41 |
| 1:J:358:VAL:O | 1:J:359:TYR:C | 2.59 | 0.41 |
| 1:J:455:ASN:HB3 | 1:J:457:TRP:CE2 | 2.56 | 0.41 |
| 1:K:227:ARG:NH2 | 1:K:261:SER:O | 2.53 | 0.41 |
| 1:L:168:ARG:CG | 1:L:168:ARG:NH1 | 2.75 | 0.41 |
| 1:N:292:LYS:HD2 | 1:N:293:ASN:ND2 | 2.37 | 0.41 |
| 1:N:600:VAL:HA | 1:N:601:PRO:HD3 | 1.85 | 0.41 |
| 1:P:445:LEU:HD12 | 1:P:480:GLU:HB2 | 2.03 | 0.41 |
| 1:Q:323:VAL:HB | 1:Q:334:SER:OG | 2.21 | 0.41 |
| 1:Q:531:GLU:HG2 | 1:Q:531:GLU:O | 2.21 | 0.41 |
| 1:B:37:ILE:O | 1:B:37:ILE:CG2 | 2.68 | 0.40 |
| 1:B:489:ILE:HD13 | 1:B:541:VAL:CG2 | 2.51 | 0.40 |
| 1:B:553:ILE:HG22 | 1:B:553:ILE:O | 2.21 | 0.40 |
| 1:B:57:LYS:O | 1:B:57:LYS:HG3 | 2.21 | 0.40 |
| 1:C:16:VAL:HG13 | 1:C:17:VAL:N | 2.36 | 0.40 |
| 1:C:72:GLY:N | 1:C:93:LEU:O | 2.53 | 0.40 |
| 1:D:157:GLU:HB3 | 1:D:161:ARG:NH1 | 2.36 | 0.40 |
| 1:E:178:ILE:HA | 1:E:268:LEU:O | 2.21 | 0.40 |
| 1:F:274:ASP:OD1 | 1:F:277:ARG:N | 2.45 | 0.40 |
| 1:F:78:LEU:HD12 | 1:F:78:LEU:HA | 1.83 | 0.40 |
| 1:H:342:ARG:HD3 | 1:H:342:ARG:HH11 | 1.69 | 0.40 |
| 1:H:534:LEU:CD1 | 1:H:576:PRO:HB3 | 2.51 | 0.40 |
| 1:I:427:ASN:N | 1:I:427:ASN:OD1 | 2.54 | 0.40 |
| 1:J:71:ILE:HB | 1:J:139:ALA:HB2 | 2.02 | 0.40 |
| 1:J:566:ILE:HG21 | 1:J:575:ILE:HD13 | 2.04 | 0.40 |
| 1:K:222:LYS:HB2 | 1:K:225:GLU:CG | 2.51 | 0.40 |
| 1:O:270:TRP:CE2 | 1:O:286:GLY:HA2 | 2.57 | 0.40 |
| 1:O:69:LEU:HD23 | 1:O:137:ILE:HG12 | 2.03 | 0.40 |
| 1:P:404:THR:HG23 | 1:P:429:GLU:HG3 | 2.03 | 0.40 |
| 1:P:447:GLU:H | 1:P:448:PRO:HA | 1.87 | 0.40 |
| 1:Q:566:ILE:CG2 | 1:Q:569:MET:HE2 | 2.51 | 0.40 |
| 1:C:547:GLU:OE2 | 1:C:550:ARG:NH1 | 2.52 | 0.40 |
| 1:C:59:HIS:HD2 | 1:C:60:GLU:HG3 | 1.85 | 0.40 |
| 1:D:175:ASN:ND2 | 1:D:237:LYS:HG2 | 2.37 | 0.40 |
| 1:D:359:TYR:C | 1:D:359:TYR:CD1 | 2.94 | 0.40 |
| 1:F:204:LEU:HD21 | 1:F:419:TYR:CE1 | 2.56 | 0.40 |
| 1:G:321:GLU:O | 1:G:322:ILE:HD13 | 2.21 | 0.40 |
| 1:J:144:THR:HG22 | 1:J:144:THR:O | 2.20 | 0.40 |
| 1:J:297:TRP:CZ2 | 1:J:299:ASP:HB2 | 2.56 | 0.40 |
| 1:J:338:LYS:HA | 1:J:338:LYS:HD2 | 1.90 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:40:PHE:CD1 | 1:J:41:ASP:N | 2.90 | 0.40 |
| 1:K:277:ARG:HG2 | 1:K:277:ARG:O | 2.21 | 0.40 |
| 1:K:299:ASP:C | 1:K:301:TRP:N | 2.75 | 0.40 |
| 1:L:457:TRP:HA | 4:L:831:HOH:O | 2.20 | 0.40 |
| 1:L:465:ASP:O | 1:L:469:LEU:HD22 | 2.21 | 0.40 |
| 1:L:445:LEU:HD12 | 1:L:480:GLU:HB2 | 2.03 | 0.40 |
| 1:L:631:ASP:C | 1:L:631:ASP:OD1 | 2.59 | 0.40 |
| 1:L:63:ASP:OD1 | 1:L:63:ASP:N | 2.36 | 0.40 |
| 1:M:194:ARG:HB3 | 1:M:201:GLU:OE1 | 2.21 | 0.40 |
| 1:M:344:TYR:N | 1:M:344:TYR:CD1 | 2.89 | 0.40 |
| 1:M:438:THR:HB | 1:M:439:ASP:OD1 | 2.22 | 0.40 |
| 1:P:198:GLU:HB3 | 1:P:200:ASP:HB2 | 2.04 | 0.40 |
| 1:P:541:VAL:HG11 | 1:P:595:ILE:HD13 | 2.03 | 0.40 |
| 1:Q:216:VAL:CA | 1:Q:302:MET:SD | 3.10 | 0.40 |
| 1:Q:287:PRO:HG2 | 1:Q:289:TRP:CH2 | 2.56 | 0.40 |
| 1:Q:460:LEU:HD22 | 1:Q:463:LEU:CD2 | 2.51 | 0.40 |
| 1:Q:474:GLY:C | 1:Q:476:GLU:N | 2.74 | 0.40 |
| 1:R:460:LEU:HD21 | 1:R:579:MET:HE1 | 2.03 | 0.40 |
| 1:R:92:ALA:C | 1:R:93:LEU:HD23 | 2.42 | 0.40 |
| 1:A:136:ILE:HA | 1:A:168:ARG:O | 2.21 | 0.40 |
| 1:B:618:LEU:HD21 | 1:B:642:GLY:HA2 | 2.03 | 0.40 |
| 1:D:631:ASP:OD1 | 1:D:631:ASP:C | 2.59 | 0.40 |
| 1:E:578:TRP:CG | 1:E:591:GLY:HA3 | 2.57 | 0.40 |
| 1:G:548:ILE:HG22 | 1:G:549:LEU:HD22 | 2.02 | 0.40 |
| 1:H:297:TRP:CE3 | 1:H:298:ARG:HA | 2.56 | 0.40 |
| 1:J:261:SER:OG | 1:J:315:GLU:HA | 2.21 | 0.40 |
| 1:J:392:LEU:HA | 1:J:392:LEU:HD23 | 1.90 | 0.40 |
| 1:K:175:ASN:O | 1:K:271:TRP:HA | 2.22 | 0.40 |
| 1:K:549:LEU:HD12 | 1:K:560:GLN:HB3 | 2.02 | 0.40 |
| 1:K:58:LYS:NZ | 1:K:86:GLY:O | 2.45 | 0.40 |
| 1:L:269:MET:HG2 | 1:L:306:TYR:CE1 | 2.56 | 0.40 |
| 1:M:434:VAL:HG12 | 1:M:469:LEU:HD12 | 2.03 | 0.40 |
| 1:N:140:GLU:OE1 | 1:N:301:TRP:CZ2 | 2.71 | 0.40 |
| 1:N:194:ARG:HB3 | 1:N:201:GLU:HG3 | 2.04 | 0.40 |
| 1:O:185:LEU:O | 1:O:185:LEU:HD23 | 2.21 | 0.40 |
| 1:O:549:LEU:HA | 1:O:549:LEU:HD12 | 1.81 | 0.40 |
| 1:O:612:TYR:CG | 1:O:613:PHE:N | 2.88 | 0.40 |
| 1:P:122:ARG:O | 1:P:125:ASP:HB2 | 2.22 | 0.40 |
| 1:Q:179:VAL:HA | 1:Q:180:PRO:HD2 | 1.88 | 0.40 |
| 1:Q:372:ASP:O | 1:Q:376:LYS:HB2 | 2.21 | 0.40 |
| 1:Q:47:LEU:O | 1:Q:51:LYS:HB2 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:612:TYR:OH | 1:R:615:ILE:CD1 | 2.70 | 0.40 |
| 1:B:91:THR:HG23 | 1:B:119:ILE:CD1 | 2.52 | 0.40 |
| 1:C:275:MET:CE | 1:C:283:ILE:H | 2.34 | 0.40 |
| 1:D:181:VAL:O | 1:D:265:ASP:N | 2.54 | 0.40 |
| 1:E:122:ARG:O | 1:E:124:THR:N | 2.55 | 0.40 |
| 1:G:227:ARG:NH2 | 1:G:261:SER:O | 2.55 | 0.40 |
| 1:G:310:GLU:OE1 | 1:G:335:ASN:OD1 | 2.40 | 0.40 |
| 1:G:35:ASP:OD2 | 1:G:299:ASP:N | 2.40 | 0.40 |
| 1:G:448:PRO:O | 1:G:448:PRO:CG | 2.69 | 0.40 |
| 1:H:315:GLU:HB3 | 1:H:318:GLN:HB2 | 2.03 | 0.40 |
| 1:H:460:LEU:HD21 | 1:H:579:MET:HE3 | 2.03 | 0.40 |
| 1:H:470:LYS:HD2 | 1:H:555:GLY:HA3 | 2.04 | 0.40 |
| 1:I:181:VAL:HG12 | 1:I:266:ALA:O | 2.22 | 0.40 |
| 1:K:497:GLN:CD | 1:K:497:GLN:H | 2.25 | 0.40 |
| 1:M:280:THR:CG2 | 1:M:281:THR:HG22 | 2.26 | 0.40 |
| 1:M:388:GLU:HB3 | 1:M:450:TYR:HA | 2.03 | 0.40 |
| 1:N:114:ASP:N | 1:N:114:ASP:OD1 | 2.55 | 0.40 |
| 1:N:233:ILE:HG12 | 1:N:256:ALA:HB2 | 2.04 | 0.40 |
| 1:N:346:VAL:O | 1:N:347:CYS:C | 2.60 | 0.40 |
| 1:N:420:ILE:HA | 1:N:425:LEU:HD12 | 2.03 | 0.40 |
| 1:O:375:ASP:HA | 1:O:399:THR:OG1 | 2.21 | 0.40 |
| 1:P:455:ASN:HA | 1:P:456:PRO:HD3 | 1.89 | 0.40 |
| 1:R:111:PRO:HD2 | 1:R:112:TRP:CZ3 | 2.57 | 0.40 |
| 1:R:531:GLU:HA | 1:R:609:GLN:O | 2.21 | 0.40 |
| 1:B:168:ARG:NH2 | 1:B:276:ASP:O | 2.55 | 0.40 |
| 1:B:404:THR:HG23 | 1:B:429:GLU:HG3 | 2.03 | 0.40 |
| 1:C:156:LYS:NZ | 1:C:246:ILE:O | 2.46 | 0.40 |
| 1:D:384:ALA:O | 1:D:444:VAL:HA | 2.21 | 0.40 |
| 1:D:565:ASN:ND2 | 1:D:644:SER:HB3 | 2.37 | 0.40 |
| 1:E:193:PRO:HA | 1:E:362:ASN:ND2 | 2.36 | 0.40 |
| 1:F:259:HIS:CD2 | 1:F:260:SER:OG | 2.70 | 0.40 |
| 1:F:39:ASP:C | 1:F:39:ASP:OD1 | 2.60 | 0.40 |
| 1:G:73:THR:HA | 2:G:701:SAH:N | 2.36 | 0.40 |
| 1:I:162:LEU:N | 1:I:162:LEU:CD1 | 2.85 | 0.40 |
| 1:I:619:ARG:HH11 | 1:I:619:ARG:HG2 | 1.86 | 0.40 |
| 1:J:264:ILE:HD12 | 1:J:312:LYS:CG | 2.52 | 0.40 |
| 1:K:627:HIS:HB2 | 1:K:640:GLN:HB2 | 2.03 | 0.40 |
| 1:M:145:GLU:O | 1:M:146:LEU:HB3 | 2.21 | 0.40 |
| 1:M:174:GLY:HA3 | 1:M:273:ILE:HG22 | 2.03 | 0.40 |
| 1:M:388:GLU:HG2 | 1:M:451:MET:HG3 | 2.04 | 0.40 |
| 1:M:96:PHE:CE2 | 1:M:98:PRO:HD2 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:N:141:VAL:O | 1:N:141:VAL:CG1 | 2.69 | 0.40 |
| 1:N:242:HIS:HB3 | 1:N:245:LYS:CG | 2.50 | 0.40 |
| 1:N:357:THR:O | 1:N:361:VAL:HG23 | 2.22 | 0.40 |
| 1:O:310:GLU:OE2 | 1:O:338:LYS:HG2 | 2.22 | 0.40 |
| 1:O:557:VAL:CG2 | 1:O:632:LYS:HB2 | 2.49 | 0.40 |
| 1:Q:410:GLU:HG3 | 1:Q:413:ARG:HH22 | 1.87 | 0.40 |
| 1:Q:443:ILE:CG1 | 1:Q:444:VAL:N | 2.85 | 0.40 |
| 1:Q:468:VAL:O | 1:Q:471:MET:HB3 | 2.21 | 0.40 |
| 1:R:278:ASN:HB2 | 1:R:280:THR:HG22 | 2.01 | 0.40 |
| 1:R:377:LEU:HB3 | 1:R:443:ILE:HD13 | 2.03 | 0.40 |
| 1:R:600:VAL:HA | 1:R:601:PRO:HD2 | 1.82 | 0.40 |

All (2) 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:D:554:ASP:OD1 | 1:C:550:ARG:NH2[3_554] | 2.01 | 0.19 |
| 1:N:554:ASP:OD1 | 1:P:550:ARG:NH2[3_654] | 2.09 | 0.11 |

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1 | A | 637/655 (97%) | 600 (94%) | 34 (5%) | 3 (0%) | 29 | 41 |
| 1 | B | 634/655 (97%) | 561 (88%) | 62 (10%) | 11 (2%) | 9 | 11 |
| 1 | C | 635/655 (97%) | 578 (91%) | 47 (7%) | 10 (2%) | 9 | 13 |
| 1 | D | 633/655 (97%) | 595 (94%) | 34 (5%) | 4 (1%) | 25 | 36 |
| 1 | E | 630/655 (96%) | 569 (90%) | 53 (8%) | 8 (1%) | 12 | 17 |
| 1 | F | 634/655 (97%) | 563 (89%) | 62 (10%) | 9 (1%) | 11 | 15 |
| 1 | G | 630/655 (96%) | 575 (91%) | 50 (8%) | 5 (1%) | 19 | 29 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|----------|----------|-------------|----|
| 1 | H | 635/655 (97%) | 590 (93%) | 39 (6%) | 6 (1%) | 17 | 25 |
| 1 | I | 642/655 (98%) | 572 (89%) | 58 (9%) | 12 (2%) | 8 | 10 |
| 1 | J | 642/655 (98%) | 578 (90%) | 54 (8%) | 10 (2%) | 9 | 13 |
| 1 | K | 637/655 (97%) | 570 (90%) | 53 (8%) | 14 (2%) | 6 | 7 |
| 1 | L | 642/655 (98%) | 607 (94%) | 34 (5%) | 1 (0%) | 47 | 62 |
| 1 | M | 625/655 (95%) | 551 (88%) | 65 (10%) | 9 (1%) | 11 | 15 |
| 1 | N | 634/655 (97%) | 558 (88%) | 67 (11%) | 9 (1%) | 11 | 15 |
| 1 | O | 637/655 (97%) | 567 (89%) | 61 (10%) | 9 (1%) | 11 | 15 |
| 1 | P | 630/655 (96%) | 576 (91%) | 48 (8%) | 6 (1%) | 15 | 23 |
| 1 | Q | 626/655 (96%) | 526 (84%) | 81 (13%) | 19 (3%) | 4 | 3 |
| 1 | R | 634/655 (97%) | 567 (89%) | 52 (8%) | 15 (2%) | 6 | 6 |
| All | All | 11417/11790 (97%) | 10303 (90%) | 954 (8%) | 160 (1%) | 11 | 15 |

All (160) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 63 | ASP |
| 1 | B | 59 | HIS |
| 1 | B | 60 | GLU |
| 1 | B | 278 | ASN |
| 1 | F | 290 | LYS |
| 1 | G | 87 | ALA |
| 1 | I | 279 | GLY |
| 1 | M | 35 | ASP |
| 1 | M | 36 | MET |
| 1 | M | 438 | THR |
| 1 | M | 616 | THR |
| 1 | N | 88 | ASP |
| 1 | O | 568 | ASN |
| 1 | P | 438 | THR |
| 1 | Q | 144 | THR |
| 1 | Q | 259 | HIS |
| 1 | Q | 336 | VAL |
| 1 | R | 88 | ASP |
| 1 | R | 219 | SER |
| 1 | R | 400 | ALA |
| 1 | J | 141 | VAL |
| 1 | K | 300 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 555 | GLY |
| 1 | D | 277 | ARG |
| 1 | D | 453 | ALA |
| 1 | B | 77 | LEU |
| 1 | B | 288 | LYS |
| 1 | B | 555 | GLY |
| 1 | C | 63 | ASP |
| 1 | C | 289 | TRP |
| 1 | C | 290 | LYS |
| 1 | C | 617 | ALA |
| 1 | F | 197 | GLY |
| 1 | F | 278 | ASN |
| 1 | F | 398 | LYS |
| 1 | E | 87 | ALA |
| 1 | E | 109 | ASN |
| 1 | E | 123 | SER |
| 1 | E | 183 | SER |
| 1 | H | 113 | SER |
| 1 | I | 286 | GLY |
| 1 | I | 453 | ALA |
| 1 | M | 146 | LEU |
| 1 | N | 264 | ILE |
| 1 | N | 291 | ASN |
| 1 | N | 474 | GLY |
| 1 | O | 141 | VAL |
| 1 | O | 380 | GLY |
| 1 | O | 461 | ARG |
| 1 | O | 478 | ARG |
| 1 | O | 617 | ALA |
| 1 | P | 108 | SER |
| 1 | P | 123 | SER |
| 1 | P | 452 | SER |
| 1 | Q | 56 | GLU |
| 1 | Q | 219 | SER |
| 1 | Q | 258 | ALA |
| 1 | Q | 277 | ARG |
| 1 | R | 346 | VAL |
| 1 | J | 130 | GLY |
| 1 | J | 396 | ALA |
| 1 | J | 598 | ALA |
| 1 | K | 85 | GLU |
| 1 | K | 113 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 286 | GLY |
| 1 | K | 535 | TRP |
| 1 | B | 41 | ASP |
| 1 | B | 42 | ARG |
| 1 | B | 124 | THR |
| 1 | C | 243 | GLU |
| 1 | F | 148 | GLY |
| 1 | G | 113 | SER |
| 1 | G | 496 | LEU |
| 1 | H | 242 | HIS |
| 1 | I | 111 | PRO |
| 1 | I | 533 | SER |
| 1 | M | 276 | ASP |
| 1 | M | 289 | TRP |
| 1 | Q | 224 | HIS |
| 1 | Q | 227 | ARG |
| 1 | Q | 232 | PRO |
| 1 | Q | 340 | LYS |
| 1 | R | 614 | PRO |
| 1 | J | 597 | SER |
| 1 | J | 632 | LYS |
| 1 | J | 643 | LYS |
| 1 | K | 144 | THR |
| 1 | K | 345 | CYS |
| 1 | K | 453 | ALA |
| 1 | K | 511 | LEU |
| 1 | A | 291 | ASN |
| 1 | B | 277 | ARG |
| 1 | C | 33 | PHE |
| 1 | C | 278 | ASN |
| 1 | C | 316 | MET |
| 1 | C | 475 | ASP |
| 1 | F | 185 | LEU |
| 1 | E | 288 | LYS |
| 1 | E | 453 | ALA |
| 1 | G | 277 | ARG |
| 1 | H | 84 | ARG |
| 1 | H | 277 | ARG |
| 1 | I | 277 | ARG |
| 1 | I | 594 | SER |
| 1 | I | 616 | THR |
| 1 | M | 302 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 453 | ALA |
| 1 | N | 55 | ALA |
| 1 | N | 83 | ALA |
| 1 | N | 133 | ARG |
| 1 | O | 616 | THR |
| 1 | Q | 87 | ALA |
| 1 | Q | 243 | GLU |
| 1 | Q | 293 | ASN |
| 1 | Q | 338 | LYS |
| 1 | R | 52 | THR |
| 1 | R | 85 | GLU |
| 1 | R | 160 | GLU |
| 1 | R | 497 | GLN |
| 1 | R | 643 | LYS |
| 1 | J | 316 | MET |
| 1 | K | 74 | GLY |
| 1 | K | 617 | ALA |
| 1 | B | 52 | THR |
| 1 | C | 632 | LYS |
| 1 | F | 379 | LYS |
| 1 | E | 108 | SER |
| 1 | G | 57 | LYS |
| 1 | H | 55 | ALA |
| 1 | I | 556 | ARG |
| 1 | P | 7 | ASN |
| 1 | Q | 146 | LEU |
| 1 | Q | 632 | LYS |
| 1 | R | 26 | GLN |
| 1 | R | 243 | GLU |
| 1 | J | 424 | LYS |
| 1 | K | 290 | LYS |
| 1 | K | 523 | THR |
| 1 | H | 350 | HIS |
| 1 | I | 309 | PRO |
| 1 | N | 242 | HIS |
| 1 | N | 244 | GLU |
| 1 | O | 441 | PRO |
| 1 | O | 614 | PRO |
| 1 | R | 557 | VAL |
| 1 | J | 33 | PHE |
| 1 | A | 64 | GLY |
| 1 | E | 279 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | R | 111 | PRO |
| 1 | L | 111 | PRO |
| 1 | D | 141 | VAL |
| 1 | F | 615 | ILE |
| 1 | P | 34 | GLY |
| 1 | K | 197 | GLY |
| 1 | F | 141 | VAL |
| 1 | I | 553 | ILE |
| 1 | R | 232 | PRO |
| 1 | I | 232 | PRO |
| 1 | Q | 111 | PRO |
| 1 | Q | 165 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|---|
| 1 | A | 556/569 (98%) | 479 (86%) | 77 (14%) | 3 | 4 |
| 1 | B | 553/569 (97%) | 474 (86%) | 79 (14%) | 3 | 4 |
| 1 | C | 554/569 (97%) | 484 (87%) | 70 (13%) | 4 | 5 |
| 1 | D | 552/569 (97%) | 488 (88%) | 64 (12%) | 5 | 7 |
| 1 | E | 551/569 (97%) | 459 (83%) | 92 (17%) | 2 | 2 |
| 1 | F | 553/569 (97%) | 471 (85%) | 82 (15%) | 3 | 3 |
| 1 | G | 552/569 (97%) | 473 (86%) | 79 (14%) | 3 | 4 |
| 1 | H | 554/569 (97%) | 481 (87%) | 73 (13%) | 4 | 4 |
| 1 | I | 557/569 (98%) | 476 (86%) | 81 (14%) | 3 | 3 |
| 1 | J | 557/569 (98%) | 481 (86%) | 76 (14%) | 3 | 4 |
| 1 | K | 556/569 (98%) | 465 (84%) | 91 (16%) | 2 | 2 |
| 1 | L | 557/569 (98%) | 483 (87%) | 74 (13%) | 4 | 4 |
| 1 | M | 550/569 (97%) | 470 (86%) | 80 (14%) | 3 | 3 |
| 1 | N | 553/569 (97%) | 455 (82%) | 98 (18%) | 2 | 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|---|
| 1 | O | 556/569 (98%) | 472 (85%) | 84 (15%) | 3 | 3 |
| 1 | P | 551/569 (97%) | 469 (85%) | 82 (15%) | 3 | 3 |
| 1 | Q | 548/569 (96%) | 465 (85%) | 83 (15%) | 3 | 3 |
| 1 | R | 553/569 (97%) | 467 (84%) | 86 (16%) | 2 | 3 |
| All | All | 9963/10242 (97%) | 8512 (85%) | 1451 (15%) | 3 | 3 |

All (1451) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 5 | LYS |
| 1 | A | 16 | VAL |
| 1 | A | 20 | GLU |
| 1 | A | 42 | ARG |
| 1 | A | 45 | LYS |
| 1 | A | 47 | LEU |
| 1 | A | 91 | THR |
| 1 | A | 107 | THR |
| 1 | A | 109 | ASN |
| 1 | A | 110 | SER |
| 1 | A | 117 | THR |
| 1 | A | 121 | GLU |
| 1 | A | 140 | GLU |
| 1 | A | 141 | VAL |
| 1 | A | 160 | GLU |
| 1 | A | 168 | ARG |
| 1 | A | 169 | VAL |
| 1 | A | 173 | THR |
| 1 | A | 176 | VAL |
| 1 | A | 185 | LEU |
| 1 | A | 187 | LYS |
| 1 | A | 191 | ASP |
| 1 | A | 210 | THR |
| 1 | A | 216 | VAL |
| 1 | A | 223 | THR |
| 1 | A | 245 | LYS |
| 1 | A | 253 | VAL |
| 1 | A | 263 | THR |
| 1 | A | 269 | MET |
| 1 | A | 281 | THR |
| 1 | A | 290 | LYS |
| 1 | A | 298 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 305 | VAL |
| 1 | A | 308 | LEU |
| 1 | A | 314 | VAL |
| 1 | A | 336 | VAL |
| 1 | A | 338 | LYS |
| 1 | A | 343 | SER |
| 1 | A | 349 | LEU |
| 1 | A | 355 | ARG |
| 1 | A | 363 | GLU |
| 1 | A | 385 | THR |
| 1 | A | 392 | LEU |
| 1 | A | 398 | LYS |
| 1 | A | 399 | THR |
| 1 | A | 424 | LYS |
| 1 | A | 428 | VAL |
| 1 | A | 437 | LEU |
| 1 | A | 444 | VAL |
| 1 | A | 445 | LEU |
| 1 | A | 451 | MET |
| 1 | A | 463 | LEU |
| 1 | A | 469 | LEU |
| 1 | A | 471 | MET |
| 1 | A | 476 | GLU |
| 1 | A | 478 | ARG |
| 1 | A | 479 | VAL |
| 1 | A | 485 | VAL |
| 1 | A | 486 | LEU |
| 1 | A | 497 | GLN |
| 1 | A | 523 | THR |
| 1 | A | 532 | GLN |
| 1 | A | 541 | VAL |
| 1 | A | 546 | VAL |
| 1 | A | 549 | LEU |
| 1 | A | 554 | ASP |
| 1 | A | 556 | ARG |
| 1 | A | 558 | SER |
| 1 | A | 561 | LYS |
| 1 | A | 564 | VAL |
| 1 | A | 582 | GLU |
| 1 | A | 593 | LEU |
| 1 | A | 611 | VAL |
| 1 | A | 616 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 618 | LEU |
| 1 | A | 621 | ASP |
| 1 | A | 632 | LYS |
| 1 | D | 9 | LYS |
| 1 | D | 16 | VAL |
| 1 | D | 19 | GLU |
| 1 | D | 20 | GLU |
| 1 | D | 47 | LEU |
| 1 | D | 61 | ASN |
| 1 | D | 78 | LEU |
| 1 | D | 85 | GLU |
| 1 | D | 91 | THR |
| 1 | D | 114 | ASP |
| 1 | D | 117 | THR |
| 1 | D | 140 | GLU |
| 1 | D | 141 | VAL |
| 1 | D | 160 | GLU |
| 1 | D | 162 | LEU |
| 1 | D | 168 | ARG |
| 1 | D | 169 | VAL |
| 1 | D | 173 | THR |
| 1 | D | 185 | LEU |
| 1 | D | 187 | LYS |
| 1 | D | 210 | THR |
| 1 | D | 227 | ARG |
| 1 | D | 230 | SER |
| 1 | D | 263 | THR |
| 1 | D | 269 | MET |
| 1 | D | 281 | THR |
| 1 | D | 292 | LYS |
| 1 | D | 298 | ARG |
| 1 | D | 308 | LEU |
| 1 | D | 314 | VAL |
| 1 | D | 331 | LEU |
| 1 | D | 355 | ARG |
| 1 | D | 368 | GLN |
| 1 | D | 385 | THR |
| 1 | D | 392 | LEU |
| 1 | D | 398 | LYS |
| 1 | D | 399 | THR |
| 1 | D | 428 | VAL |
| 1 | D | 437 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 438 | THR |
| 1 | D | 440 | SER |
| 1 | D | 445 | LEU |
| 1 | D | 451 | MET |
| 1 | D | 463 | LEU |
| 1 | D | 469 | LEU |
| 1 | D | 476 | GLU |
| 1 | D | 478 | ARG |
| 1 | D | 479 | VAL |
| 1 | D | 486 | LEU |
| 1 | D | 497 | GLN |
| 1 | D | 506 | VAL |
| 1 | D | 540 | ILE |
| 1 | D | 541 | VAL |
| 1 | D | 546 | VAL |
| 1 | D | 549 | LEU |
| 1 | D | 557 | VAL |
| 1 | D | 561 | LYS |
| 1 | D | 562 | CYS |
| 1 | D | 568 | ASN |
| 1 | D | 593 | LEU |
| 1 | D | 597 | SER |
| 1 | D | 611 | VAL |
| 1 | D | 618 | LEU |
| 1 | D | 622 | LYS |
| 1 | B | 16 | VAL |
| 1 | B | 19 | GLU |
| 1 | B | 31 | SER |
| 1 | B | 43 | ASN |
| 1 | B | 45 | LYS |
| 1 | B | 47 | LEU |
| 1 | B | 52 | THR |
| 1 | B | 56 | GLU |
| 1 | B | 62 | THR |
| 1 | B | 67 | HIS |
| 1 | B | 71 | ILE |
| 1 | B | 75 | THR |
| 1 | B | 78 | LEU |
| 1 | B | 84 | ARG |
| 1 | B | 88 | ASP |
| 1 | B | 101 | ASP |
| 1 | B | 107 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 108 | SER |
| 1 | B | 114 | ASP |
| 1 | B | 117 | THR |
| 1 | B | 140 | GLU |
| 1 | B | 162 | LEU |
| 1 | B | 169 | VAL |
| 1 | B | 173 | THR |
| 1 | B | 176 | VAL |
| 1 | B | 181 | VAL |
| 1 | B | 185 | LEU |
| 1 | B | 187 | LYS |
| 1 | B | 191 | ASP |
| 1 | B | 208 | SER |
| 1 | B | 210 | THR |
| 1 | B | 216 | VAL |
| 1 | B | 223 | THR |
| 1 | B | 230 | SER |
| 1 | B | 233 | ILE |
| 1 | B | 244 | GLU |
| 1 | B | 259 | HIS |
| 1 | B | 260 | SER |
| 1 | B | 263 | THR |
| 1 | B | 269 | MET |
| 1 | B | 293 | ASN |
| 1 | B | 298 | ARG |
| 1 | B | 308 | LEU |
| 1 | B | 331 | LEU |
| 1 | B | 336 | VAL |
| 1 | B | 351 | SER |
| 1 | B | 355 | ARG |
| 1 | B | 369 | LYS |
| 1 | B | 371 | LYS |
| 1 | B | 383 | VAL |
| 1 | B | 385 | THR |
| 1 | B | 428 | VAL |
| 1 | B | 436 | SER |
| 1 | B | 437 | LEU |
| 1 | B | 440 | SER |
| 1 | B | 451 | MET |
| 1 | B | 452 | SER |
| 1 | B | 463 | LEU |
| 1 | B | 469 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 476 | GLU |
| 1 | B | 479 | VAL |
| 1 | B | 480 | GLU |
| 1 | B | 497 | GLN |
| 1 | B | 503 | VAL |
| 1 | B | 505 | THR |
| 1 | B | 507 | ASN |
| 1 | B | 541 | VAL |
| 1 | B | 546 | VAL |
| 1 | B | 550 | ARG |
| 1 | B | 557 | VAL |
| 1 | B | 562 | CYS |
| 1 | B | 570 | SER |
| 1 | B | 579 | MET |
| 1 | B | 611 | VAL |
| 1 | B | 614 | PRO |
| 1 | B | 616 | THR |
| 1 | B | 627 | HIS |
| 1 | B | 629 | LEU |
| 1 | B | 640 | GLN |
| 1 | C | 16 | VAL |
| 1 | C | 20 | GLU |
| 1 | C | 24 | MET |
| 1 | C | 45 | LYS |
| 1 | C | 47 | LEU |
| 1 | C | 58 | LYS |
| 1 | C | 62 | THR |
| 1 | C | 65 | LYS |
| 1 | C | 78 | LEU |
| 1 | C | 89 | LYS |
| 1 | C | 104 | ARG |
| 1 | C | 107 | THR |
| 1 | C | 114 | ASP |
| 1 | C | 117 | THR |
| 1 | C | 123 | SER |
| 1 | C | 140 | GLU |
| 1 | C | 162 | LEU |
| 1 | C | 168 | ARG |
| 1 | C | 173 | THR |
| 1 | C | 176 | VAL |
| 1 | C | 208 | SER |
| 1 | C | 210 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 230 | SER |
| 1 | C | 253 | VAL |
| 1 | C | 260 | SER |
| 1 | C | 269 | MET |
| 1 | C | 272 | ASP |
| 1 | C | 280 | THR |
| 1 | C | 288 | LYS |
| 1 | C | 290 | LYS |
| 1 | C | 293 | ASN |
| 1 | C | 298 | ARG |
| 1 | C | 305 | VAL |
| 1 | C | 308 | LEU |
| 1 | C | 311 | LYS |
| 1 | C | 319 | THR |
| 1 | C | 326 | HIS |
| 1 | C | 330 | SER |
| 1 | C | 338 | LYS |
| 1 | C | 355 | ARG |
| 1 | C | 363 | GLU |
| 1 | C | 383 | VAL |
| 1 | C | 392 | LEU |
| 1 | C | 428 | VAL |
| 1 | C | 434 | VAL |
| 1 | C | 437 | LEU |
| 1 | C | 444 | VAL |
| 1 | C | 445 | LEU |
| 1 | C | 451 | MET |
| 1 | C | 469 | LEU |
| 1 | C | 479 | VAL |
| 1 | C | 492 | LYS |
| 1 | C | 497 | GLN |
| 1 | C | 503 | VAL |
| 1 | C | 533 | SER |
| 1 | C | 540 | ILE |
| 1 | C | 549 | LEU |
| 1 | C | 557 | VAL |
| 1 | C | 561 | LYS |
| 1 | C | 562 | CYS |
| 1 | C | 568 | ASN |
| 1 | C | 572 | SER |
| 1 | C | 579 | MET |
| 1 | C | 593 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 597 | SER |
| 1 | C | 619 | ARG |
| 1 | C | 621 | ASP |
| 1 | C | 622 | LYS |
| 1 | C | 629 | LEU |
| 1 | C | 643 | LYS |
| 1 | F | 1 | MET |
| 1 | F | 16 | VAL |
| 1 | F | 20 | GLU |
| 1 | F | 24 | MET |
| 1 | F | 45 | LYS |
| 1 | F | 47 | LEU |
| 1 | F | 62 | THR |
| 1 | F | 78 | LEU |
| 1 | F | 85 | GLU |
| 1 | F | 89 | LYS |
| 1 | F | 108 | SER |
| 1 | F | 113 | SER |
| 1 | F | 116 | ILE |
| 1 | F | 117 | THR |
| 1 | F | 133 | ARG |
| 1 | F | 140 | GLU |
| 1 | F | 162 | LEU |
| 1 | F | 169 | VAL |
| 1 | F | 173 | THR |
| 1 | F | 176 | VAL |
| 1 | F | 187 | LYS |
| 1 | F | 196 | ASN |
| 1 | F | 210 | THR |
| 1 | F | 216 | VAL |
| 1 | F | 243 | GLU |
| 1 | F | 244 | GLU |
| 1 | F | 253 | VAL |
| 1 | F | 259 | HIS |
| 1 | F | 263 | THR |
| 1 | F | 269 | MET |
| 1 | F | 275 | MET |
| 1 | F | 277 | ARG |
| 1 | F | 278 | ASN |
| 1 | F | 290 | LYS |
| 1 | F | 292 | LYS |
| 1 | F | 293 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 298 | ARG |
| 1 | F | 310 | GLU |
| 1 | F | 316 | MET |
| 1 | F | 320 | PHE |
| 1 | F | 326 | HIS |
| 1 | F | 331 | LEU |
| 1 | F | 334 | SER |
| 1 | F | 335 | ASN |
| 1 | F | 336 | VAL |
| 1 | F | 341 | SER |
| 1 | F | 349 | LEU |
| 1 | F | 352 | MET |
| 1 | F | 355 | ARG |
| 1 | F | 363 | GLU |
| 1 | F | 383 | VAL |
| 1 | F | 385 | THR |
| 1 | F | 392 | LEU |
| 1 | F | 436 | SER |
| 1 | F | 437 | LEU |
| 1 | F | 444 | VAL |
| 1 | F | 445 | LEU |
| 1 | F | 451 | MET |
| 1 | F | 463 | LEU |
| 1 | F | 469 | LEU |
| 1 | F | 476 | GLU |
| 1 | F | 478 | ARG |
| 1 | F | 479 | VAL |
| 1 | F | 486 | LEU |
| 1 | F | 494 | GLU |
| 1 | F | 497 | GLN |
| 1 | F | 503 | VAL |
| 1 | F | 533 | SER |
| 1 | F | 540 | ILE |
| 1 | F | 541 | VAL |
| 1 | F | 546 | VAL |
| 1 | F | 549 | LEU |
| 1 | F | 550 | ARG |
| 1 | F | 557 | VAL |
| 1 | F | 564 | VAL |
| 1 | F | 595 | ILE |
| 1 | F | 602 | GLU |
| 1 | F | 618 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 622 | LYS |
| 1 | F | 624 | LEU |
| 1 | F | 632 | LYS |
| 1 | F | 634 | THR |
| 1 | E | 1 | MET |
| 1 | E | 9 | LYS |
| 1 | E | 16 | VAL |
| 1 | E | 20 | GLU |
| 1 | E | 30 | ARG |
| 1 | E | 40 | PHE |
| 1 | E | 45 | LYS |
| 1 | E | 47 | LEU |
| 1 | E | 56 | GLU |
| 1 | E | 84 | ARG |
| 1 | E | 85 | GLU |
| 1 | E | 91 | THR |
| 1 | E | 93 | LEU |
| 1 | E | 104 | ARG |
| 1 | E | 107 | THR |
| 1 | E | 109 | ASN |
| 1 | E | 117 | THR |
| 1 | E | 121 | GLU |
| 1 | E | 140 | GLU |
| 1 | E | 144 | THR |
| 1 | E | 146 | LEU |
| 1 | E | 160 | GLU |
| 1 | E | 162 | LEU |
| 1 | E | 173 | THR |
| 1 | E | 176 | VAL |
| 1 | E | 181 | VAL |
| 1 | E | 185 | LEU |
| 1 | E | 187 | LYS |
| 1 | E | 199 | LYS |
| 1 | E | 208 | SER |
| 1 | E | 210 | THR |
| 1 | E | 216 | VAL |
| 1 | E | 230 | SER |
| 1 | E | 259 | HIS |
| 1 | E | 260 | SER |
| 1 | E | 269 | MET |
| 1 | E | 272 | ASP |
| 1 | E | 278 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 290 | LYS |
| 1 | E | 298 | ARG |
| 1 | E | 305 | VAL |
| 1 | E | 308 | LEU |
| 1 | E | 314 | VAL |
| 1 | E | 317 | ASN |
| 1 | E | 319 | THR |
| 1 | E | 331 | LEU |
| 1 | E | 338 | LYS |
| 1 | E | 341 | SER |
| 1 | E | 343 | SER |
| 1 | E | 349 | LEU |
| 1 | E | 355 | ARG |
| 1 | E | 363 | GLU |
| 1 | E | 371 | LYS |
| 1 | E | 379 | LYS |
| 1 | E | 383 | VAL |
| 1 | E | 385 | THR |
| 1 | E | 392 | LEU |
| 1 | E | 399 | THR |
| 1 | E | 428 | VAL |
| 1 | E | 437 | LEU |
| 1 | E | 439 | ASP |
| 1 | E | 440 | SER |
| 1 | E | 444 | VAL |
| 1 | E | 445 | LEU |
| 1 | E | 451 | MET |
| 1 | E | 452 | SER |
| 1 | E | 454 | MET |
| 1 | E | 463 | LEU |
| 1 | E | 469 | LEU |
| 1 | E | 470 | LYS |
| 1 | E | 476 | GLU |
| 1 | E | 478 | ARG |
| 1 | E | 479 | VAL |
| 1 | E | 486 | LEU |
| 1 | E | 497 | GLN |
| 1 | E | 531 | GLU |
| 1 | E | 541 | VAL |
| 1 | E | 549 | LEU |
| 1 | E | 556 | ARG |
| 1 | E | 557 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 561 | LYS |
| 1 | E | 562 | CYS |
| 1 | E | 571 | SER |
| 1 | E | 577 | MET |
| 1 | E | 587 | ASN |
| 1 | E | 593 | LEU |
| 1 | E | 616 | THR |
| 1 | E | 618 | LEU |
| 1 | E | 621 | ASP |
| 1 | E | 623 | SER |
| 1 | E | 632 | LYS |
| 1 | E | 643 | LYS |
| 1 | G | 1 | MET |
| 1 | G | 16 | VAL |
| 1 | G | 26 | GLN |
| 1 | G | 30 | ARG |
| 1 | G | 45 | LYS |
| 1 | G | 47 | LEU |
| 1 | G | 67 | HIS |
| 1 | G | 78 | LEU |
| 1 | G | 84 | ARG |
| 1 | G | 85 | GLU |
| 1 | G | 117 | THR |
| 1 | G | 122 | ARG |
| 1 | G | 127 | SER |
| 1 | G | 128 | GLN |
| 1 | G | 140 | GLU |
| 1 | G | 172 | SER |
| 1 | G | 176 | VAL |
| 1 | G | 181 | VAL |
| 1 | G | 185 | LEU |
| 1 | G | 191 | ASP |
| 1 | G | 199 | LYS |
| 1 | G | 200 | ASP |
| 1 | G | 206 | ARG |
| 1 | G | 210 | THR |
| 1 | G | 214 | PHE |
| 1 | G | 216 | VAL |
| 1 | G | 230 | SER |
| 1 | G | 243 | GLU |
| 1 | G | 253 | VAL |
| 1 | G | 260 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 261 | SER |
| 1 | G | 263 | THR |
| 1 | G | 269 | MET |
| 1 | G | 277 | ARG |
| 1 | G | 294 | ASN |
| 1 | G | 298 | ARG |
| 1 | G | 305 | VAL |
| 1 | G | 308 | LEU |
| 1 | G | 314 | VAL |
| 1 | G | 319 | THR |
| 1 | G | 336 | VAL |
| 1 | G | 339 | ASP |
| 1 | G | 341 | SER |
| 1 | G | 351 | SER |
| 1 | G | 355 | ARG |
| 1 | G | 371 | LYS |
| 1 | G | 383 | VAL |
| 1 | G | 385 | THR |
| 1 | G | 392 | LEU |
| 1 | G | 399 | THR |
| 1 | G | 424 | LYS |
| 1 | G | 428 | VAL |
| 1 | G | 433 | LYS |
| 1 | G | 437 | LEU |
| 1 | G | 444 | VAL |
| 1 | G | 451 | MET |
| 1 | G | 463 | LEU |
| 1 | G | 469 | LEU |
| 1 | G | 486 | LEU |
| 1 | G | 492 | LYS |
| 1 | G | 497 | GLN |
| 1 | G | 511 | LEU |
| 1 | G | 512 | SER |
| 1 | G | 533 | SER |
| 1 | G | 540 | ILE |
| 1 | G | 541 | VAL |
| 1 | G | 546 | VAL |
| 1 | G | 549 | LEU |
| 1 | G | 557 | VAL |
| 1 | G | 562 | CYS |
| 1 | G | 564 | VAL |
| 1 | G | 570 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 577 | MET |
| 1 | G | 587 | ASN |
| 1 | G | 593 | LEU |
| 1 | G | 597 | SER |
| 1 | G | 611 | VAL |
| 1 | G | 616 | THR |
| 1 | G | 629 | LEU |
| 1 | H | 1 | MET |
| 1 | H | 9 | LYS |
| 1 | H | 16 | VAL |
| 1 | H | 20 | GLU |
| 1 | H | 26 | GLN |
| 1 | H | 45 | LYS |
| 1 | H | 47 | LEU |
| 1 | H | 78 | LEU |
| 1 | H | 85 | GLU |
| 1 | H | 110 | SER |
| 1 | H | 114 | ASP |
| 1 | H | 117 | THR |
| 1 | H | 140 | GLU |
| 1 | H | 141 | VAL |
| 1 | H | 173 | THR |
| 1 | H | 181 | VAL |
| 1 | H | 185 | LEU |
| 1 | H | 210 | THR |
| 1 | H | 216 | VAL |
| 1 | H | 243 | GLU |
| 1 | H | 244 | GLU |
| 1 | H | 253 | VAL |
| 1 | H | 260 | SER |
| 1 | H | 263 | THR |
| 1 | H | 269 | MET |
| 1 | H | 281 | THR |
| 1 | H | 290 | LYS |
| 1 | H | 292 | LYS |
| 1 | H | 293 | ASN |
| 1 | H | 298 | ARG |
| 1 | H | 305 | VAL |
| 1 | H | 308 | LEU |
| 1 | H | 319 | THR |
| 1 | H | 336 | VAL |
| 1 | H | 338 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 339 | ASP |
| 1 | H | 341 | SER |
| 1 | H | 351 | SER |
| 1 | H | 355 | ARG |
| 1 | H | 378 | SER |
| 1 | H | 385 | THR |
| 1 | H | 392 | LEU |
| 1 | H | 398 | LYS |
| 1 | H | 411 | ARG |
| 1 | H | 428 | VAL |
| 1 | H | 437 | LEU |
| 1 | H | 444 | VAL |
| 1 | H | 445 | LEU |
| 1 | H | 452 | SER |
| 1 | H | 463 | LEU |
| 1 | H | 469 | LEU |
| 1 | H | 475 | ASP |
| 1 | H | 478 | ARG |
| 1 | H | 479 | VAL |
| 1 | H | 485 | VAL |
| 1 | H | 486 | LEU |
| 1 | H | 490 | PRO |
| 1 | H | 497 | GLN |
| 1 | H | 541 | VAL |
| 1 | H | 546 | VAL |
| 1 | H | 549 | LEU |
| 1 | H | 556 | ARG |
| 1 | H | 562 | CYS |
| 1 | H | 564 | VAL |
| 1 | H | 570 | SER |
| 1 | H | 593 | LEU |
| 1 | H | 611 | VAL |
| 1 | H | 616 | THR |
| 1 | H | 618 | LEU |
| 1 | H | 621 | ASP |
| 1 | H | 632 | LYS |
| 1 | H | 643 | LYS |
| 1 | H | 644 | SER |
| 1 | I | 16 | VAL |
| 1 | I | 19 | GLU |
| 1 | I | 30 | ARG |
| 1 | I | 31 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 47 | LEU |
| 1 | I | 53 | THR |
| 1 | I | 56 | GLU |
| 1 | I | 63 | ASP |
| 1 | I | 78 | LEU |
| 1 | I | 85 | GLU |
| 1 | I | 97 | LYS |
| 1 | I | 104 | ARG |
| 1 | I | 114 | ASP |
| 1 | I | 115 | LYS |
| 1 | I | 117 | THR |
| 1 | I | 140 | GLU |
| 1 | I | 162 | LEU |
| 1 | I | 167 | CYS |
| 1 | I | 168 | ARG |
| 1 | I | 169 | VAL |
| 1 | I | 172 | SER |
| 1 | I | 173 | THR |
| 1 | I | 176 | VAL |
| 1 | I | 185 | LEU |
| 1 | I | 191 | ASP |
| 1 | I | 210 | THR |
| 1 | I | 243 | GLU |
| 1 | I | 261 | SER |
| 1 | I | 269 | MET |
| 1 | I | 277 | ARG |
| 1 | I | 278 | ASN |
| 1 | I | 280 | THR |
| 1 | I | 287 | PRO |
| 1 | I | 290 | LYS |
| 1 | I | 293 | ASN |
| 1 | I | 298 | ARG |
| 1 | I | 308 | LEU |
| 1 | I | 314 | VAL |
| 1 | I | 316 | MET |
| 1 | I | 325 | ASN |
| 1 | I | 331 | LEU |
| 1 | I | 336 | VAL |
| 1 | I | 351 | SER |
| 1 | I | 355 | ARG |
| 1 | I | 368 | GLN |
| 1 | I | 369 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 383 | VAL |
| 1 | I | 385 | THR |
| 1 | I | 392 | LEU |
| 1 | I | 398 | LYS |
| 1 | I | 399 | THR |
| 1 | I | 424 | LYS |
| 1 | I | 428 | VAL |
| 1 | I | 437 | LEU |
| 1 | I | 438 | THR |
| 1 | I | 445 | LEU |
| 1 | I | 451 | MET |
| 1 | I | 463 | LEU |
| 1 | I | 469 | LEU |
| 1 | I | 476 | GLU |
| 1 | I | 478 | ARG |
| 1 | I | 479 | VAL |
| 1 | I | 486 | LEU |
| 1 | I | 497 | GLN |
| 1 | I | 541 | VAL |
| 1 | I | 546 | VAL |
| 1 | I | 549 | LEU |
| 1 | I | 550 | ARG |
| 1 | I | 554 | ASP |
| 1 | I | 556 | ARG |
| 1 | I | 557 | VAL |
| 1 | I | 561 | LYS |
| 1 | I | 564 | VAL |
| 1 | I | 568 | ASN |
| 1 | I | 572 | SER |
| 1 | I | 579 | MET |
| 1 | I | 587 | ASN |
| 1 | I | 593 | LEU |
| 1 | I | 597 | SER |
| 1 | I | 618 | LEU |
| 1 | I | 624 | LEU |
| 1 | M | 30 | ARG |
| 1 | M | 37 | ILE |
| 1 | M | 43 | ASN |
| 1 | M | 45 | LYS |
| 1 | M | 52 | THR |
| 1 | M | 56 | GLU |
| 1 | M | 65 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 97 | LYS |
| 1 | M | 106 | ILE |
| 1 | M | 117 | THR |
| 1 | M | 119 | ILE |
| 1 | M | 124 | THR |
| 1 | M | 126 | VAL |
| 1 | M | 140 | GLU |
| 1 | M | 162 | LEU |
| 1 | M | 169 | VAL |
| 1 | M | 173 | THR |
| 1 | M | 175 | ASN |
| 1 | M | 178 | ILE |
| 1 | M | 185 | LEU |
| 1 | M | 191 | ASP |
| 1 | M | 194 | ARG |
| 1 | M | 199 | LYS |
| 1 | M | 200 | ASP |
| 1 | M | 206 | ARG |
| 1 | M | 210 | THR |
| 1 | M | 216 | VAL |
| 1 | M | 225 | GLU |
| 1 | M | 237 | LYS |
| 1 | M | 253 | VAL |
| 1 | M | 263 | THR |
| 1 | M | 268 | LEU |
| 1 | M | 269 | MET |
| 1 | M | 275 | MET |
| 1 | M | 281 | THR |
| 1 | M | 298 | ARG |
| 1 | M | 305 | VAL |
| 1 | M | 308 | LEU |
| 1 | M | 317 | ASN |
| 1 | M | 319 | THR |
| 1 | M | 326 | HIS |
| 1 | M | 338 | LYS |
| 1 | M | 351 | SER |
| 1 | M | 352 | MET |
| 1 | M | 355 | ARG |
| 1 | M | 369 | LYS |
| 1 | M | 371 | LYS |
| 1 | M | 383 | VAL |
| 1 | M | 385 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 399 | THR |
| 1 | M | 401 | LYS |
| 1 | M | 411 | ARG |
| 1 | M | 437 | LEU |
| 1 | M | 438 | THR |
| 1 | M | 439 | ASP |
| 1 | M | 444 | VAL |
| 1 | M | 445 | LEU |
| 1 | M | 451 | MET |
| 1 | M | 452 | SER |
| 1 | M | 478 | ARG |
| 1 | M | 479 | VAL |
| 1 | M | 483 | MET |
| 1 | M | 485 | VAL |
| 1 | M | 486 | LEU |
| 1 | M | 497 | GLN |
| 1 | M | 507 | ASN |
| 1 | M | 533 | SER |
| 1 | M | 540 | ILE |
| 1 | M | 542 | LYS |
| 1 | M | 547 | GLU |
| 1 | M | 549 | LEU |
| 1 | M | 554 | ASP |
| 1 | M | 562 | CYS |
| 1 | M | 568 | ASN |
| 1 | M | 579 | MET |
| 1 | M | 592 | LEU |
| 1 | M | 593 | LEU |
| 1 | M | 611 | VAL |
| 1 | M | 618 | LEU |
| 1 | M | 622 | LYS |
| 1 | N | 5 | LYS |
| 1 | N | 6 | ILE |
| 1 | N | 9 | LYS |
| 1 | N | 20 | GLU |
| 1 | N | 30 | ARG |
| 1 | N | 31 | SER |
| 1 | N | 47 | LEU |
| 1 | N | 58 | LYS |
| 1 | N | 62 | THR |
| 1 | N | 66 | VAL |
| 1 | N | 75 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 78 | LEU |
| 1 | N | 84 | ARG |
| 1 | N | 97 | LYS |
| 1 | N | 101 | ASP |
| 1 | N | 107 | THR |
| 1 | N | 108 | SER |
| 1 | N | 133 | ARG |
| 1 | N | 140 | GLU |
| 1 | N | 160 | GLU |
| 1 | N | 167 | CYS |
| 1 | N | 168 | ARG |
| 1 | N | 169 | VAL |
| 1 | N | 185 | LEU |
| 1 | N | 191 | ASP |
| 1 | N | 194 | ARG |
| 1 | N | 200 | ASP |
| 1 | N | 202 | GLU |
| 1 | N | 204 | LEU |
| 1 | N | 210 | THR |
| 1 | N | 214 | PHE |
| 1 | N | 237 | LYS |
| 1 | N | 244 | GLU |
| 1 | N | 245 | LYS |
| 1 | N | 253 | VAL |
| 1 | N | 259 | HIS |
| 1 | N | 269 | MET |
| 1 | N | 272 | ASP |
| 1 | N | 278 | ASN |
| 1 | N | 281 | THR |
| 1 | N | 294 | ASN |
| 1 | N | 298 | ARG |
| 1 | N | 305 | VAL |
| 1 | N | 308 | LEU |
| 1 | N | 313 | LYS |
| 1 | N | 314 | VAL |
| 1 | N | 317 | ASN |
| 1 | N | 325 | ASN |
| 1 | N | 331 | LEU |
| 1 | N | 336 | VAL |
| 1 | N | 341 | SER |
| 1 | N | 343 | SER |
| 1 | N | 349 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 355 | ARG |
| 1 | N | 357 | THR |
| 1 | N | 363 | GLU |
| 1 | N | 371 | LYS |
| 1 | N | 383 | VAL |
| 1 | N | 385 | THR |
| 1 | N | 392 | LEU |
| 1 | N | 398 | LYS |
| 1 | N | 424 | LYS |
| 1 | N | 428 | VAL |
| 1 | N | 434 | VAL |
| 1 | N | 435 | THR |
| 1 | N | 436 | SER |
| 1 | N | 437 | LEU |
| 1 | N | 444 | VAL |
| 1 | N | 445 | LEU |
| 1 | N | 451 | MET |
| 1 | N | 454 | MET |
| 1 | N | 463 | LEU |
| 1 | N | 469 | LEU |
| 1 | N | 471 | MET |
| 1 | N | 475 | ASP |
| 1 | N | 476 | GLU |
| 1 | N | 478 | ARG |
| 1 | N | 479 | VAL |
| 1 | N | 486 | LEU |
| 1 | N | 492 | LYS |
| 1 | N | 494 | GLU |
| 1 | N | 497 | GLN |
| 1 | N | 540 | ILE |
| 1 | N | 541 | VAL |
| 1 | N | 546 | VAL |
| 1 | N | 549 | LEU |
| 1 | N | 553 | ILE |
| 1 | N | 557 | VAL |
| 1 | N | 564 | VAL |
| 1 | N | 593 | LEU |
| 1 | N | 597 | SER |
| 1 | N | 611 | VAL |
| 1 | N | 616 | THR |
| 1 | N | 618 | LEU |
| 1 | N | 621 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 629 | LEU |
| 1 | N | 632 | LYS |
| 1 | N | 633 | SER |
| 1 | O | 1 | MET |
| 1 | O | 9 | LYS |
| 1 | O | 16 | VAL |
| 1 | O | 19 | GLU |
| 1 | O | 45 | LYS |
| 1 | O | 47 | LEU |
| 1 | O | 78 | LEU |
| 1 | O | 85 | GLU |
| 1 | O | 109 | ASN |
| 1 | O | 114 | ASP |
| 1 | O | 117 | THR |
| 1 | O | 120 | SER |
| 1 | O | 127 | SER |
| 1 | O | 128 | GLN |
| 1 | O | 140 | GLU |
| 1 | O | 141 | VAL |
| 1 | O | 156 | LYS |
| 1 | O | 162 | LEU |
| 1 | O | 169 | VAL |
| 1 | O | 176 | VAL |
| 1 | O | 185 | LEU |
| 1 | O | 187 | LYS |
| 1 | O | 191 | ASP |
| 1 | O | 206 | ARG |
| 1 | O | 210 | THR |
| 1 | O | 216 | VAL |
| 1 | O | 221 | MET |
| 1 | O | 223 | THR |
| 1 | O | 230 | SER |
| 1 | O | 233 | ILE |
| 1 | O | 269 | MET |
| 1 | O | 275 | MET |
| 1 | O | 281 | THR |
| 1 | O | 288 | LYS |
| 1 | O | 292 | LYS |
| 1 | O | 298 | ARG |
| 1 | O | 305 | VAL |
| 1 | O | 308 | LEU |
| 1 | O | 310 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 313 | LYS |
| 1 | O | 317 | ASN |
| 1 | O | 319 | THR |
| 1 | O | 338 | LYS |
| 1 | O | 355 | ARG |
| 1 | O | 375 | ASP |
| 1 | O | 377 | LEU |
| 1 | O | 382 | HIS |
| 1 | O | 385 | THR |
| 1 | O | 399 | THR |
| 1 | O | 401 | LYS |
| 1 | O | 420 | ILE |
| 1 | O | 426 | THR |
| 1 | O | 436 | SER |
| 1 | O | 438 | THR |
| 1 | O | 445 | LEU |
| 1 | O | 451 | MET |
| 1 | O | 463 | LEU |
| 1 | O | 472 | MET |
| 1 | O | 478 | ARG |
| 1 | O | 486 | LEU |
| 1 | O | 487 | LYS |
| 1 | O | 497 | GLN |
| 1 | O | 501 | SER |
| 1 | O | 528 | ILE |
| 1 | O | 541 | VAL |
| 1 | O | 544 | ASP |
| 1 | O | 546 | VAL |
| 1 | O | 549 | LEU |
| 1 | O | 550 | ARG |
| 1 | O | 556 | ARG |
| 1 | O | 558 | SER |
| 1 | O | 559 | SER |
| 1 | O | 563 | VAL |
| 1 | O | 567 | ASP |
| 1 | O | 577 | MET |
| 1 | O | 579 | MET |
| 1 | O | 587 | ASN |
| 1 | O | 588 | LEU |
| 1 | O | 597 | SER |
| 1 | O | 602 | GLU |
| 1 | O | 621 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | O | 623 | SER |
| 1 | O | 624 | LEU |
| 1 | O | 643 | LYS |
| 1 | P | 16 | VAL |
| 1 | P | 45 | LYS |
| 1 | P | 47 | LEU |
| 1 | P | 58 | LYS |
| 1 | P | 93 | LEU |
| 1 | P | 104 | ARG |
| 1 | P | 106 | ILE |
| 1 | P | 108 | SER |
| 1 | P | 112 | TRP |
| 1 | P | 115 | LYS |
| 1 | P | 117 | THR |
| 1 | P | 123 | SER |
| 1 | P | 133 | ARG |
| 1 | P | 138 | VAL |
| 1 | P | 140 | GLU |
| 1 | P | 156 | LYS |
| 1 | P | 160 | GLU |
| 1 | P | 169 | VAL |
| 1 | P | 173 | THR |
| 1 | P | 176 | VAL |
| 1 | P | 181 | VAL |
| 1 | P | 187 | LYS |
| 1 | P | 200 | ASP |
| 1 | P | 210 | THR |
| 1 | P | 216 | VAL |
| 1 | P | 243 | GLU |
| 1 | P | 249 | ASP |
| 1 | P | 253 | VAL |
| 1 | P | 263 | THR |
| 1 | P | 269 | MET |
| 1 | P | 275 | MET |
| 1 | P | 290 | LYS |
| 1 | P | 292 | LYS |
| 1 | P | 298 | ARG |
| 1 | P | 305 | VAL |
| 1 | P | 308 | LEU |
| 1 | P | 314 | VAL |
| 1 | P | 316 | MET |
| 1 | P | 317 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 318 | GLN |
| 1 | P | 319 | THR |
| 1 | P | 349 | LEU |
| 1 | P | 351 | SER |
| 1 | P | 352 | MET |
| 1 | P | 355 | ARG |
| 1 | P | 369 | LYS |
| 1 | P | 383 | VAL |
| 1 | P | 392 | LEU |
| 1 | P | 398 | LYS |
| 1 | P | 399 | THR |
| 1 | P | 433 | LYS |
| 1 | P | 436 | SER |
| 1 | P | 437 | LEU |
| 1 | P | 440 | SER |
| 1 | P | 444 | VAL |
| 1 | P | 445 | LEU |
| 1 | P | 451 | MET |
| 1 | P | 452 | SER |
| 1 | P | 463 | LEU |
| 1 | P | 469 | LEU |
| 1 | P | 470 | LYS |
| 1 | P | 476 | GLU |
| 1 | P | 478 | ARG |
| 1 | P | 497 | GLN |
| 1 | P | 505 | THR |
| 1 | P | 506 | VAL |
| 1 | P | 540 | ILE |
| 1 | P | 549 | LEU |
| 1 | P | 550 | ARG |
| 1 | P | 556 | ARG |
| 1 | P | 562 | CYS |
| 1 | P | 564 | VAL |
| 1 | P | 565 | ASN |
| 1 | P | 570 | SER |
| 1 | P | 593 | LEU |
| 1 | P | 611 | VAL |
| 1 | P | 618 | LEU |
| 1 | P | 621 | ASP |
| 1 | P | 632 | LYS |
| 1 | P | 640 | GLN |
| 1 | P | 643 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 644 | SER |
| 1 | Q | 16 | VAL |
| 1 | Q | 30 | ARG |
| 1 | Q | 47 | LEU |
| 1 | Q | 56 | GLU |
| 1 | Q | 59 | HIS |
| 1 | Q | 78 | LEU |
| 1 | Q | 90 | VAL |
| 1 | Q | 112 | TRP |
| 1 | Q | 117 | THR |
| 1 | Q | 119 | ILE |
| 1 | Q | 122 | ARG |
| 1 | Q | 140 | GLU |
| 1 | Q | 153 | ARG |
| 1 | Q | 156 | LYS |
| 1 | Q | 160 | GLU |
| 1 | Q | 167 | CYS |
| 1 | Q | 168 | ARG |
| 1 | Q | 178 | ILE |
| 1 | Q | 191 | ASP |
| 1 | Q | 210 | THR |
| 1 | Q | 231 | GLU |
| 1 | Q | 233 | ILE |
| 1 | Q | 247 | ILE |
| 1 | Q | 259 | HIS |
| 1 | Q | 264 | ILE |
| 1 | Q | 269 | MET |
| 1 | Q | 273 | ILE |
| 1 | Q | 275 | MET |
| 1 | Q | 277 | ARG |
| 1 | Q | 290 | LYS |
| 1 | Q | 293 | ASN |
| 1 | Q | 294 | ASN |
| 1 | Q | 298 | ARG |
| 1 | Q | 305 | VAL |
| 1 | Q | 316 | MET |
| 1 | Q | 317 | ASN |
| 1 | Q | 318 | GLN |
| 1 | Q | 319 | THR |
| 1 | Q | 322 | ILE |
| 1 | Q | 325 | ASN |
| 1 | Q | 330 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Q | 334 | SER |
| 1 | Q | 338 | LYS |
| 1 | Q | 339 | ASP |
| 1 | Q | 340 | LYS |
| 1 | Q | 349 | LEU |
| 1 | Q | 351 | SER |
| 1 | Q | 355 | ARG |
| 1 | Q | 368 | GLN |
| 1 | Q | 379 | LYS |
| 1 | Q | 383 | VAL |
| 1 | Q | 392 | LEU |
| 1 | Q | 410 | GLU |
| 1 | Q | 420 | ILE |
| 1 | Q | 428 | VAL |
| 1 | Q | 437 | LEU |
| 1 | Q | 444 | VAL |
| 1 | Q | 451 | MET |
| 1 | Q | 469 | LEU |
| 1 | Q | 476 | GLU |
| 1 | Q | 478 | ARG |
| 1 | Q | 479 | VAL |
| 1 | Q | 480 | GLU |
| 1 | Q | 486 | LEU |
| 1 | Q | 497 | GLN |
| 1 | Q | 531 | GLU |
| 1 | Q | 533 | SER |
| 1 | Q | 540 | ILE |
| 1 | Q | 541 | VAL |
| 1 | Q | 546 | VAL |
| 1 | Q | 549 | LEU |
| 1 | Q | 554 | ASP |
| 1 | Q | 556 | ARG |
| 1 | Q | 563 | VAL |
| 1 | Q | 564 | VAL |
| 1 | Q | 571 | SER |
| 1 | Q | 588 | LEU |
| 1 | Q | 593 | LEU |
| 1 | Q | 611 | VAL |
| 1 | Q | 615 | ILE |
| 1 | Q | 618 | LEU |
| 1 | Q | 625 | CYS |
| 1 | Q | 632 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | R | 1 | MET |
| 1 | R | 5 | LYS |
| 1 | R | 13 | ARG |
| 1 | R | 19 | GLU |
| 1 | R | 44 | ASP |
| 1 | R | 45 | LYS |
| 1 | R | 47 | LEU |
| 1 | R | 51 | LYS |
| 1 | R | 53 | THR |
| 1 | R | 58 | LYS |
| 1 | R | 59 | HIS |
| 1 | R | 63 | ASP |
| 1 | R | 65 | LYS |
| 1 | R | 67 | HIS |
| 1 | R | 69 | LEU |
| 1 | R | 78 | LEU |
| 1 | R | 93 | LEU |
| 1 | R | 109 | ASN |
| 1 | R | 114 | ASP |
| 1 | R | 115 | LYS |
| 1 | R | 116 | ILE |
| 1 | R | 117 | THR |
| 1 | R | 124 | THR |
| 1 | R | 140 | GLU |
| 1 | R | 146 | LEU |
| 1 | R | 160 | GLU |
| 1 | R | 169 | VAL |
| 1 | R | 172 | SER |
| 1 | R | 176 | VAL |
| 1 | R | 178 | ILE |
| 1 | R | 185 | LEU |
| 1 | R | 191 | ASP |
| 1 | R | 199 | LYS |
| 1 | R | 206 | ARG |
| 1 | R | 210 | THR |
| 1 | R | 222 | LYS |
| 1 | R | 233 | ILE |
| 1 | R | 244 | GLU |
| 1 | R | 251 | SER |
| 1 | R | 253 | VAL |
| 1 | R | 269 | MET |
| 1 | R | 292 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | R | 293 | ASN |
| 1 | R | 294 | ASN |
| 1 | R | 298 | ARG |
| 1 | R | 305 | VAL |
| 1 | R | 308 | LEU |
| 1 | R | 315 | GLU |
| 1 | R | 317 | ASN |
| 1 | R | 331 | LEU |
| 1 | R | 335 | ASN |
| 1 | R | 349 | LEU |
| 1 | R | 355 | ARG |
| 1 | R | 364 | MET |
| 1 | R | 371 | LYS |
| 1 | R | 375 | ASP |
| 1 | R | 383 | VAL |
| 1 | R | 385 | THR |
| 1 | R | 392 | LEU |
| 1 | R | 398 | LYS |
| 1 | R | 401 | LYS |
| 1 | R | 420 | ILE |
| 1 | R | 433 | LYS |
| 1 | R | 437 | LEU |
| 1 | R | 451 | MET |
| 1 | R | 469 | LEU |
| 1 | R | 476 | GLU |
| 1 | R | 486 | LEU |
| 1 | R | 497 | GLN |
| 1 | R | 503 | VAL |
| 1 | R | 528 | ILE |
| 1 | R | 546 | VAL |
| 1 | R | 549 | LEU |
| 1 | R | 553 | ILE |
| 1 | R | 556 | ARG |
| 1 | R | 560 | GLN |
| 1 | R | 564 | VAL |
| 1 | R | 579 | MET |
| 1 | R | 615 | ILE |
| 1 | R | 616 | THR |
| 1 | R | 621 | ASP |
| 1 | R | 622 | LYS |
| 1 | R | 624 | LEU |
| 1 | R | 625 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | R | 638 | ASN |
| 1 | R | 643 | LYS |
| 1 | J | 5 | LYS |
| 1 | J | 9 | LYS |
| 1 | J | 16 | VAL |
| 1 | J | 45 | LYS |
| 1 | J | 47 | LEU |
| 1 | J | 60 | GLU |
| 1 | J | 62 | THR |
| 1 | J | 78 | LEU |
| 1 | J | 91 | THR |
| 1 | J | 107 | THR |
| 1 | J | 108 | SER |
| 1 | J | 115 | LYS |
| 1 | J | 132 | SER |
| 1 | J | 140 | GLU |
| 1 | J | 141 | VAL |
| 1 | J | 173 | THR |
| 1 | J | 176 | VAL |
| 1 | J | 181 | VAL |
| 1 | J | 185 | LEU |
| 1 | J | 191 | ASP |
| 1 | J | 199 | LYS |
| 1 | J | 210 | THR |
| 1 | J | 216 | VAL |
| 1 | J | 221 | MET |
| 1 | J | 222 | LYS |
| 1 | J | 230 | SER |
| 1 | J | 244 | GLU |
| 1 | J | 251 | SER |
| 1 | J | 260 | SER |
| 1 | J | 261 | SER |
| 1 | J | 263 | THR |
| 1 | J | 269 | MET |
| 1 | J | 280 | THR |
| 1 | J | 281 | THR |
| 1 | J | 288 | LYS |
| 1 | J | 298 | ARG |
| 1 | J | 308 | LEU |
| 1 | J | 311 | LYS |
| 1 | J | 319 | THR |
| 1 | J | 338 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 339 | ASP |
| 1 | J | 351 | SER |
| 1 | J | 355 | ARG |
| 1 | J | 379 | LYS |
| 1 | J | 383 | VAL |
| 1 | J | 385 | THR |
| 1 | J | 398 | LYS |
| 1 | J | 399 | THR |
| 1 | J | 428 | VAL |
| 1 | J | 437 | LEU |
| 1 | J | 439 | ASP |
| 1 | J | 445 | LEU |
| 1 | J | 451 | MET |
| 1 | J | 461 | ARG |
| 1 | J | 469 | LEU |
| 1 | J | 476 | GLU |
| 1 | J | 478 | ARG |
| 1 | J | 485 | VAL |
| 1 | J | 486 | LEU |
| 1 | J | 492 | LYS |
| 1 | J | 497 | GLN |
| 1 | J | 509 | PHE |
| 1 | J | 540 | ILE |
| 1 | J | 541 | VAL |
| 1 | J | 557 | VAL |
| 1 | J | 558 | SER |
| 1 | J | 577 | MET |
| 1 | J | 582 | GLU |
| 1 | J | 593 | LEU |
| 1 | J | 611 | VAL |
| 1 | J | 616 | THR |
| 1 | J | 618 | LEU |
| 1 | J | 625 | CYS |
| 1 | J | 629 | LEU |
| 1 | J | 632 | LYS |
| 1 | J | 638 | ASN |
| 1 | K | 3 | LEU |
| 1 | K | 15 | TRP |
| 1 | K | 24 | MET |
| 1 | K | 31 | SER |
| 1 | K | 45 | LYS |
| 1 | K | 47 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 60 | GLU |
| 1 | K | 65 | LYS |
| 1 | K | 66 | VAL |
| 1 | K | 91 | THR |
| 1 | K | 107 | THR |
| 1 | K | 112 | TRP |
| 1 | K | 140 | GLU |
| 1 | K | 141 | VAL |
| 1 | K | 156 | LYS |
| 1 | K | 160 | GLU |
| 1 | K | 162 | LEU |
| 1 | K | 169 | VAL |
| 1 | K | 176 | VAL |
| 1 | K | 181 | VAL |
| 1 | K | 185 | LEU |
| 1 | K | 191 | ASP |
| 1 | K | 210 | THR |
| 1 | K | 216 | VAL |
| 1 | K | 223 | THR |
| 1 | K | 225 | GLU |
| 1 | K | 227 | ARG |
| 1 | K | 243 | GLU |
| 1 | K | 244 | GLU |
| 1 | K | 253 | VAL |
| 1 | K | 257 | VAL |
| 1 | K | 259 | HIS |
| 1 | K | 263 | THR |
| 1 | K | 268 | LEU |
| 1 | K | 269 | MET |
| 1 | K | 273 | ILE |
| 1 | K | 281 | THR |
| 1 | K | 290 | LYS |
| 1 | K | 292 | LYS |
| 1 | K | 298 | ARG |
| 1 | K | 305 | VAL |
| 1 | K | 308 | LEU |
| 1 | K | 311 | LYS |
| 1 | K | 312 | LYS |
| 1 | K | 314 | VAL |
| 1 | K | 319 | THR |
| 1 | K | 321 | GLU |
| 1 | K | 322 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 331 | LEU |
| 1 | K | 341 | SER |
| 1 | K | 355 | ARG |
| 1 | K | 363 | GLU |
| 1 | K | 364 | MET |
| 1 | K | 366 | GLU |
| 1 | K | 383 | VAL |
| 1 | K | 385 | THR |
| 1 | K | 392 | LEU |
| 1 | K | 399 | THR |
| 1 | K | 401 | LYS |
| 1 | K | 424 | LYS |
| 1 | K | 428 | VAL |
| 1 | K | 437 | LEU |
| 1 | K | 444 | VAL |
| 1 | K | 445 | LEU |
| 1 | K | 451 | MET |
| 1 | K | 469 | LEU |
| 1 | K | 471 | MET |
| 1 | K | 475 | ASP |
| 1 | K | 479 | VAL |
| 1 | K | 486 | LEU |
| 1 | K | 497 | GLN |
| 1 | K | 503 | VAL |
| 1 | K | 506 | VAL |
| 1 | K | 532 | GLN |
| 1 | K | 544 | ASP |
| 1 | K | 546 | VAL |
| 1 | K | 556 | ARG |
| 1 | K | 558 | SER |
| 1 | K | 562 | CYS |
| 1 | K | 564 | VAL |
| 1 | K | 567 | ASP |
| 1 | K | 577 | MET |
| 1 | K | 579 | MET |
| 1 | K | 589 | SER |
| 1 | K | 593 | LEU |
| 1 | K | 596 | SER |
| 1 | K | 597 | SER |
| 1 | K | 621 | ASP |
| 1 | K | 624 | LEU |
| 1 | K | 632 | LYS |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | K | 643 | LYS |
| 1 | L | 47 | LEU |
| 1 | L | 60 | GLU |
| 1 | L | 62 | THR |
| 1 | L | 78 | LEU |
| 1 | L | 85 | GLU |
| 1 | L | 91 | THR |
| 1 | L | 107 | THR |
| 1 | L | 113 | SER |
| 1 | L | 114 | ASP |
| 1 | L | 117 | THR |
| 1 | L | 124 | THR |
| 1 | L | 128 | GLN |
| 1 | L | 129 | ILE |
| 1 | L | 140 | GLU |
| 1 | L | 141 | VAL |
| 1 | L | 162 | LEU |
| 1 | L | 168 | ARG |
| 1 | L | 169 | VAL |
| 1 | L | 173 | THR |
| 1 | L | 181 | VAL |
| 1 | L | 185 | LEU |
| 1 | L | 193 | PRO |
| 1 | L | 210 | THR |
| 1 | L | 216 | VAL |
| 1 | L | 221 | MET |
| 1 | L | 223 | THR |
| 1 | L | 225 | GLU |
| 1 | L | 228 | GLU |
| 1 | L | 260 | SER |
| 1 | L | 263 | THR |
| 1 | L | 269 | MET |
| 1 | L | 281 | THR |
| 1 | L | 290 | LYS |
| 1 | L | 298 | ARG |
| 1 | L | 305 | VAL |
| 1 | L | 308 | LEU |
| 1 | L | 316 | MET |
| 1 | L | 317 | ASN |
| 1 | L | 319 | THR |
| 1 | L | 331 | LEU |
| 1 | L | 349 | LEU |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 355 | ARG |
| 1 | L | 369 | LYS |
| 1 | L | 385 | THR |
| 1 | L | 392 | LEU |
| 1 | L | 399 | THR |
| 1 | L | 428 | VAL |
| 1 | L | 433 | LYS |
| 1 | L | 437 | LEU |
| 1 | L | 440 | SER |
| 1 | L | 444 | VAL |
| 1 | L | 445 | LEU |
| 1 | L | 451 | MET |
| 1 | L | 452 | SER |
| 1 | L | 463 | LEU |
| 1 | L | 469 | LEU |
| 1 | L | 476 | GLU |
| 1 | L | 479 | VAL |
| 1 | L | 485 | VAL |
| 1 | L | 486 | LEU |
| 1 | L | 497 | GLN |
| 1 | L | 503 | VAL |
| 1 | L | 541 | VAL |
| 1 | L | 549 | LEU |
| 1 | L | 556 | ARG |
| 1 | L | 557 | VAL |
| 1 | L | 562 | CYS |
| 1 | L | 564 | VAL |
| 1 | L | 593 | LEU |
| 1 | L | 611 | VAL |
| 1 | L | 616 | THR |
| 1 | L | 618 | LEU |
| 1 | L | 624 | LEU |
| 1 | L | 633 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (309) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 43 | ASN |
| 1 | A | 67 | HIS |
| 1 | A | 109 | ASN |
| 1 | A | 175 | ASN |
| 1 | A | 242 | HIS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 259 | HIS |
| 1 | A | 294 | ASN |
| 1 | A | 303 | GLN |
| 1 | A | 335 | ASN |
| 1 | A | 362 | ASN |
| 1 | A | 459 | HIS |
| 1 | A | 482 | HIS |
| 1 | A | 497 | GLN |
| 1 | A | 498 | ASN |
| 1 | A | 507 | ASN |
| 1 | A | 587 | ASN |
| 1 | D | 43 | ASN |
| 1 | D | 67 | HIS |
| 1 | D | 175 | ASN |
| 1 | D | 190 | ASN |
| 1 | D | 242 | HIS |
| 1 | D | 259 | HIS |
| 1 | D | 293 | ASN |
| 1 | D | 303 | GLN |
| 1 | D | 335 | ASN |
| 1 | D | 362 | ASN |
| 1 | D | 459 | HIS |
| 1 | D | 482 | HIS |
| 1 | D | 497 | GLN |
| 1 | D | 507 | ASN |
| 1 | D | 560 | GLN |
| 1 | D | 565 | ASN |
| 1 | B | 175 | ASN |
| 1 | B | 190 | ASN |
| 1 | B | 242 | HIS |
| 1 | B | 259 | HIS |
| 1 | B | 291 | ASN |
| 1 | B | 294 | ASN |
| 1 | B | 303 | GLN |
| 1 | B | 335 | ASN |
| 1 | B | 362 | ASN |
| 1 | B | 455 | ASN |
| 1 | B | 459 | HIS |
| 1 | B | 482 | HIS |
| 1 | B | 497 | GLN |
| 1 | B | 498 | ASN |
| 1 | B | 507 | ASN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 560 | GLN |
| 1 | C | 43 | ASN |
| 1 | C | 59 | HIS |
| 1 | C | 61 | ASN |
| 1 | C | 67 | HIS |
| 1 | C | 109 | ASN |
| 1 | C | 190 | ASN |
| 1 | C | 242 | HIS |
| 1 | C | 259 | HIS |
| 1 | C | 294 | ASN |
| 1 | C | 303 | GLN |
| 1 | C | 335 | ASN |
| 1 | C | 362 | ASN |
| 1 | C | 459 | HIS |
| 1 | C | 482 | HIS |
| 1 | C | 497 | GLN |
| 1 | C | 498 | ASN |
| 1 | C | 507 | ASN |
| 1 | C | 560 | GLN |
| 1 | C | 568 | ASN |
| 1 | F | 43 | ASN |
| 1 | F | 61 | ASN |
| 1 | F | 242 | HIS |
| 1 | F | 259 | HIS |
| 1 | F | 278 | ASN |
| 1 | F | 303 | GLN |
| 1 | F | 362 | ASN |
| 1 | F | 368 | GLN |
| 1 | F | 455 | ASN |
| 1 | F | 459 | HIS |
| 1 | F | 482 | HIS |
| 1 | F | 497 | GLN |
| 1 | F | 507 | ASN |
| 1 | F | 565 | ASN |
| 1 | F | 587 | ASN |
| 1 | F | 620 | ASN |
| 1 | E | 43 | ASN |
| 1 | E | 67 | HIS |
| 1 | E | 109 | ASN |
| 1 | E | 175 | ASN |
| 1 | E | 259 | HIS |
| 1 | E | 278 | ASN |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 303 | GLN |
| 1 | E | 317 | ASN |
| 1 | E | 335 | ASN |
| 1 | E | 362 | ASN |
| 1 | E | 459 | HIS |
| 1 | E | 482 | HIS |
| 1 | E | 497 | GLN |
| 1 | E | 507 | ASN |
| 1 | E | 560 | GLN |
| 1 | E | 587 | ASN |
| 1 | E | 638 | ASN |
| 1 | G | 43 | ASN |
| 1 | G | 67 | HIS |
| 1 | G | 109 | ASN |
| 1 | G | 190 | ASN |
| 1 | G | 259 | HIS |
| 1 | G | 293 | ASN |
| 1 | G | 294 | ASN |
| 1 | G | 300 | HIS |
| 1 | G | 303 | GLN |
| 1 | G | 335 | ASN |
| 1 | G | 362 | ASN |
| 1 | G | 459 | HIS |
| 1 | G | 482 | HIS |
| 1 | G | 497 | GLN |
| 1 | G | 560 | GLN |
| 1 | G | 587 | ASN |
| 1 | H | 26 | GLN |
| 1 | H | 43 | ASN |
| 1 | H | 67 | HIS |
| 1 | H | 109 | ASN |
| 1 | H | 175 | ASN |
| 1 | H | 190 | ASN |
| 1 | H | 224 | HIS |
| 1 | H | 294 | ASN |
| 1 | H | 303 | GLN |
| 1 | H | 335 | ASN |
| 1 | H | 362 | ASN |
| 1 | H | 459 | HIS |
| 1 | H | 482 | HIS |
| 1 | H | 497 | GLN |
| 1 | H | 507 | ASN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 26 | GLN |
| 1 | I | 43 | ASN |
| 1 | I | 67 | HIS |
| 1 | I | 190 | ASN |
| 1 | I | 242 | HIS |
| 1 | I | 259 | HIS |
| 1 | I | 278 | ASN |
| 1 | I | 294 | ASN |
| 1 | I | 300 | HIS |
| 1 | I | 303 | GLN |
| 1 | I | 335 | ASN |
| 1 | I | 362 | ASN |
| 1 | I | 459 | HIS |
| 1 | I | 482 | HIS |
| 1 | I | 497 | GLN |
| 1 | I | 498 | ASN |
| 1 | I | 507 | ASN |
| 1 | I | 560 | GLN |
| 1 | I | 568 | ASN |
| 1 | I | 587 | ASN |
| 1 | I | 640 | GLN |
| 1 | M | 43 | ASN |
| 1 | M | 67 | HIS |
| 1 | M | 109 | ASN |
| 1 | M | 175 | ASN |
| 1 | M | 190 | ASN |
| 1 | M | 259 | HIS |
| 1 | M | 278 | ASN |
| 1 | M | 303 | GLN |
| 1 | M | 335 | ASN |
| 1 | M | 362 | ASN |
| 1 | M | 459 | HIS |
| 1 | M | 482 | HIS |
| 1 | M | 497 | GLN |
| 1 | M | 507 | ASN |
| 1 | M | 560 | GLN |
| 1 | M | 568 | ASN |
| 1 | N | 26 | GLN |
| 1 | N | 43 | ASN |
| 1 | N | 175 | ASN |
| 1 | N | 190 | ASN |
| 1 | N | 259 | HIS |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | N | 291 | ASN |
| 1 | N | 293 | ASN |
| 1 | N | 294 | ASN |
| 1 | N | 303 | GLN |
| 1 | N | 335 | ASN |
| 1 | N | 362 | ASN |
| 1 | N | 459 | HIS |
| 1 | N | 482 | HIS |
| 1 | N | 497 | GLN |
| 1 | N | 498 | ASN |
| 1 | N | 507 | ASN |
| 1 | N | 560 | GLN |
| 1 | N | 565 | ASN |
| 1 | O | 43 | ASN |
| 1 | O | 67 | HIS |
| 1 | O | 109 | ASN |
| 1 | O | 175 | ASN |
| 1 | O | 190 | ASN |
| 1 | O | 303 | GLN |
| 1 | O | 335 | ASN |
| 1 | O | 362 | ASN |
| 1 | O | 459 | HIS |
| 1 | O | 497 | GLN |
| 1 | O | 498 | ASN |
| 1 | O | 507 | ASN |
| 1 | O | 560 | GLN |
| 1 | O | 565 | ASN |
| 1 | O | 587 | ASN |
| 1 | O | 620 | ASN |
| 1 | O | 638 | ASN |
| 1 | O | 640 | GLN |
| 1 | P | 43 | ASN |
| 1 | P | 67 | HIS |
| 1 | P | 175 | ASN |
| 1 | P | 190 | ASN |
| 1 | P | 259 | HIS |
| 1 | P | 294 | ASN |
| 1 | P | 303 | GLN |
| 1 | P | 317 | ASN |
| 1 | P | 362 | ASN |
| 1 | P | 459 | HIS |
| 1 | P | 482 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 497 | GLN |
| 1 | P | 498 | ASN |
| 1 | P | 507 | ASN |
| 1 | P | 560 | GLN |
| 1 | P | 565 | ASN |
| 1 | P | 587 | ASN |
| 1 | P | 640 | GLN |
| 1 | Q | 43 | ASN |
| 1 | Q | 67 | HIS |
| 1 | Q | 175 | ASN |
| 1 | Q | 190 | ASN |
| 1 | Q | 196 | ASN |
| 1 | Q | 224 | HIS |
| 1 | Q | 242 | HIS |
| 1 | Q | 259 | HIS |
| 1 | Q | 291 | ASN |
| 1 | Q | 293 | ASN |
| 1 | Q | 300 | HIS |
| 1 | Q | 303 | GLN |
| 1 | Q | 335 | ASN |
| 1 | Q | 362 | ASN |
| 1 | Q | 455 | ASN |
| 1 | Q | 459 | HIS |
| 1 | Q | 482 | HIS |
| 1 | Q | 497 | GLN |
| 1 | Q | 498 | ASN |
| 1 | Q | 532 | GLN |
| 1 | Q | 560 | GLN |
| 1 | Q | 568 | ASN |
| 1 | R | 43 | ASN |
| 1 | R | 61 | ASN |
| 1 | R | 109 | ASN |
| 1 | R | 175 | ASN |
| 1 | R | 190 | ASN |
| 1 | R | 224 | HIS |
| 1 | R | 242 | HIS |
| 1 | R | 259 | HIS |
| 1 | R | 293 | ASN |
| 1 | R | 294 | ASN |
| 1 | R | 300 | HIS |
| 1 | R | 303 | GLN |
| 1 | R | 362 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | R | 459 | HIS |
| 1 | R | 482 | HIS |
| 1 | R | 497 | GLN |
| 1 | R | 498 | ASN |
| 1 | R | 560 | GLN |
| 1 | R | 638 | ASN |
| 1 | J | 43 | ASN |
| 1 | J | 67 | HIS |
| 1 | J | 175 | ASN |
| 1 | J | 190 | ASN |
| 1 | J | 242 | HIS |
| 1 | J | 300 | HIS |
| 1 | J | 303 | GLN |
| 1 | J | 362 | ASN |
| 1 | J | 459 | HIS |
| 1 | J | 482 | HIS |
| 1 | J | 497 | GLN |
| 1 | J | 498 | ASN |
| 1 | J | 627 | HIS |
| 1 | K | 43 | ASN |
| 1 | K | 67 | HIS |
| 1 | K | 190 | ASN |
| 1 | K | 259 | HIS |
| 1 | K | 294 | ASN |
| 1 | K | 303 | GLN |
| 1 | K | 335 | ASN |
| 1 | K | 362 | ASN |
| 1 | K | 459 | HIS |
| 1 | K | 482 | HIS |
| 1 | K | 497 | GLN |
| 1 | K | 498 | ASN |
| 1 | K | 532 | GLN |
| 1 | K | 560 | GLN |
| 1 | K | 587 | ASN |
| 1 | L | 26 | GLN |
| 1 | L | 43 | ASN |
| 1 | L | 61 | ASN |
| 1 | L | 67 | HIS |
| 1 | L | 175 | ASN |
| 1 | L | 190 | ASN |
| 1 | L | 242 | HIS |
| 1 | L | 259 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 294 | ASN |
| 1 | L | 303 | GLN |
| 1 | L | 317 | ASN |
| 1 | L | 335 | ASN |
| 1 | L | 362 | ASN |
| 1 | L | 459 | HIS |
| 1 | L | 482 | HIS |
| 1 | L | 497 | GLN |
| 1 | L | 507 | ASN |
| 1 | L | 560 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

36 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 | $\# Z > 2$ |
| 3 | PO4 | O | 702 | - | 4,4,4 | 0.81 | 0 | 6,6,6 | 0.39 | 0 |
| 3 | PO4 | N | 702 | - | 4,4,4 | 0.96 | 0 | 6,6,6 | 0.71 | 0 |
| 2 | SAH | O | 701 | - | 21,28,28 | 1.16 | 3 (14%) | 20,40,40 | 1.64 | 5 (25%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | SAH | N | 701 | - | 21,28,28 | 1.25 | 3 (14%) | 20,40,40 | 1.71 | 5 (25%) |
| 2 | SAH | P | 701 | - | 21,28,28 | 1.21 | 2 (9%) | 20,40,40 | 1.68 | 6 (30%) |
| 2 | SAH | Q | 701 | - | 21,28,28 | 1.03 | 1 (4%) | 20,40,40 | 1.57 | 4 (20%) |
| 2 | SAH | C | 701 | - | 21,28,28 | 1.19 | 1 (4%) | 20,40,40 | 1.43 | 5 (25%) |
| 3 | PO4 | F | 702 | - | 4,4,4 | 0.99 | 0 | 6,6,6 | 1.39 | 1 (16%) |
| 2 | SAH | D | 701 | - | 21,28,28 | 1.24 | 3 (14%) | 20,40,40 | 1.64 | 5 (25%) |
| 2 | SAH | F | 701 | - | 21,28,28 | 1.06 | 2 (9%) | 20,40,40 | 1.55 | 4 (20%) |
| 3 | PO4 | P | 702 | - | 4,4,4 | 0.87 | 0 | 6,6,6 | 0.98 | 0 |
| 3 | PO4 | C | 702 | - | 4,4,4 | 0.74 | 0 | 6,6,6 | 1.15 | 1 (16%) |
| 3 | PO4 | A | 702 | - | 4,4,4 | 0.67 | 0 | 6,6,6 | 1.31 | 1 (16%) |
| 2 | SAH | L | 701 | - | 21,28,28 | 1.38 | 3 (14%) | 20,40,40 | 1.89 | 8 (40%) |
| 3 | PO4 | G | 702 | - | 4,4,4 | 1.05 | 0 | 6,6,6 | 0.97 | 0 |
| 3 | PO4 | H | 702 | - | 4,4,4 | 0.69 | 0 | 6,6,6 | 1.47 | 1 (16%) |
| 3 | PO4 | L | 702 | - | 4,4,4 | 1.07 | 0 | 6,6,6 | 0.89 | 0 |
| 3 | PO4 | D | 702 | - | 4,4,4 | 1.04 | 0 | 6,6,6 | 1.69 | 2 (33%) |
| 3 | PO4 | K | 702 | - | 4,4,4 | 0.93 | 0 | 6,6,6 | 0.60 | 0 |
| 2 | SAH | B | 701 | - | 21,28,28 | 0.99 | 1 (4%) | 20,40,40 | 1.54 | 4 (20%) |
| 3 | PO4 | I | 702 | - | 4,4,4 | 1.13 | 0 | 6,6,6 | 1.46 | 2 (33%) |
| 2 | SAH | G | 701 | - | 21,28,28 | 1.26 | 3 (14%) | 20,40,40 | 1.61 | 4 (20%) |
| 3 | PO4 | M | 702 | - | 4,4,4 | 0.76 | 0 | 6,6,6 | 0.80 | 0 |
| 2 | SAH | H | 701 | - | 21,28,28 | 1.42 | 4 (19%) | 20,40,40 | 1.66 | 4 (20%) |
| 2 | SAH | K | 701 | - | 21,28,28 | 1.24 | 2 (9%) | 20,40,40 | 1.65 | 5 (25%) |
| 2 | SAH | E | 701 | - | 21,28,28 | 1.11 | 1 (4%) | 20,40,40 | 1.75 | 6 (30%) |
| 2 | SAH | I | 701 | - | 21,28,28 | 1.21 | 3 (14%) | 20,40,40 | 2.15 | 8 (40%) |
| 3 | PO4 | E | 702 | - | 4,4,4 | 0.66 | 0 | 6,6,6 | 0.91 | 0 |
| 3 | PO4 | J | 702 | - | 4,4,4 | 1.02 | 0 | 6,6,6 | 0.76 | 0 |
| 3 | PO4 | Q | 702 | - | 4,4,4 | 0.96 | 0 | 6,6,6 | 0.55 | 0 |
| 2 | SAH | A | 701 | - | 21,28,28 | 1.30 | 3 (14%) | 20,40,40 | 1.62 | 5 (25%) |
| 2 | SAH | J | 701 | - | 21,28,28 | 0.96 | 2 (9%) | 20,40,40 | 1.58 | 5 (25%) |
| 3 | PO4 | R | 702 | - | 4,4,4 | 0.68 | 0 | 6,6,6 | 0.78 | 0 |
| 2 | SAH | R | 701 | - | 21,28,28 | 1.02 | 1 (4%) | 20,40,40 | 1.55 | 4 (20%) |
| 2 | SAH | M | 701 | - | 21,28,28 | 1.56 | 5 (23%) | 20,40,40 | 1.81 | 6 (30%) |
| 3 | PO4 | B | 702 | - | 4,4,4 | 0.82 | 0 | 6,6,6 | 1.08 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2 | SAH | B | 701 | - | - | 1/7/31/31 | 0/3/3/3 |
| 2 | SAH | D | 701 | - | - | 0/7/31/31 | 0/3/3/3 |
| 2 | SAH | G | 701 | - | - | 2/7/31/31 | 0/3/3/3 |
| 2 | SAH | F | 701 | - | - | 2/7/31/31 | 0/3/3/3 |
| 2 | SAH | A | 701 | - | - | 0/7/31/31 | 0/3/3/3 |
| 2 | SAH | H | 701 | - | - | 2/7/31/31 | 0/3/3/3 |
| 2 | SAH | K | 701 | - | - | 0/7/31/31 | 0/3/3/3 |
| 2 | SAH | J | 701 | - | - | 1/7/31/31 | 0/3/3/3 |
| 2 | SAH | E | 701 | - | - | 0/7/31/31 | 0/3/3/3 |
| 2 | SAH | L | 701 | - | - | 2/7/31/31 | 0/3/3/3 |
| 2 | SAH | O | 701 | - | - | 0/7/31/31 | 0/3/3/3 |
| 2 | SAH | N | 701 | - | - | 3/7/31/31 | 0/3/3/3 |
| 2 | SAH | I | 701 | - | - | 0/7/31/31 | 0/3/3/3 |
| 2 | SAH | P | 701 | - | - | 2/7/31/31 | 0/3/3/3 |
| 2 | SAH | R | 701 | - | - | 2/7/31/31 | 0/3/3/3 |
| 2 | SAH | M | 701 | - | - | 3/7/31/31 | 0/3/3/3 |
| 2 | SAH | Q | 701 | - | - | 2/7/31/31 | 0/3/3/3 |
| 2 | SAH | C | 701 | - | - | 1/7/31/31 | 0/3/3/3 |

All (43) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | H | 701 | SAH | C2-N3 | 3.85 | 1.38 | 1.32 |
| 2 | L | 701 | SAH | O4'-C1' | 3.83 | 1.46 | 1.41 |
| 2 | C | 701 | SAH | O4'-C1' | 3.74 | 1.46 | 1.41 |
| 2 | K | 701 | SAH | C2'-C1' | -3.40 | 1.48 | 1.53 |
| 2 | M | 701 | SAH | C4-N3 | 3.17 | 1.40 | 1.35 |
| 2 | N | 701 | SAH | O4'-C1' | 3.13 | 1.45 | 1.41 |
| 2 | M | 701 | SAH | O4'-C1' | 3.11 | 1.45 | 1.41 |
| 2 | M | 701 | SAH | C5-C4 | 2.95 | 1.48 | 1.40 |
| 2 | P | 701 | SAH | C5-C4 | 2.86 | 1.48 | 1.40 |
| 2 | M | 701 | SAH | C2-N3 | 2.77 | 1.36 | 1.32 |
| 2 | I | 701 | SAH | C2'-C1' | -2.77 | 1.49 | 1.53 |
| 2 | G | 701 | SAH | C5-C4 | 2.72 | 1.48 | 1.40 |
| 2 | L | 701 | SAH | C5-C4 | 2.66 | 1.48 | 1.40 |
| 2 | A | 701 | SAH | C5-C4 | 2.65 | 1.47 | 1.40 |
| 2 | N | 701 | SAH | C4-N3 | 2.62 | 1.39 | 1.35 |
| 2 | K | 701 | SAH | O4'-C1' | 2.58 | 1.44 | 1.41 |
| 2 | R | 701 | SAH | C5-C4 | 2.55 | 1.47 | 1.40 |
| 2 | O | 701 | SAH | O4'-C1' | 2.51 | 1.44 | 1.41 |
| 2 | H | 701 | SAH | C2'-C1' | -2.48 | 1.50 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | D | 701 | SAH | C5-C4 | 2.44 | 1.47 | 1.40 |
| 2 | F | 701 | SAH | C2-N3 | 2.42 | 1.36 | 1.32 |
| 2 | A | 701 | SAH | C2'-C1' | -2.39 | 1.50 | 1.53 |
| 2 | E | 701 | SAH | C5-C4 | 2.38 | 1.47 | 1.40 |
| 2 | D | 701 | SAH | C2-N3 | 2.34 | 1.35 | 1.32 |
| 2 | H | 701 | SAH | C5-C4 | 2.34 | 1.47 | 1.40 |
| 2 | G | 701 | SAH | C2'-C1' | -2.31 | 1.50 | 1.53 |
| 2 | B | 701 | SAH | C5-C4 | 2.29 | 1.47 | 1.40 |
| 2 | L | 701 | SAH | C2'-C1' | -2.27 | 1.50 | 1.53 |
| 2 | J | 701 | SAH | C5-C4 | 2.27 | 1.46 | 1.40 |
| 2 | N | 701 | SAH | C5-C4 | 2.25 | 1.46 | 1.40 |
| 2 | O | 701 | SAH | C5-C4 | 2.20 | 1.46 | 1.40 |
| 2 | I | 701 | SAH | C5-C4 | 2.17 | 1.46 | 1.40 |
| 2 | Q | 701 | SAH | C5-C4 | 2.15 | 1.46 | 1.40 |
| 2 | I | 701 | SAH | O4'-C4' | -2.15 | 1.40 | 1.45 |
| 2 | D | 701 | SAH | C2'-C1' | -2.14 | 1.50 | 1.53 |
| 2 | F | 701 | SAH | O4'-C1' | 2.07 | 1.44 | 1.41 |
| 2 | P | 701 | SAH | C2-N3 | 2.05 | 1.35 | 1.32 |
| 2 | H | 701 | SAH | O4'-C4' | -2.04 | 1.40 | 1.45 |
| 2 | M | 701 | SAH | C2-N1 | 2.03 | 1.37 | 1.33 |
| 2 | O | 701 | SAH | C2-N3 | 2.03 | 1.35 | 1.32 |
| 2 | G | 701 | SAH | O4'-C1' | 2.01 | 1.43 | 1.41 |
| 2 | A | 701 | SAH | C2-N3 | 2.01 | 1.35 | 1.32 |
| 2 | J | 701 | SAH | O4'-C1' | 2.00 | 1.43 | 1.41 |

All (101) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | N | 701 | SAH | N3-C2-N1 | -4.37 | 121.85 | 128.68 |
| 2 | I | 701 | SAH | N3-C2-N1 | -4.34 | 121.90 | 128.68 |
| 2 | I | 701 | SAH | C1'-N9-C4 | -4.22 | 119.23 | 126.64 |
| 2 | L | 701 | SAH | N3-C2-N1 | -4.04 | 122.36 | 128.68 |
| 2 | O | 701 | SAH | N3-C2-N1 | -4.00 | 122.42 | 128.68 |
| 2 | M | 701 | SAH | N3-C2-N1 | -3.86 | 122.64 | 128.68 |
| 2 | Q | 701 | SAH | N3-C2-N1 | -3.79 | 122.75 | 128.68 |
| 2 | M | 701 | SAH | N6-C6-N1 | 3.72 | 126.30 | 118.57 |
| 2 | H | 701 | SAH | N3-C2-N1 | -3.71 | 122.88 | 128.68 |
| 2 | R | 701 | SAH | N3-C2-N1 | -3.71 | 122.88 | 128.68 |
| 2 | F | 701 | SAH | N3-C2-N1 | -3.69 | 122.92 | 128.68 |
| 2 | E | 701 | SAH | N3-C2-N1 | -3.64 | 123.00 | 128.68 |
| 2 | P | 701 | SAH | N3-C2-N1 | -3.59 | 123.06 | 128.68 |
| 2 | K | 701 | SAH | N3-C2-N1 | -3.49 | 123.22 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | G | 701 | SAH | N3-C2-N1 | -3.48 | 123.24 | 128.68 |
| 2 | D | 701 | SAH | O4'-C1'-C2' | -3.42 | 101.93 | 106.93 |
| 2 | B | 701 | SAH | N3-C2-N1 | -3.40 | 123.36 | 128.68 |
| 2 | C | 701 | SAH | N3-C2-N1 | -3.38 | 123.39 | 128.68 |
| 2 | P | 701 | SAH | C1'-N9-C4 | -3.35 | 120.75 | 126.64 |
| 2 | A | 701 | SAH | N3-C2-N1 | -3.27 | 123.57 | 128.68 |
| 2 | K | 701 | SAH | C1'-N9-C4 | -3.25 | 120.92 | 126.64 |
| 2 | A | 701 | SAH | O3'-C3'-C4' | -3.14 | 101.96 | 111.05 |
| 2 | G | 701 | SAH | C4-C5-N7 | -3.09 | 106.18 | 109.40 |
| 2 | E | 701 | SAH | C3'-C2'-C1' | 3.06 | 105.59 | 100.98 |
| 2 | L | 701 | SAH | C4-C5-N7 | -2.99 | 106.28 | 109.40 |
| 2 | I | 701 | SAH | CB-CG-SD | -2.97 | 106.64 | 113.31 |
| 2 | L | 701 | SAH | O2'-C2'-C1' | -2.96 | 99.93 | 110.85 |
| 2 | I | 701 | SAH | C2'-C3'-C4' | 2.95 | 108.38 | 102.64 |
| 2 | O | 701 | SAH | C2'-C3'-C4' | 2.94 | 108.36 | 102.64 |
| 2 | I | 701 | SAH | C4-C5-N7 | -2.94 | 106.34 | 109.40 |
| 2 | D | 701 | SAH | CB-CG-SD | -2.94 | 106.72 | 113.31 |
| 3 | H | 702 | PO4 | O4-P-O2 | 2.93 | 117.39 | 107.97 |
| 2 | J | 701 | SAH | N3-C2-N1 | -2.91 | 124.13 | 128.68 |
| 2 | D | 701 | SAH | O3'-C3'-C4' | -2.87 | 102.76 | 111.05 |
| 2 | H | 701 | SAH | O4'-C1'-C2' | -2.86 | 102.75 | 106.93 |
| 2 | G | 701 | SAH | CB-CG-SD | -2.82 | 106.99 | 113.31 |
| 2 | E | 701 | SAH | C4'-C5'-SD | -2.73 | 103.99 | 113.78 |
| 2 | N | 701 | SAH | C2-N1-C6 | 2.67 | 123.33 | 118.75 |
| 2 | I | 701 | SAH | O3'-C3'-C4' | -2.67 | 103.33 | 111.05 |
| 2 | D | 701 | SAH | N3-C2-N1 | -2.65 | 124.54 | 128.68 |
| 2 | L | 701 | SAH | C1'-N9-C4 | -2.64 | 122.01 | 126.64 |
| 2 | L | 701 | SAH | CB-CG-SD | -2.62 | 107.42 | 113.31 |
| 2 | J | 701 | SAH | O3'-C3'-C4' | -2.62 | 103.47 | 111.05 |
| 2 | B | 701 | SAH | O3'-C3'-C2' | -2.61 | 103.38 | 111.82 |
| 3 | D | 702 | PO4 | O4-P-O3 | 2.60 | 116.31 | 107.97 |
| 2 | J | 701 | SAH | C1'-N9-C4 | -2.59 | 122.08 | 126.64 |
| 2 | L | 701 | SAH | O3'-C3'-C4' | -2.58 | 103.60 | 111.05 |
| 2 | F | 701 | SAH | C2'-C3'-C4' | 2.57 | 107.63 | 102.64 |
| 2 | E | 701 | SAH | O3'-C3'-C4' | -2.56 | 103.65 | 111.05 |
| 2 | F | 701 | SAH | C1'-N9-C4 | -2.55 | 122.16 | 126.64 |
| 2 | B | 701 | SAH | C2'-C3'-C4' | 2.54 | 107.58 | 102.64 |
| 2 | N | 701 | SAH | N6-C6-N1 | 2.54 | 123.84 | 118.57 |
| 2 | H | 701 | SAH | CB-CG-SD | -2.52 | 107.66 | 113.31 |
| 2 | C | 701 | SAH | C4-C5-N7 | -2.51 | 106.79 | 109.40 |
| 2 | N | 701 | SAH | C1'-N9-C4 | -2.48 | 122.29 | 126.64 |
| 3 | A | 702 | PO4 | O4-P-O3 | 2.48 | 115.91 | 107.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | C | 701 | SAH | O3'-C3'-C4' | -2.47 | 103.91 | 111.05 |
| 2 | I | 701 | SAH | C2-N1-C6 | 2.46 | 122.97 | 118.75 |
| 2 | M | 701 | SAH | O4'-C1'-C2' | -2.45 | 103.34 | 106.93 |
| 2 | R | 701 | SAH | C2-N1-C6 | 2.45 | 122.95 | 118.75 |
| 3 | D | 702 | PO4 | O3-P-O1 | -2.44 | 101.97 | 110.89 |
| 2 | G | 701 | SAH | C2-N1-C6 | 2.43 | 122.92 | 118.75 |
| 2 | A | 701 | SAH | C1'-N9-C4 | -2.43 | 122.36 | 126.64 |
| 2 | P | 701 | SAH | C2'-C3'-C4' | 2.42 | 107.34 | 102.64 |
| 2 | H | 701 | SAH | C4-C5-N7 | -2.42 | 106.88 | 109.40 |
| 2 | J | 701 | SAH | C2'-C3'-C4' | 2.40 | 107.31 | 102.64 |
| 2 | M | 701 | SAH | C3'-C2'-C1' | 2.40 | 104.59 | 100.98 |
| 2 | P | 701 | SAH | C4-C5-N7 | -2.39 | 106.90 | 109.40 |
| 2 | M | 701 | SAH | C2-N1-C6 | 2.39 | 122.85 | 118.75 |
| 2 | L | 701 | SAH | O4'-C1'-C2' | -2.39 | 103.44 | 106.93 |
| 2 | B | 701 | SAH | C4-C5-N7 | -2.38 | 106.92 | 109.40 |
| 2 | M | 701 | SAH | C5-C6-N6 | -2.36 | 116.77 | 120.35 |
| 2 | E | 701 | SAH | C1'-N9-C4 | -2.34 | 122.52 | 126.64 |
| 2 | E | 701 | SAH | C4-C5-N7 | -2.34 | 106.96 | 109.40 |
| 2 | A | 701 | SAH | C2'-C3'-C4' | 2.33 | 107.18 | 102.64 |
| 2 | K | 701 | SAH | N6-C6-N1 | 2.31 | 123.37 | 118.57 |
| 2 | C | 701 | SAH | O4'-C1'-C2' | -2.29 | 103.58 | 106.93 |
| 2 | I | 701 | SAH | C5'-SD-CG | -2.27 | 95.46 | 102.27 |
| 2 | R | 701 | SAH | CB-CG-SD | -2.26 | 108.24 | 113.31 |
| 2 | K | 701 | SAH | C2-N1-C6 | 2.25 | 122.60 | 118.75 |
| 2 | P | 701 | SAH | O3'-C3'-C4' | -2.24 | 104.57 | 111.05 |
| 2 | Q | 701 | SAH | N6-C6-N1 | 2.23 | 123.20 | 118.57 |
| 2 | K | 701 | SAH | C2'-C3'-C4' | 2.21 | 106.93 | 102.64 |
| 2 | P | 701 | SAH | C2-N1-C6 | 2.19 | 122.51 | 118.75 |
| 3 | I | 702 | PO4 | O4-P-O1 | 2.19 | 118.92 | 110.89 |
| 2 | J | 701 | SAH | C4-C5-N7 | -2.18 | 107.12 | 109.40 |
| 2 | O | 701 | SAH | N6-C6-N1 | 2.18 | 123.11 | 118.57 |
| 2 | O | 701 | SAH | CB-CG-SD | -2.17 | 108.44 | 113.31 |
| 2 | Q | 701 | SAH | C3'-C2'-C1' | 2.16 | 104.24 | 100.98 |
| 2 | A | 701 | SAH | C2-N1-C6 | 2.16 | 122.44 | 118.75 |
| 3 | F | 702 | PO4 | O4-P-O2 | 2.14 | 114.83 | 107.97 |
| 2 | Q | 701 | SAH | CB-CG-SD | -2.13 | 108.53 | 113.31 |
| 2 | N | 701 | SAH | CB-CG-SD | -2.13 | 108.54 | 113.31 |
| 3 | I | 702 | PO4 | O2-P-O1 | -2.07 | 103.32 | 110.89 |
| 2 | O | 701 | SAH | C1'-N9-C4 | -2.07 | 123.01 | 126.64 |
| 2 | D | 701 | SAH | C4-C5-N7 | -2.06 | 107.25 | 109.40 |
| 2 | C | 701 | SAH | C2'-C3'-C4' | 2.05 | 106.63 | 102.64 |
| 2 | L | 701 | SAH | C2-N1-C6 | 2.05 | 122.26 | 118.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | F | 701 | SAH | C4-C5-N7 | -2.04 | 107.28 | 109.40 |
| 2 | R | 701 | SAH | C4-C5-N7 | -2.03 | 107.28 | 109.40 |
| 3 | C | 702 | PO4 | O4-P-O2 | 2.01 | 114.41 | 107.97 |

There are no chirality outliers.

All (23) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 2 | N | 701 | SAH | O4'-C4'-C5'-SD |
| 2 | N | 701 | SAH | C3'-C4'-C5'-SD |
| 2 | P | 701 | SAH | O4'-C4'-C5'-SD |
| 2 | P | 701 | SAH | C3'-C4'-C5'-SD |
| 2 | Q | 701 | SAH | O4'-C4'-C5'-SD |
| 2 | Q | 701 | SAH | C3'-C4'-C5'-SD |
| 2 | F | 701 | SAH | O4'-C4'-C5'-SD |
| 2 | G | 701 | SAH | O4'-C4'-C5'-SD |
| 2 | G | 701 | SAH | C3'-C4'-C5'-SD |
| 2 | R | 701 | SAH | O4'-C4'-C5'-SD |
| 2 | R | 701 | SAH | C3'-C4'-C5'-SD |
| 2 | H | 701 | SAH | N-CA-CB-CG |
| 2 | F | 701 | SAH | C3'-C4'-C5'-SD |
| 2 | L | 701 | SAH | C3'-C4'-C5'-SD |
| 2 | L | 701 | SAH | O4'-C4'-C5'-SD |
| 2 | M | 701 | SAH | O4'-C4'-C5'-SD |
| 2 | H | 701 | SAH | CB-CG-SD-C5' |
| 2 | J | 701 | SAH | CB-CG-SD-C5' |
| 2 | M | 701 | SAH | N-CA-CB-CG |
| 2 | C | 701 | SAH | C3'-C4'-C5'-SD |
| 2 | B | 701 | SAH | C3'-C4'-C5'-SD |
| 2 | M | 701 | SAH | C3'-C4'-C5'-SD |
| 2 | N | 701 | SAH | CB-CG-SD-C5' |

There are no ring outliers.

15 monomers are involved in 25 short contacts:

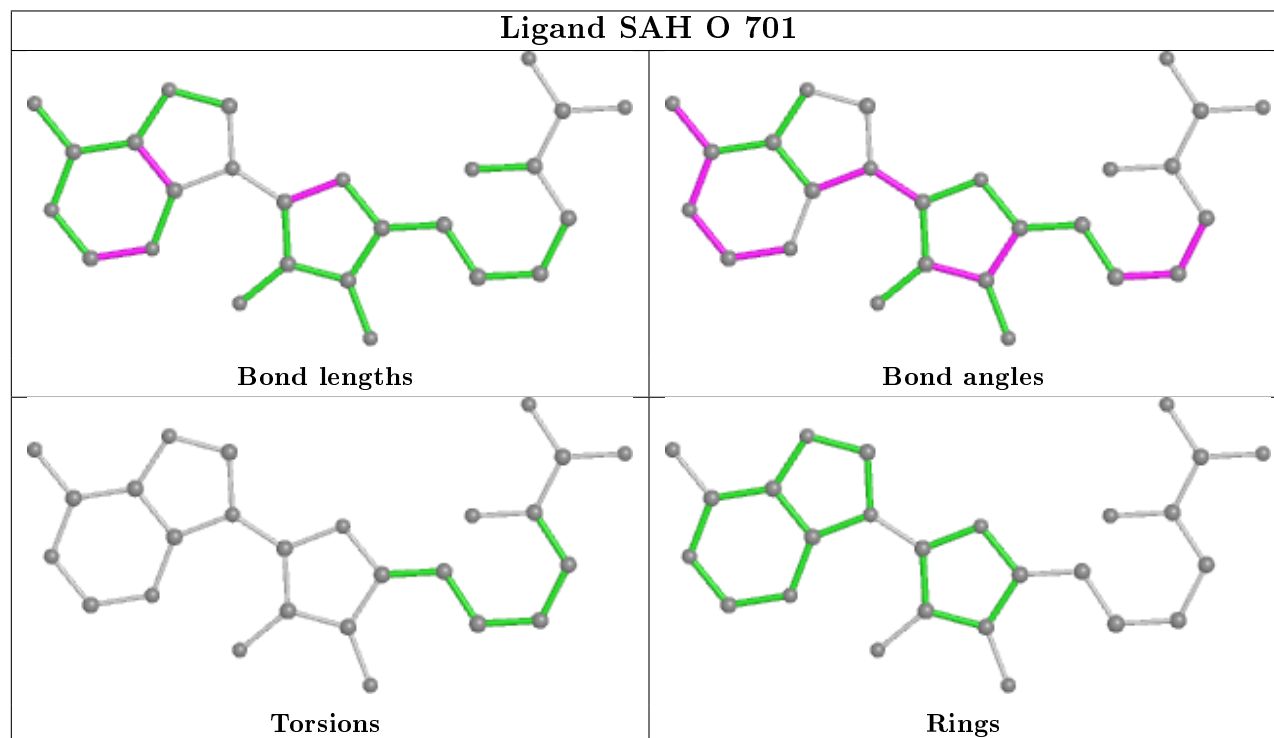
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | N | 701 | SAH | 1 | 0 |
| 2 | P | 701 | SAH | 3 | 0 |
| 2 | Q | 701 | SAH | 1 | 0 |
| 2 | C | 701 | SAH | 1 | 0 |
| 2 | F | 701 | SAH | 2 | 0 |

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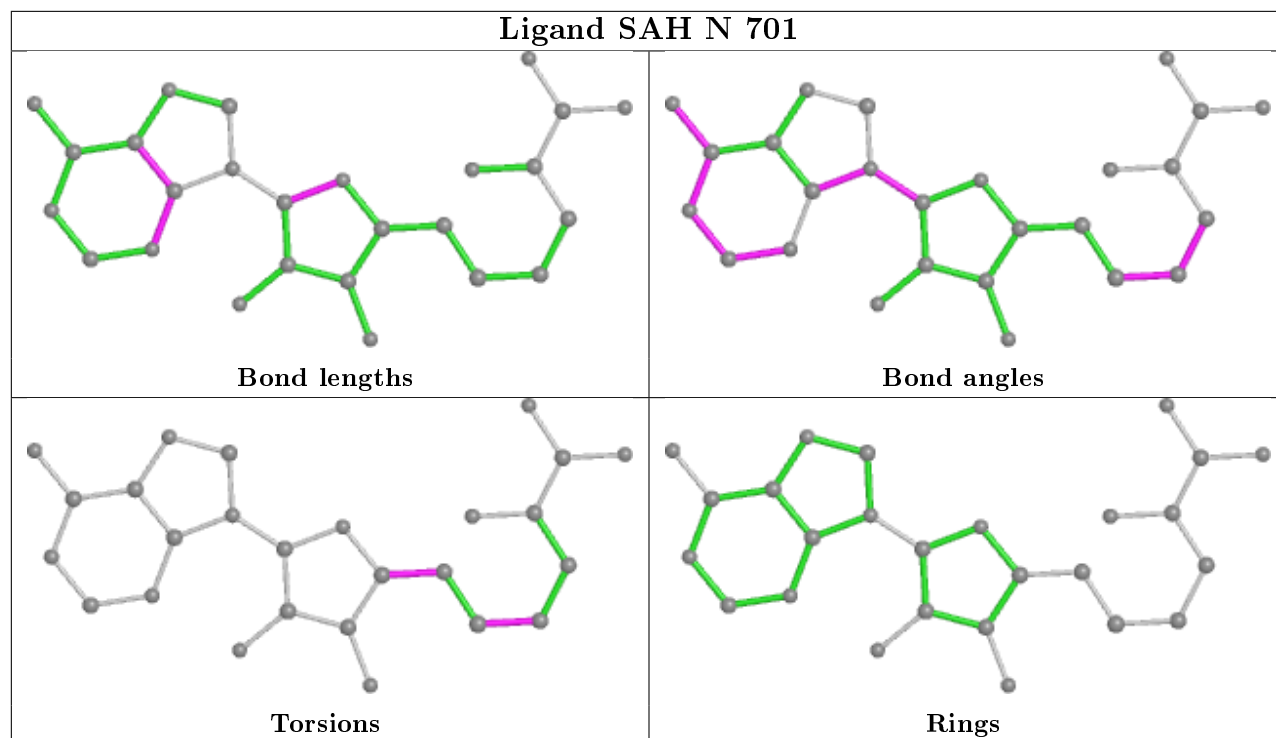
Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | B | 701 | SAH | 2 | 0 |
| 3 | I | 702 | PO4 | 1 | 0 |
| 2 | G | 701 | SAH | 2 | 0 |
| 2 | H | 701 | SAH | 1 | 0 |
| 2 | K | 701 | SAH | 3 | 0 |
| 2 | E | 701 | SAH | 3 | 0 |
| 2 | I | 701 | SAH | 1 | 0 |
| 3 | Q | 702 | PO4 | 1 | 0 |
| 2 | R | 701 | SAH | 1 | 0 |
| 2 | M | 701 | SAH | 2 | 0 |

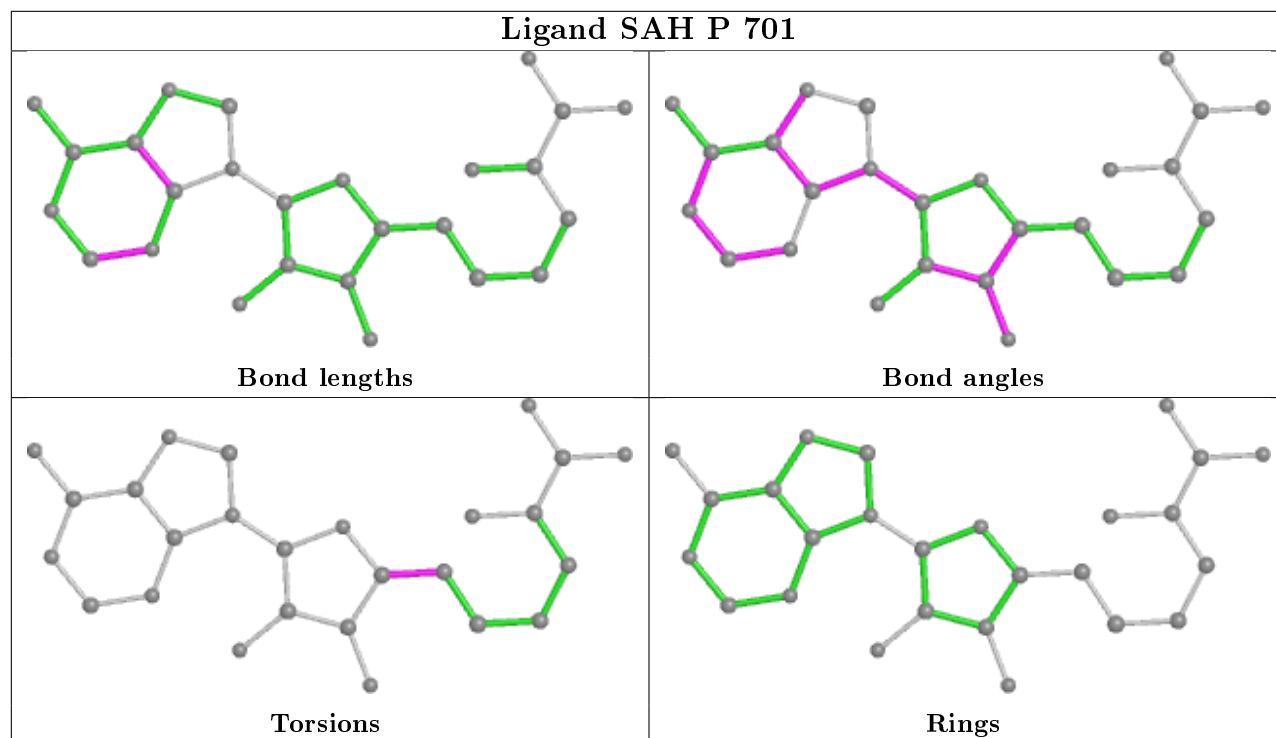
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



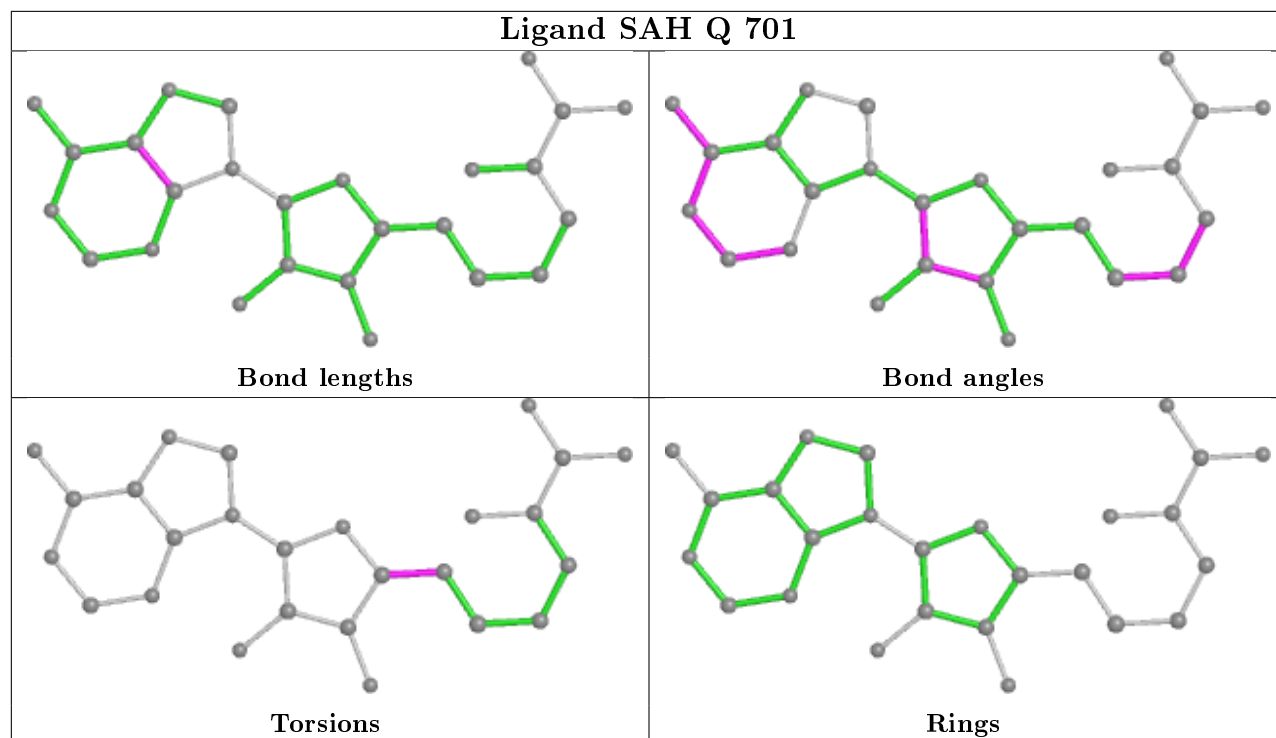
Ligand SAH N 701



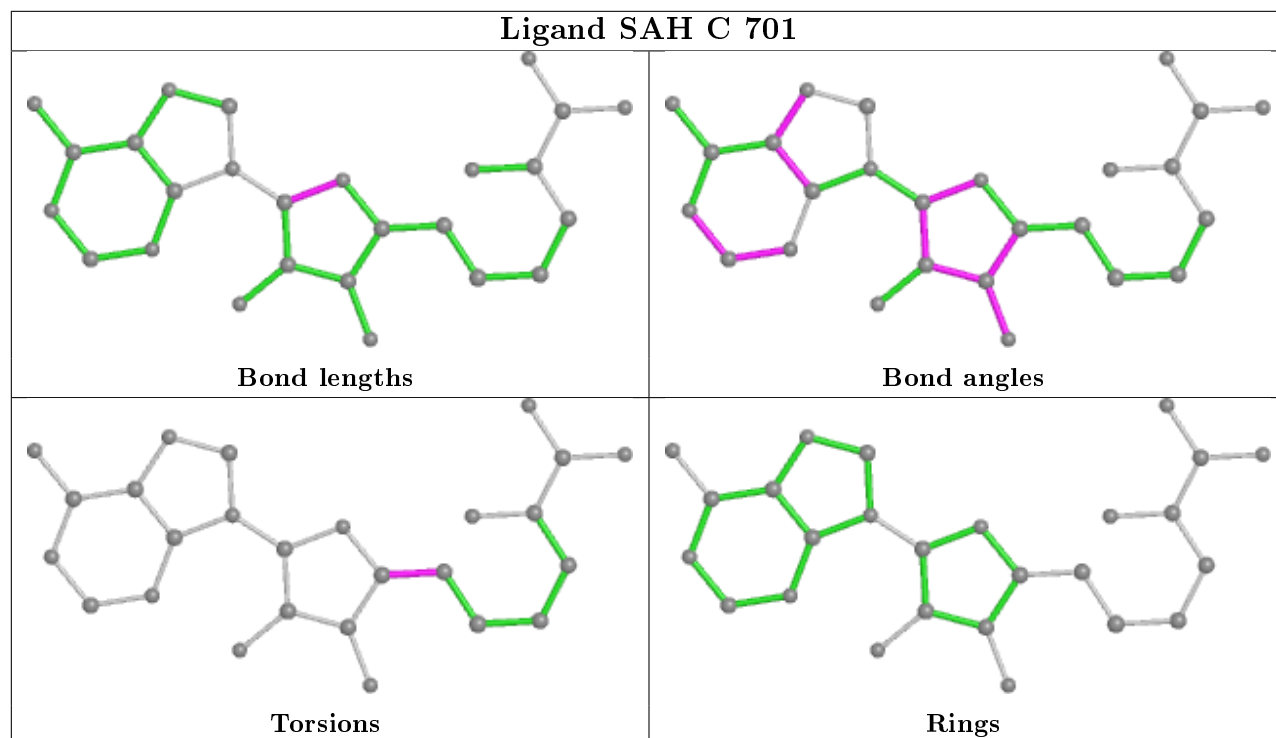
Ligand SAH P 701



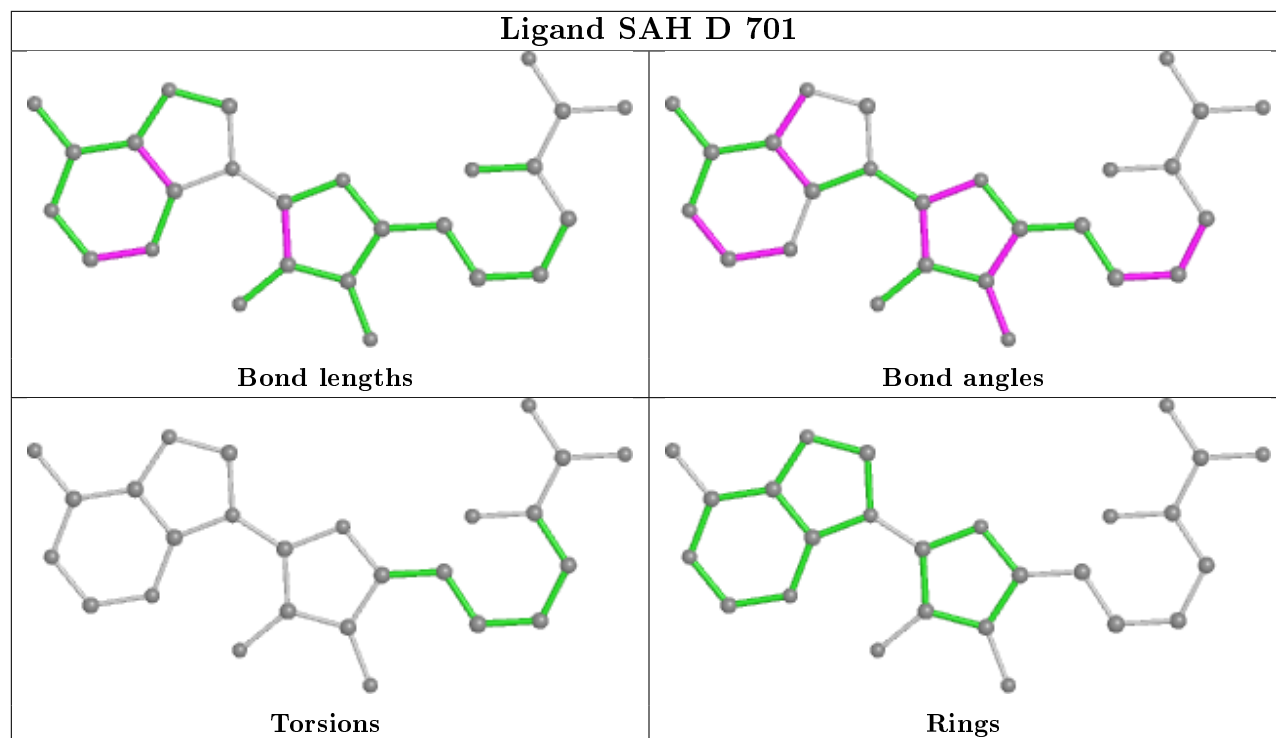
Ligand SAH Q 701



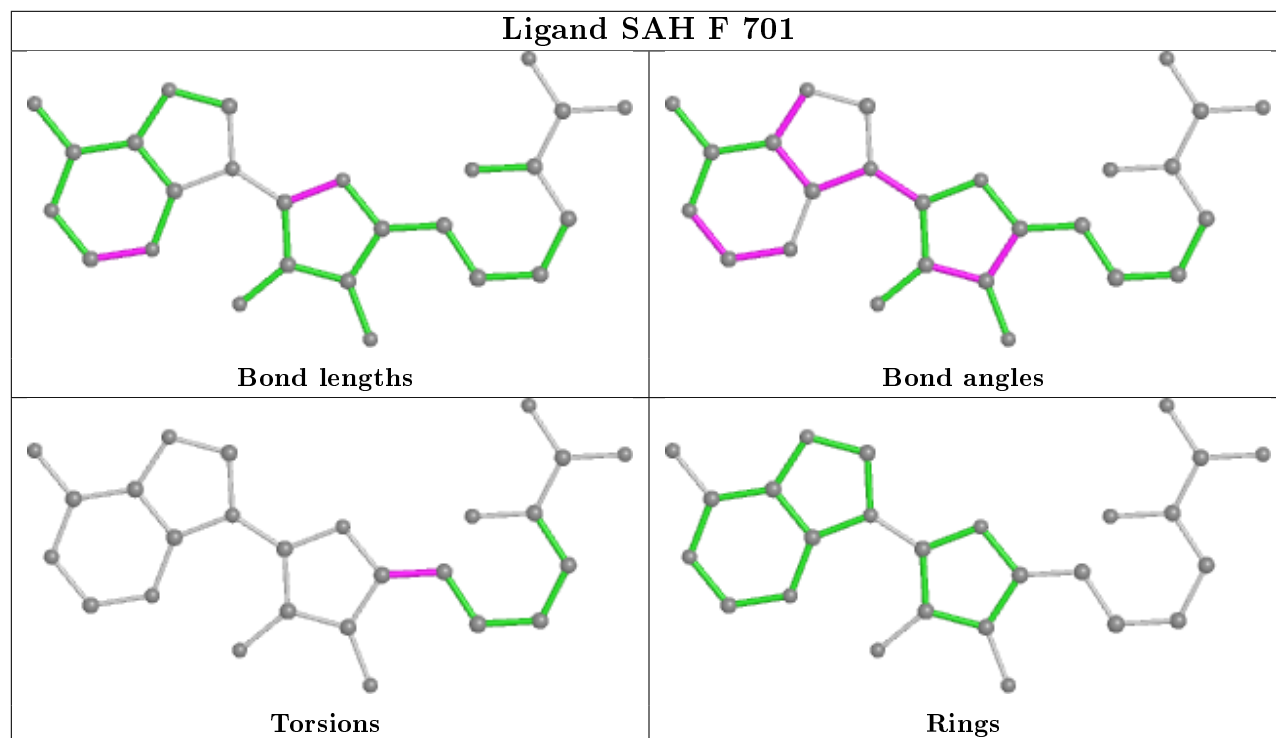
Ligand SAH C 701



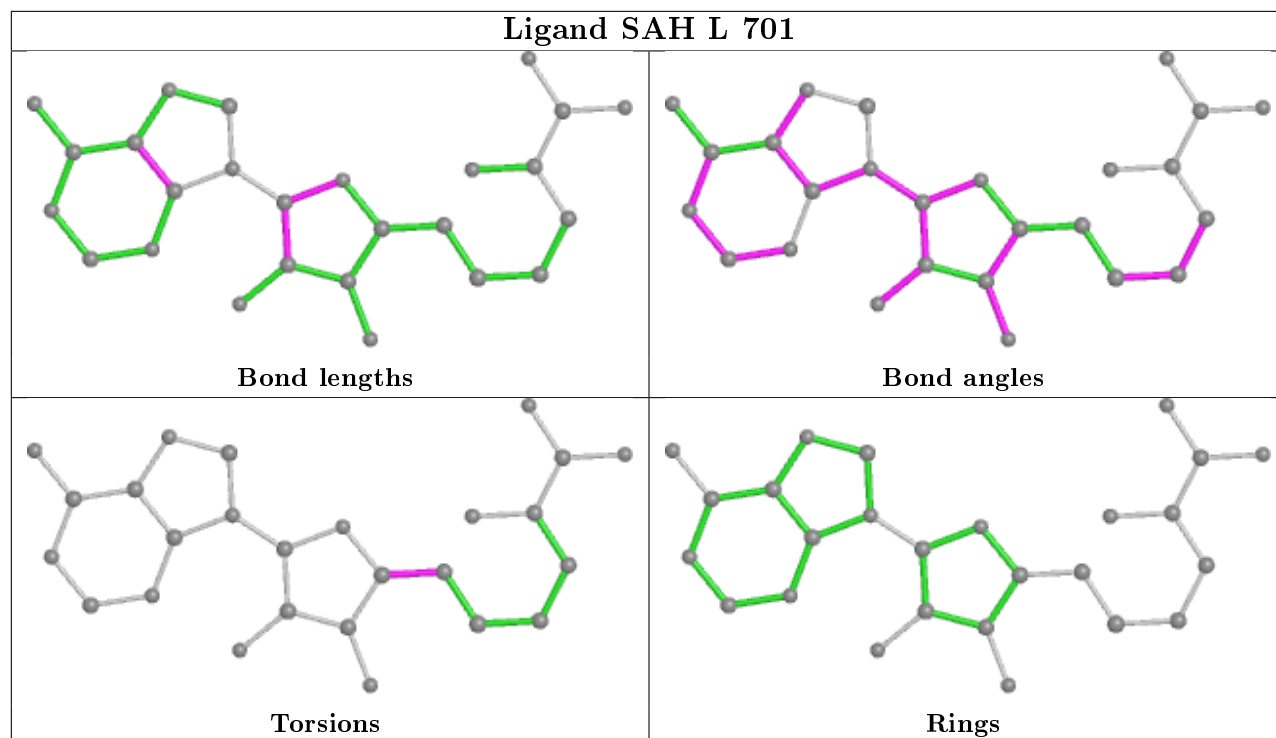
Ligand SAH D 701



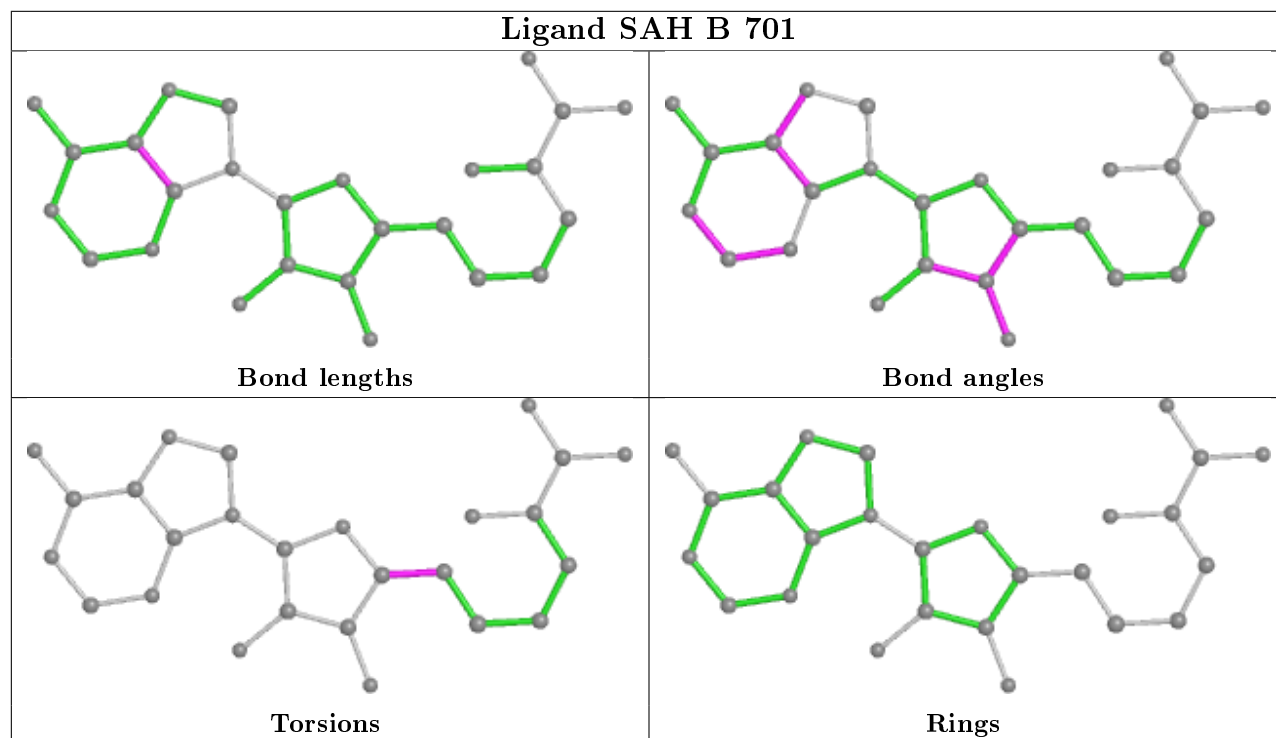
Ligand SAH F 701

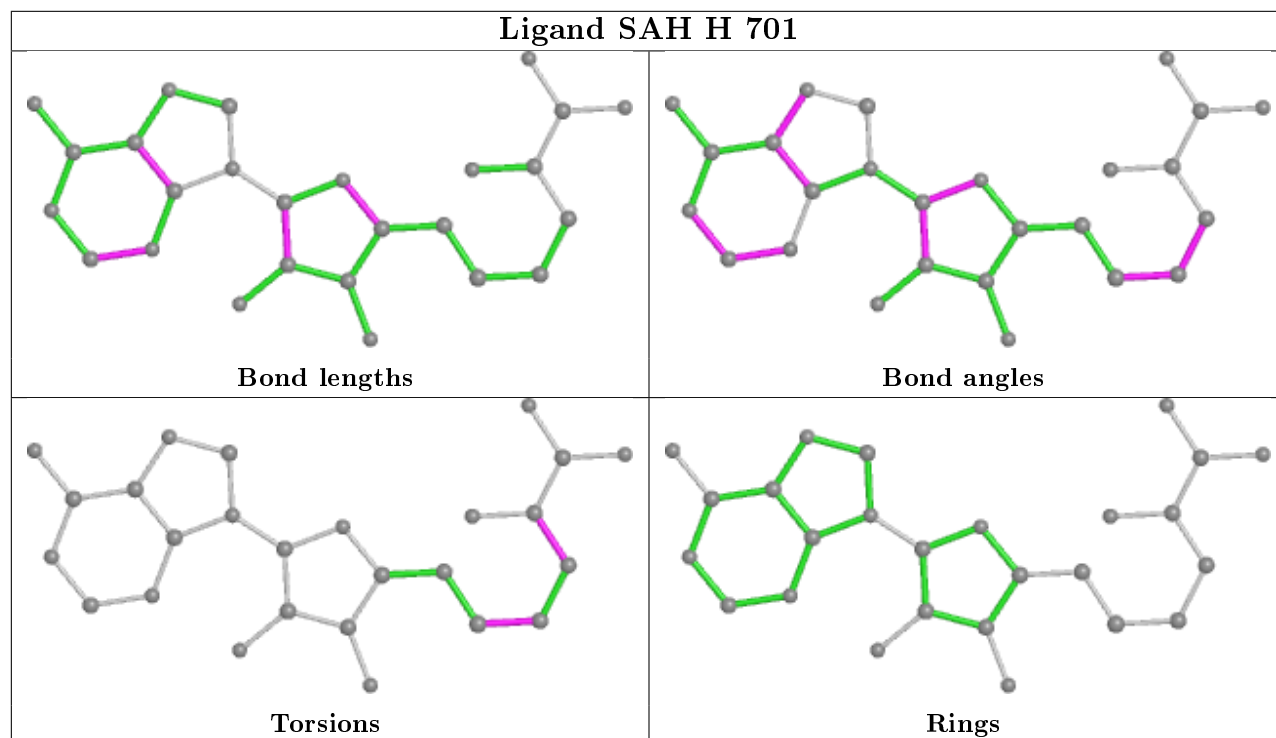
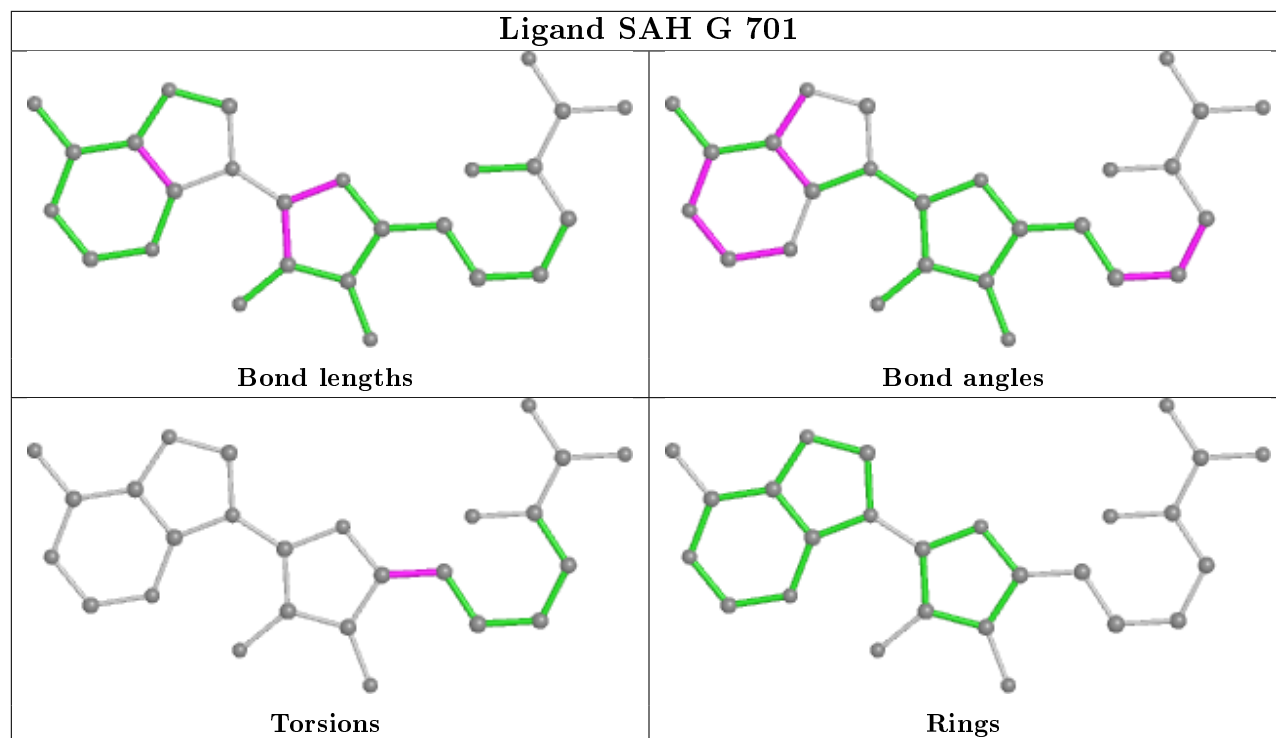


Ligand SAH L 701

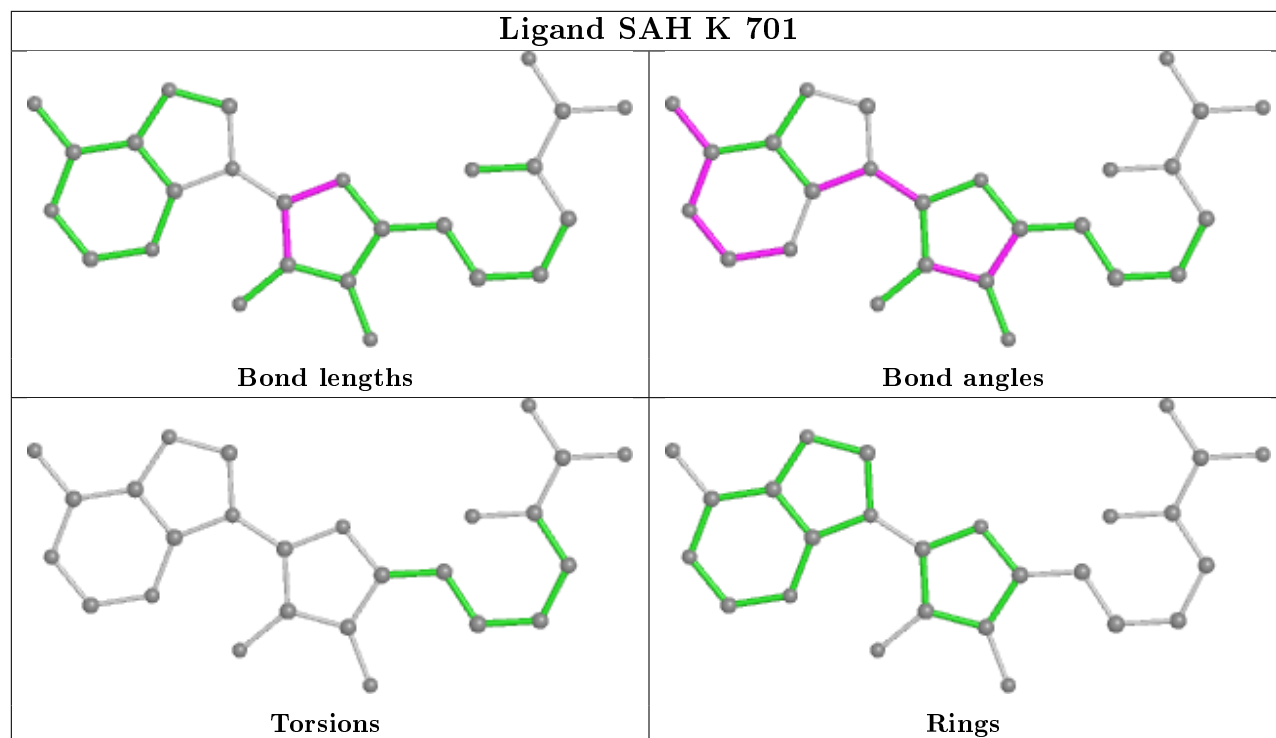


Ligand SAH B 701

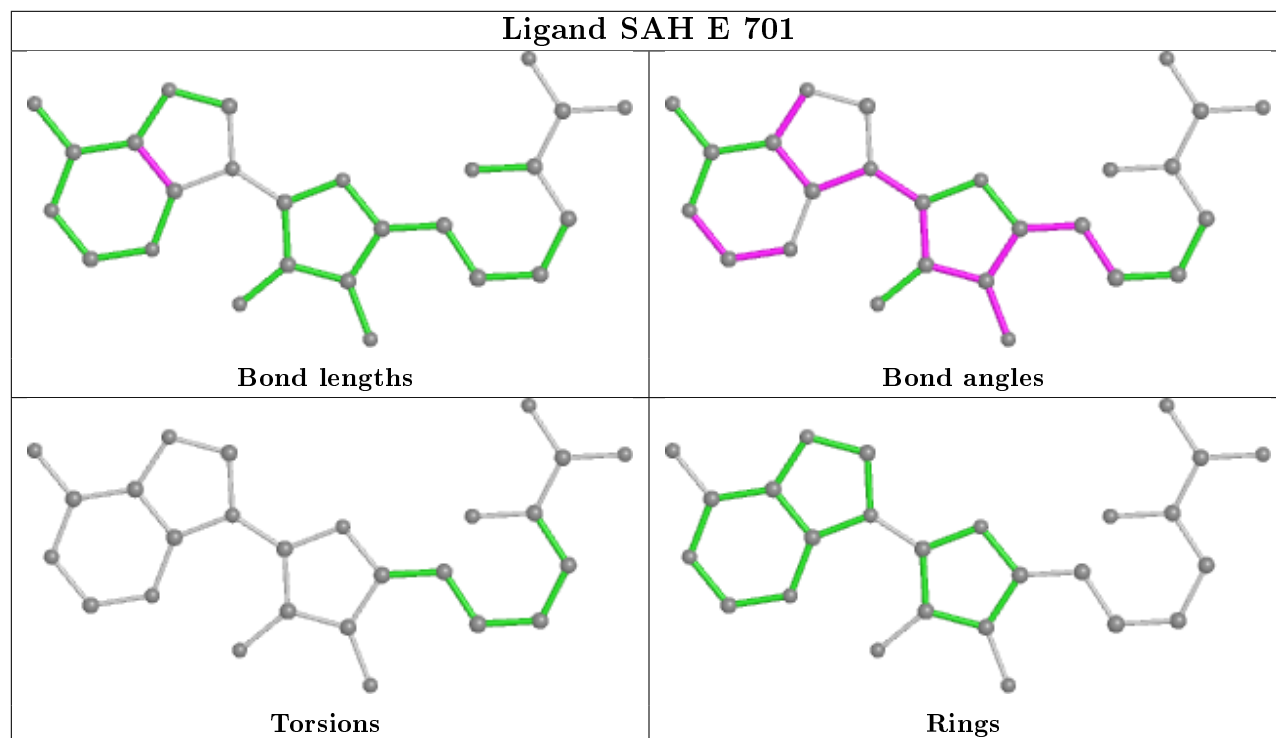




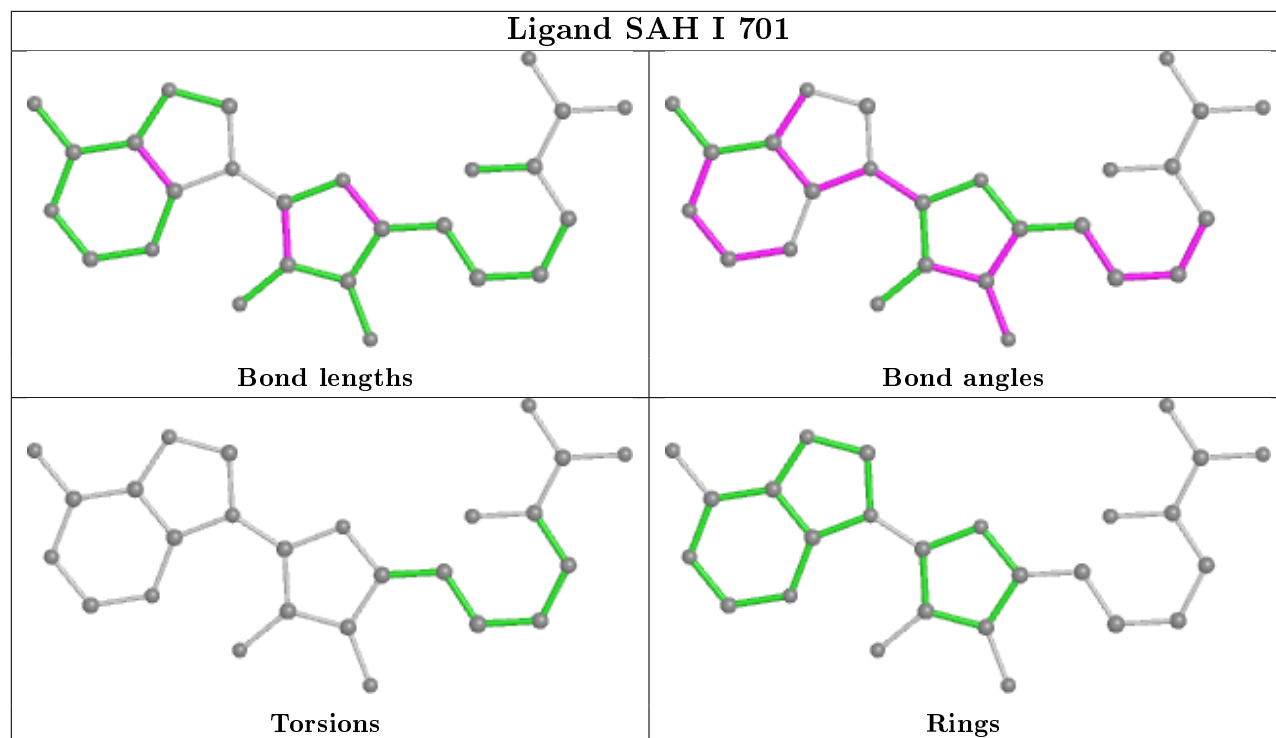
Ligand SAH K 701



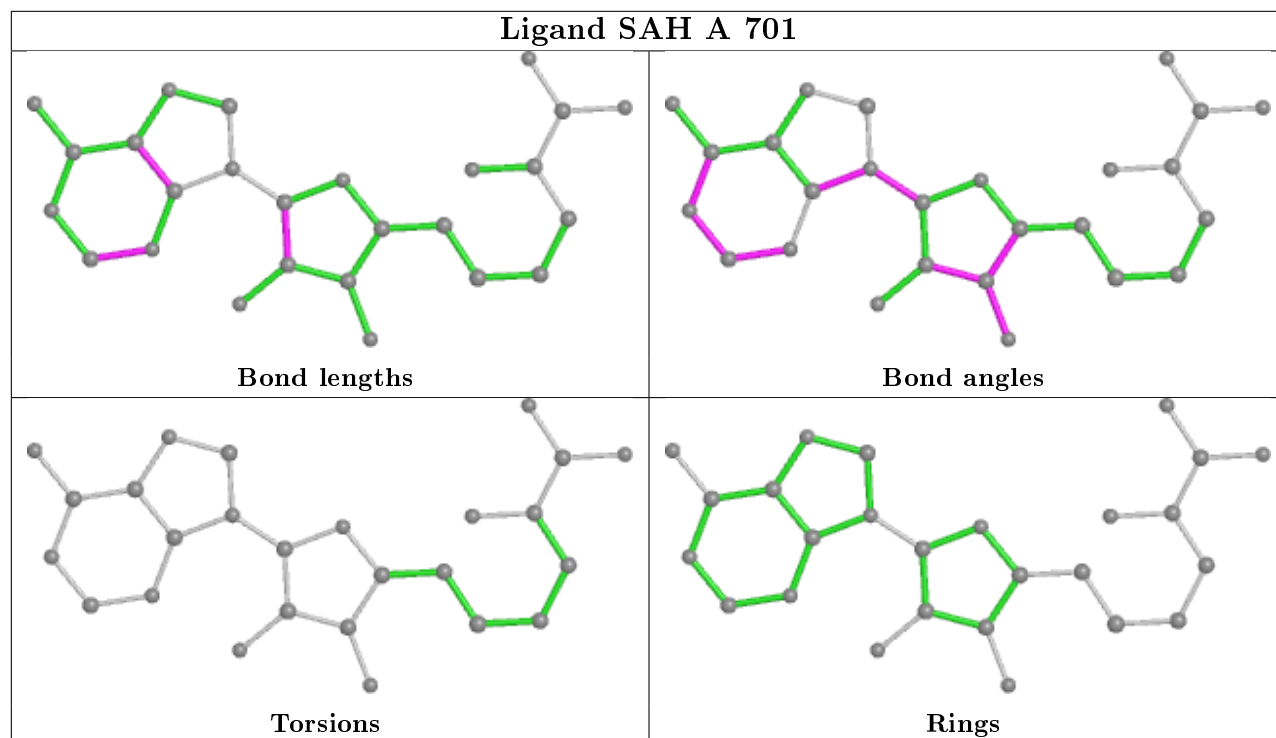
Ligand SAH E 701



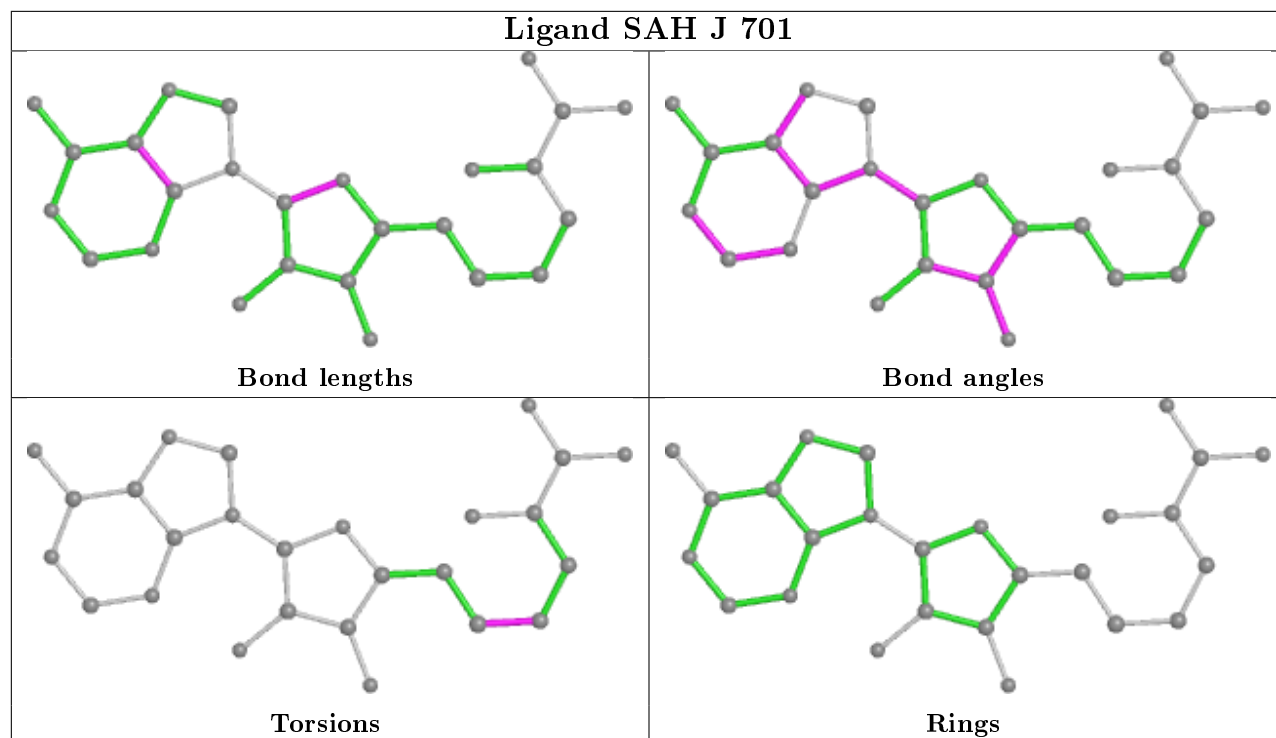
Ligand SAH I 701



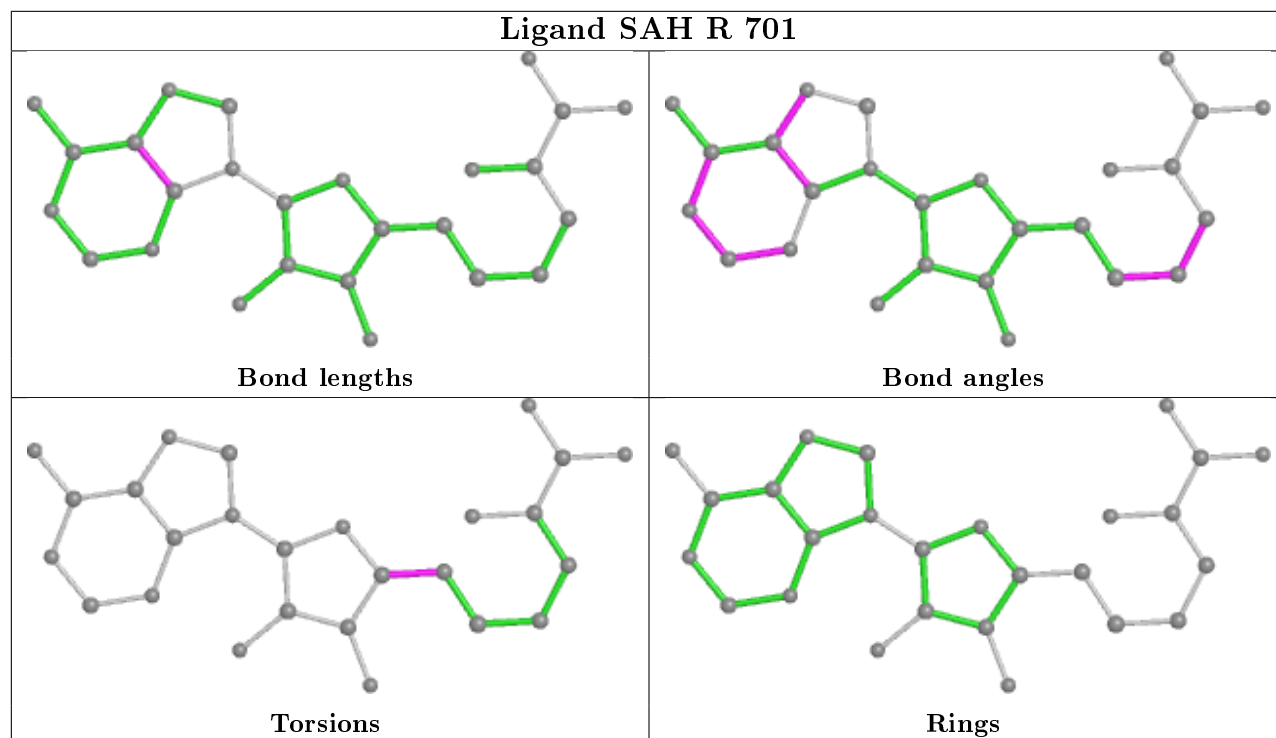
Ligand SAH A 701

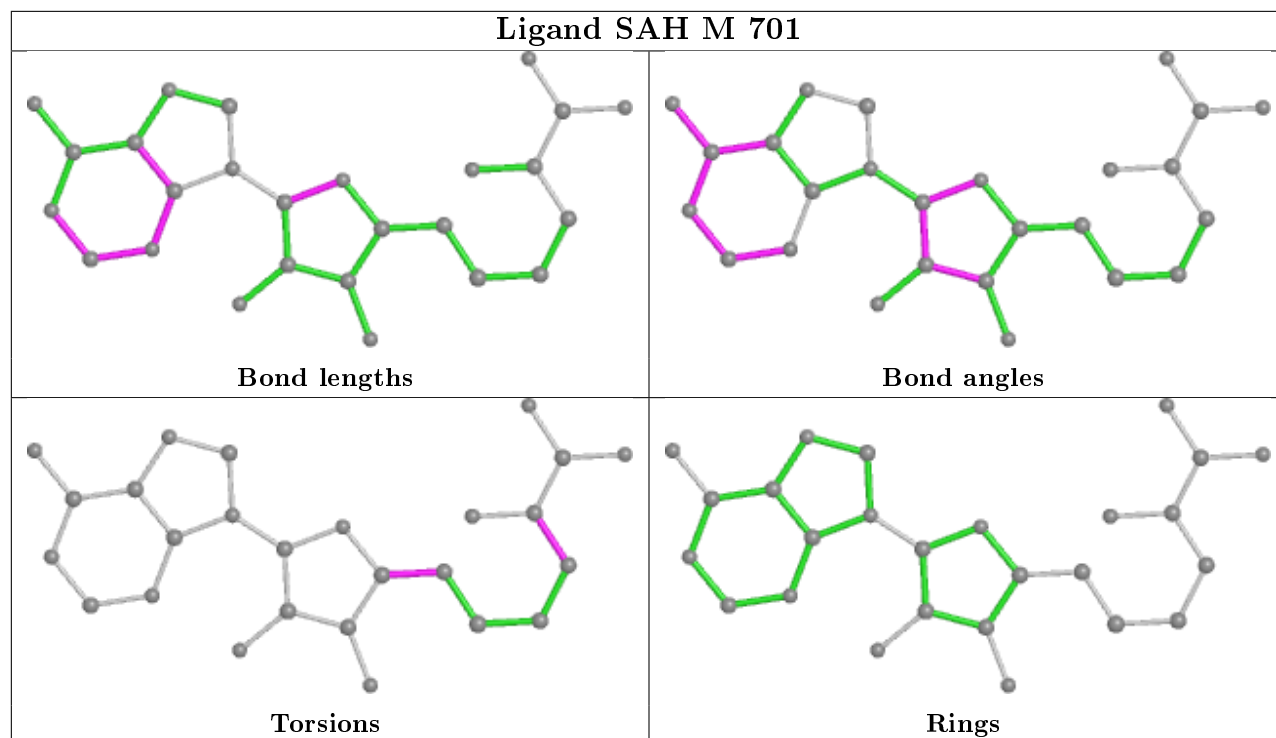


Ligand SAH J 701



Ligand SAH R 701





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 | 641/655 (97%) | -0.01 | 0 100 100 | 16, 33, 57, 83 | 0 |
| 1 | B | 638/655 (97%) | 0.10 | 6 (0%) 84 82 | 24, 43, 74, 103 | 0 |
| 1 | C | 639/655 (97%) | 0.03 | 0 100 100 | 26, 44, 68, 100 | 0 |
| 1 | D | 637/655 (97%) | -0.02 | 1 (0%) 95 94 | 19, 34, 56, 101 | 0 |
| 1 | E | 636/655 (97%) | 0.15 | 9 (1%) 75 73 | 21, 41, 80, 124 | 0 |
| 1 | F | 638/655 (97%) | 0.15 | 12 (1%) 66 64 | 27, 48, 75, 120 | 0 |
| 1 | G | 636/655 (97%) | 0.10 | 10 (1%) 72 70 | 23, 43, 81, 129 | 0 |
| 1 | H | 639/655 (97%) | -0.02 | 1 (0%) 95 94 | 18, 38, 60, 91 | 0 |
| 1 | I | 644/655 (98%) | -0.00 | 4 (0%) 89 88 | 28, 44, 68, 94 | 0 |
| 1 | J | 644/655 (98%) | 0.09 | 5 (0%) 86 84 | 29, 47, 69, 92 | 0 |
| 1 | K | 641/655 (97%) | 0.13 | 4 (0%) 89 88 | 26, 52, 77, 99 | 0 |
| 1 | L | 644/655 (98%) | -0.03 | 2 (0%) 94 93 | 19, 33, 55, 78 | 0 |
| 1 | M | 633/655 (96%) | 0.40 | 36 (5%) 23 22 | 38, 61, 84, 110 | 0 |
| 1 | N | 638/655 (97%) | 0.15 | 6 (0%) 84 82 | 36, 55, 75, 93 | 0 |
| 1 | O | 641/655 (97%) | 0.43 | 39 (6%) 21 20 | 39, 64, 96, 127 | 0 |
| 1 | P | 636/655 (97%) | 0.19 | 28 (4%) 34 33 | 30, 51, 82, 105 | 0 |
| 1 | Q | 632/655 (96%) | 0.46 | 43 (6%) 17 15 | 37, 62, 99, 124 | 0 |
| 1 | R | 638/655 (97%) | 0.59 | 59 (9%) 9 8 | 44, 69, 99, 131 | 0 |
| All | All | 11495/11790 (97%) | 0.16 | 265 (2%) 60 58 | 16, 48, 82, 131 | 0 |

All (265) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | O | 586 | ILE | 8.7 |
| 1 | E | 64 | GLY | 6.6 |
| 1 | E | 119 | ILE | 5.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | O | 644 | SER | 5.4 |
| 1 | Q | 116 | ILE | 5.3 |
| 1 | Q | 86 | GLY | 5.0 |
| 1 | O | 553 | ILE | 5.0 |
| 1 | R | 54 | ILE | 4.9 |
| 1 | R | 68 | VAL | 4.8 |
| 1 | G | 114 | ASP | 4.6 |
| 1 | R | 598 | ALA | 4.6 |
| 1 | Q | 155 | PHE | 4.5 |
| 1 | M | 107 | THR | 4.5 |
| 1 | R | 599 | GLY | 4.4 |
| 1 | R | 264 | ILE | 4.3 |
| 1 | O | 377 | LEU | 4.3 |
| 1 | Q | 329 | PHE | 4.2 |
| 1 | R | 199 | LYS | 4.2 |
| 1 | F | 317 | ASN | 4.2 |
| 1 | R | 60 | GLU | 4.2 |
| 1 | O | 595 | ILE | 4.2 |
| 1 | O | 583 | PHE | 4.1 |
| 1 | R | 40 | PHE | 4.1 |
| 1 | M | 106 | ILE | 4.1 |
| 1 | Q | 340 | LYS | 4.0 |
| 1 | R | 257 | VAL | 4.0 |
| 1 | P | 136 | ILE | 3.9 |
| 1 | O | 557 | VAL | 3.9 |
| 1 | R | 66 | VAL | 3.9 |
| 1 | F | 315 | GLU | 3.8 |
| 1 | G | 164 | LYS | 3.8 |
| 1 | Q | 311 | LYS | 3.8 |
| 1 | Q | 257 | VAL | 3.8 |
| 1 | Q | 437 | LEU | 3.7 |
| 1 | D | 62 | THR | 3.7 |
| 1 | R | 222 | LYS | 3.7 |
| 1 | Q | 236 | PHE | 3.6 |
| 1 | R | 320 | PHE | 3.6 |
| 1 | R | 162 | LEU | 3.6 |
| 1 | N | 54 | ILE | 3.5 |
| 1 | E | 118 | VAL | 3.5 |
| 1 | R | 50 | LEU | 3.5 |
| 1 | M | 66 | VAL | 3.5 |
| 1 | M | 316 | MET | 3.5 |
| 1 | M | 48 | ALA | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | F | 262 | GLY | 3.5 |
| 1 | O | 633 | SER | 3.5 |
| 1 | R | 593 | LEU | 3.4 |
| 1 | G | 121 | GLU | 3.4 |
| 1 | Q | 262 | GLY | 3.4 |
| 1 | P | 55 | ALA | 3.4 |
| 1 | O | 564 | VAL | 3.4 |
| 1 | R | 200 | ASP | 3.4 |
| 1 | O | 577 | MET | 3.4 |
| 1 | P | 137 | ILE | 3.4 |
| 1 | E | 66 | VAL | 3.4 |
| 1 | O | 620 | ASN | 3.4 |
| 1 | M | 566 | ILE | 3.3 |
| 1 | O | 426 | THR | 3.3 |
| 1 | K | 62 | THR | 3.3 |
| 1 | P | 86 | GLY | 3.2 |
| 1 | O | 566 | ILE | 3.2 |
| 1 | R | 428 | VAL | 3.2 |
| 1 | Q | 336 | VAL | 3.2 |
| 1 | M | 514 | PHE | 3.2 |
| 1 | M | 555 | GLY | 3.2 |
| 1 | P | 114 | ASP | 3.2 |
| 1 | M | 301 | TRP | 3.2 |
| 1 | Q | 119 | ILE | 3.1 |
| 1 | R | 602 | GLU | 3.1 |
| 1 | O | 517 | ILE | 3.1 |
| 1 | R | 477 | LEU | 3.1 |
| 1 | F | 336 | VAL | 3.1 |
| 1 | Q | 59 | HIS | 3.1 |
| 1 | R | 55 | ALA | 3.1 |
| 1 | O | 199 | LYS | 3.1 |
| 1 | P | 66 | VAL | 3.1 |
| 1 | I | 622 | LYS | 3.0 |
| 1 | I | 129 | ILE | 3.0 |
| 1 | M | 82 | ALA | 3.0 |
| 1 | P | 555 | GLY | 3.0 |
| 1 | R | 58 | LYS | 3.0 |
| 1 | R | 155 | PHE | 3.0 |
| 1 | Q | 90 | VAL | 3.0 |
| 1 | J | 292 | LYS | 3.0 |
| 1 | R | 88 | ASP | 3.0 |
| 1 | P | 93 | LEU | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | R | 444 | VAL | 3.0 |
| 1 | K | 489 | ILE | 3.0 |
| 1 | Q | 317 | ASN | 3.0 |
| 1 | P | 74 | GLY | 2.9 |
| 1 | N | 320 | PHE | 2.9 |
| 1 | M | 643 | LYS | 2.9 |
| 1 | P | 118 | VAL | 2.9 |
| 1 | Q | 308 | LEU | 2.9 |
| 1 | M | 238 | PHE | 2.9 |
| 1 | I | 66 | VAL | 2.8 |
| 1 | P | 454 | MET | 2.8 |
| 1 | P | 155 | PHE | 2.8 |
| 1 | E | 93 | LEU | 2.8 |
| 1 | P | 132 | SER | 2.8 |
| 1 | E | 114 | ASP | 2.8 |
| 1 | K | 454 | MET | 2.8 |
| 1 | Q | 337 | GLY | 2.8 |
| 1 | F | 189 | PHE | 2.8 |
| 1 | M | 50 | LEU | 2.8 |
| 1 | M | 180 | PRO | 2.8 |
| 1 | R | 159 | LEU | 2.8 |
| 1 | O | 379 | LYS | 2.8 |
| 1 | P | 67 | HIS | 2.8 |
| 1 | O | 585 | GLY | 2.8 |
| 1 | Q | 93 | LEU | 2.8 |
| 1 | Q | 555 | GLY | 2.8 |
| 1 | O | 483 | MET | 2.7 |
| 1 | Q | 247 | ILE | 2.7 |
| 1 | M | 314 | VAL | 2.7 |
| 1 | O | 320 | PHE | 2.7 |
| 1 | Q | 253 | VAL | 2.7 |
| 1 | J | 454 | MET | 2.7 |
| 1 | Q | 137 | ILE | 2.7 |
| 1 | O | 584 | GLY | 2.7 |
| 1 | L | 131 | GLY | 2.7 |
| 1 | O | 629 | LEU | 2.7 |
| 1 | M | 52 | THR | 2.7 |
| 1 | F | 556 | ARG | 2.7 |
| 1 | M | 206 | ARG | 2.7 |
| 1 | F | 320 | PHE | 2.7 |
| 1 | R | 234 | VAL | 2.7 |
| 1 | P | 546 | VAL | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | R | 425 | LEU | 2.6 |
| 1 | R | 471 | MET | 2.6 |
| 1 | E | 570 | SER | 2.6 |
| 1 | E | 111 | PRO | 2.6 |
| 1 | O | 347 | CYS | 2.6 |
| 1 | R | 246 | ILE | 2.6 |
| 1 | P | 240 | PHE | 2.6 |
| 1 | Q | 240 | PHE | 2.6 |
| 1 | R | 179 | VAL | 2.6 |
| 1 | Q | 556 | ARG | 2.6 |
| 1 | F | 316 | MET | 2.6 |
| 1 | M | 318 | GLN | 2.6 |
| 1 | R | 478 | ARG | 2.5 |
| 1 | G | 162 | LEU | 2.5 |
| 1 | Q | 158 | ALA | 2.5 |
| 1 | R | 296 | ALA | 2.5 |
| 1 | Q | 162 | LEU | 2.5 |
| 1 | P | 314 | VAL | 2.5 |
| 1 | L | 454 | MET | 2.5 |
| 1 | J | 227 | ARG | 2.5 |
| 1 | N | 134 | ALA | 2.5 |
| 1 | K | 114 | ASP | 2.5 |
| 1 | O | 489 | ILE | 2.5 |
| 1 | O | 540 | ILE | 2.5 |
| 1 | M | 46 | PHE | 2.5 |
| 1 | O | 565 | ASN | 2.5 |
| 1 | R | 308 | LEU | 2.5 |
| 1 | P | 68 | VAL | 2.4 |
| 1 | Q | 314 | VAL | 2.4 |
| 1 | M | 210 | THR | 2.4 |
| 1 | Q | 112 | TRP | 2.4 |
| 1 | R | 622 | LYS | 2.4 |
| 1 | M | 119 | ILE | 2.4 |
| 1 | M | 247 | ILE | 2.4 |
| 1 | O | 486 | LEU | 2.4 |
| 1 | O | 551 | PHE | 2.4 |
| 1 | Q | 238 | PHE | 2.4 |
| 1 | Q | 319 | THR | 2.4 |
| 1 | R | 85 | GLU | 2.4 |
| 1 | Q | 292 | LYS | 2.4 |
| 1 | P | 509 | PHE | 2.4 |
| 1 | M | 61 | ASN | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 133 | ARG | 2.4 |
| 1 | M | 103 | ALA | 2.4 |
| 1 | Q | 627 | HIS | 2.4 |
| 1 | R | 167 | CYS | 2.4 |
| 1 | J | 315 | GLU | 2.4 |
| 1 | B | 292 | LYS | 2.4 |
| 1 | Q | 277 | ARG | 2.4 |
| 1 | Q | 255 | GLU | 2.4 |
| 1 | M | 624 | LEU | 2.3 |
| 1 | Q | 111 | PRO | 2.3 |
| 1 | M | 65 | LYS | 2.3 |
| 1 | G | 116 | ILE | 2.3 |
| 1 | O | 545 | ALA | 2.3 |
| 1 | Q | 161 | ARG | 2.3 |
| 1 | R | 505 | THR | 2.3 |
| 1 | R | 59 | HIS | 2.3 |
| 1 | O | 192 | ILE | 2.3 |
| 1 | I | 292 | LYS | 2.3 |
| 1 | R | 142 | PHE | 2.3 |
| 1 | R | 643 | LYS | 2.3 |
| 1 | N | 294 | ASN | 2.3 |
| 1 | B | 83 | ALA | 2.3 |
| 1 | R | 511 | LEU | 2.3 |
| 1 | F | 370 | PHE | 2.3 |
| 1 | F | 613 | PHE | 2.3 |
| 1 | O | 428 | VAL | 2.3 |
| 1 | Q | 57 | LYS | 2.3 |
| 1 | N | 268 | LEU | 2.3 |
| 1 | O | 561 | LYS | 2.3 |
| 1 | R | 164 | LYS | 2.3 |
| 1 | Q | 163 | ALA | 2.3 |
| 1 | R | 62 | THR | 2.2 |
| 1 | G | 68 | VAL | 2.2 |
| 1 | M | 320 | PHE | 2.2 |
| 1 | B | 113 | SER | 2.2 |
| 1 | Q | 85 | GLU | 2.2 |
| 1 | R | 369 | LYS | 2.2 |
| 1 | P | 63 | ASP | 2.2 |
| 1 | Q | 133 | ARG | 2.2 |
| 1 | B | 199 | LYS | 2.2 |
| 1 | J | 586 | ILE | 2.2 |
| 1 | P | 133 | ARG | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 132 | SER | 2.2 |
| 1 | F | 282 | PHE | 2.2 |
| 1 | N | 319 | THR | 2.2 |
| 1 | F | 54 | ILE | 2.2 |
| 1 | O | 443 | ILE | 2.2 |
| 1 | M | 623 | SER | 2.2 |
| 1 | Q | 199 | LYS | 2.2 |
| 1 | O | 399 | THR | 2.2 |
| 1 | R | 504 | GLY | 2.2 |
| 1 | G | 161 | ARG | 2.1 |
| 1 | O | 403 | VAL | 2.1 |
| 1 | R | 443 | ILE | 2.1 |
| 1 | O | 349 | LEU | 2.1 |
| 1 | O | 477 | LEU | 2.1 |
| 1 | P | 58 | LYS | 2.1 |
| 1 | R | 571 | SER | 2.1 |
| 1 | O | 200 | ASP | 2.1 |
| 1 | G | 54 | ILE | 2.1 |
| 1 | R | 600 | VAL | 2.1 |
| 1 | P | 620 | ASN | 2.1 |
| 1 | P | 69 | LEU | 2.1 |
| 1 | Q | 267 | LEU | 2.1 |
| 1 | R | 456 | PRO | 2.1 |
| 1 | G | 59 | HIS | 2.1 |
| 1 | O | 567 | ASP | 2.1 |
| 1 | G | 158 | ALA | 2.1 |
| 1 | R | 283 | ILE | 2.1 |
| 1 | R | 38 | LEU | 2.1 |
| 1 | R | 592 | LEU | 2.1 |
| 1 | M | 471 | MET | 2.1 |
| 1 | R | 621 | ASP | 2.1 |
| 1 | R | 206 | ARG | 2.1 |
| 1 | M | 55 | ALA | 2.1 |
| 1 | P | 628 | ALA | 2.1 |
| 1 | B | 169 | VAL | 2.1 |
| 1 | P | 51 | LYS | 2.1 |
| 1 | P | 644 | SER | 2.1 |
| 1 | M | 313 | LYS | 2.1 |
| 1 | O | 622 | LYS | 2.1 |
| 1 | R | 314 | VAL | 2.1 |
| 1 | M | 116 | ILE | 2.0 |
| 1 | P | 619 | ARG | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | M | 199 | LYS | 2.0 |
| 1 | R | 340 | LYS | 2.0 |
| 1 | M | 17 | VAL | 2.0 |
| 1 | H | 556 | ARG | 2.0 |
| 1 | M | 142 | PHE | 2.0 |
| 1 | M | 168 | ARG | 2.0 |
| 1 | Q | 232 | PRO | 2.0 |
| 1 | R | 345 | CYS | 2.0 |
| 1 | R | 586 | ILE | 2.0 |
| 1 | R | 454 | MET | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2 | SAH | M | 701 | 26/26 | 0.89 | 0.16 | 36,61,74,79 | 0 |
| 2 | SAH | N | 701 | 26/26 | 0.90 | 0.12 | 40,53,58,58 | 0 |
| 2 | SAH | R | 701 | 26/26 | 0.91 | 0.17 | 47,56,92,99 | 0 |
| 3 | PO4 | M | 702 | 5/5 | 0.91 | 0.13 | 70,71,74,78 | 0 |
| 2 | SAH | Q | 701 | 26/26 | 0.92 | 0.14 | 48,64,75,76 | 0 |
| 2 | SAH | G | 701 | 26/26 | 0.93 | 0.14 | 46,63,72,72 | 0 |
| 2 | SAH | P | 701 | 26/26 | 0.93 | 0.11 | 43,53,63,65 | 0 |
| 2 | SAH | K | 701 | 26/26 | 0.94 | 0.13 | 37,41,47,51 | 0 |
| 2 | SAH | C | 701 | 26/26 | 0.95 | 0.14 | 36,48,57,59 | 0 |
| 2 | SAH | D | 701 | 26/26 | 0.95 | 0.15 | 32,37,45,46 | 0 |
| 2 | SAH | E | 701 | 26/26 | 0.95 | 0.13 | 43,53,63,65 | 0 |
| 2 | SAH | F | 701 | 26/26 | 0.95 | 0.14 | 35,46,61,64 | 0 |
| 2 | SAH | O | 701 | 26/26 | 0.95 | 0.10 | 37,41,47,52 | 0 |

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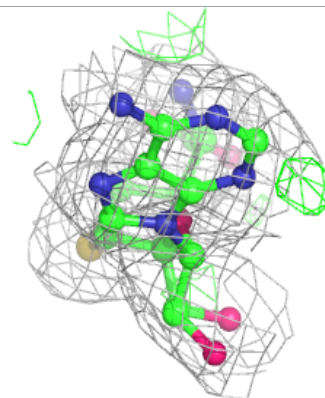
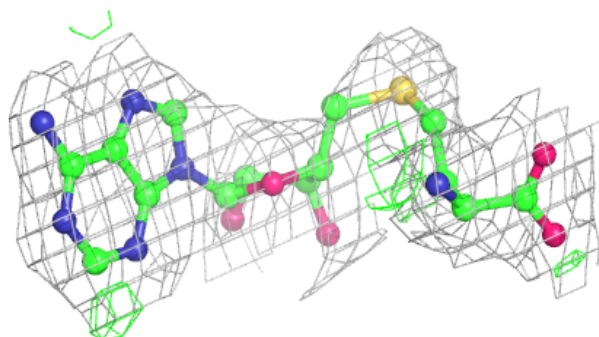
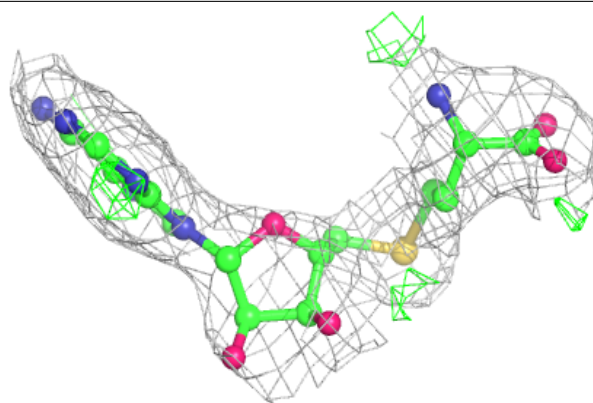
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2 | SAH | I | 701 | 26/26 | 0.96 | 0.12 | 35,38,45,47 | 0 |
| 3 | PO4 | Q | 702 | 5/5 | 0.96 | 0.12 | 59,63,72,72 | 0 |
| 2 | SAH | A | 701 | 26/26 | 0.96 | 0.13 | 27,33,38,38 | 0 |
| 2 | SAH | J | 701 | 26/26 | 0.96 | 0.11 | 34,38,44,46 | 0 |
| 3 | PO4 | R | 702 | 5/5 | 0.96 | 0.09 | 52,55,59,61 | 0 |
| 2 | SAH | B | 701 | 26/26 | 0.96 | 0.12 | 36,43,57,58 | 0 |
| 2 | SAH | H | 701 | 26/26 | 0.96 | 0.12 | 24,29,33,34 | 0 |
| 3 | PO4 | O | 702 | 5/5 | 0.97 | 0.07 | 57,58,70,72 | 0 |
| 2 | SAH | L | 701 | 26/26 | 0.97 | 0.12 | 27,33,36,39 | 0 |
| 3 | PO4 | N | 702 | 5/5 | 0.97 | 0.09 | 52,57,62,66 | 0 |
| 3 | PO4 | I | 702 | 5/5 | 0.97 | 0.14 | 36,37,44,49 | 0 |
| 3 | PO4 | J | 702 | 5/5 | 0.98 | 0.11 | 45,46,49,51 | 0 |
| 3 | PO4 | H | 702 | 5/5 | 0.98 | 0.09 | 28,34,36,37 | 0 |
| 3 | PO4 | K | 702 | 5/5 | 0.98 | 0.09 | 43,45,46,51 | 0 |
| 3 | PO4 | P | 702 | 5/5 | 0.98 | 0.12 | 43,43,45,47 | 0 |
| 3 | PO4 | C | 702 | 5/5 | 0.98 | 0.09 | 37,41,44,44 | 0 |
| 3 | PO4 | F | 702 | 5/5 | 0.98 | 0.08 | 38,42,49,56 | 0 |
| 3 | PO4 | E | 702 | 5/5 | 0.98 | 0.10 | 36,40,43,47 | 0 |
| 3 | PO4 | B | 702 | 5/5 | 0.98 | 0.13 | 36,39,45,48 | 0 |
| 3 | PO4 | L | 702 | 5/5 | 0.99 | 0.12 | 32,32,35,37 | 0 |
| 3 | PO4 | D | 702 | 5/5 | 0.99 | 0.12 | 31,35,36,37 | 0 |
| 3 | PO4 | G | 702 | 5/5 | 0.99 | 0.11 | 42,42,49,50 | 0 |
| 3 | PO4 | A | 702 | 5/5 | 0.99 | 0.12 | 31,32,37,39 | 0 |

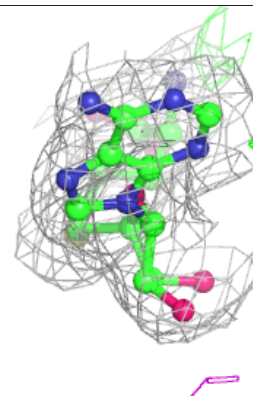
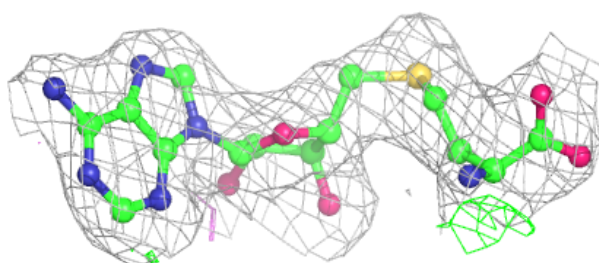
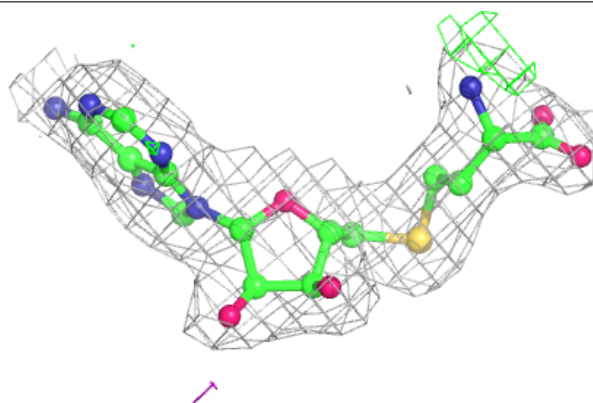
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH M 701:

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

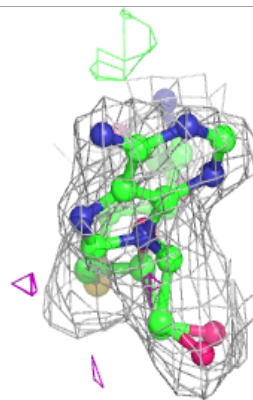
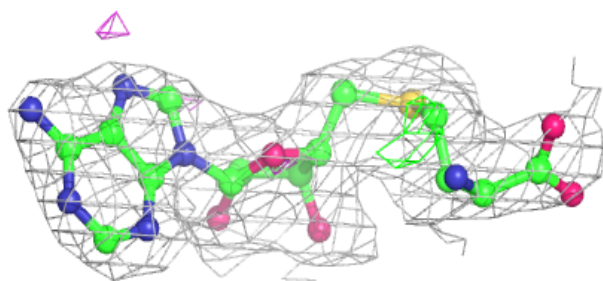
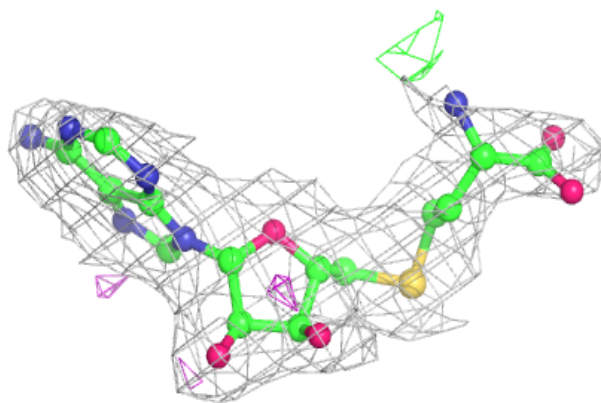
**Electron density around SAH N 701:**

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

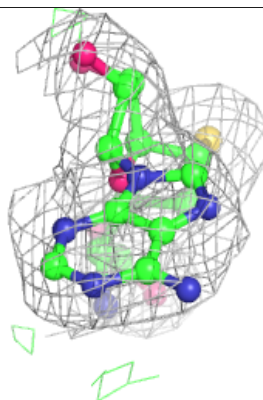
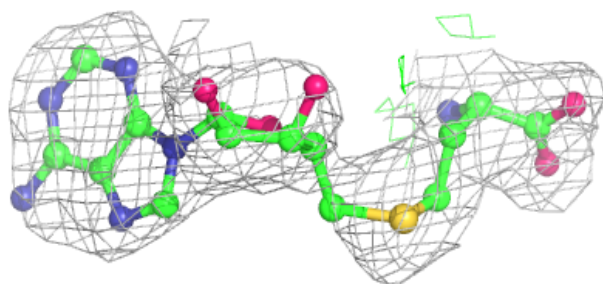
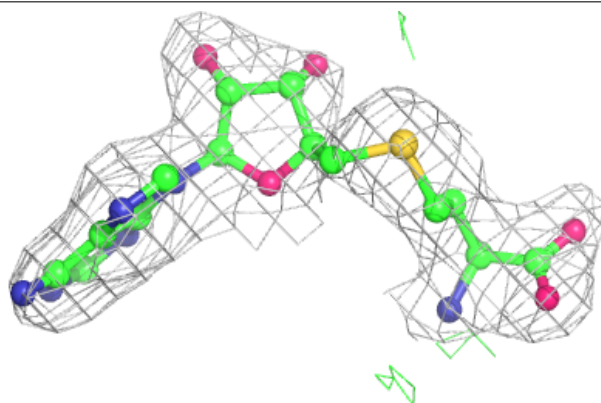


Electron density around SAH R 701:

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

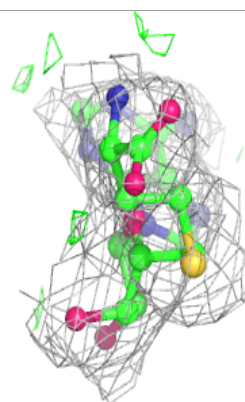
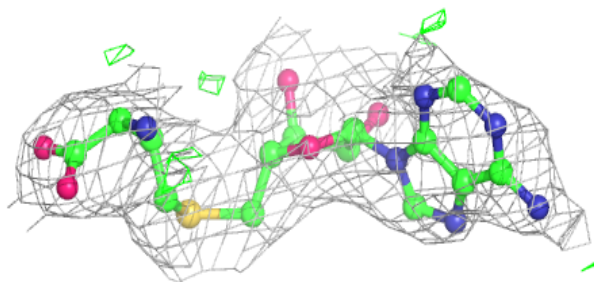
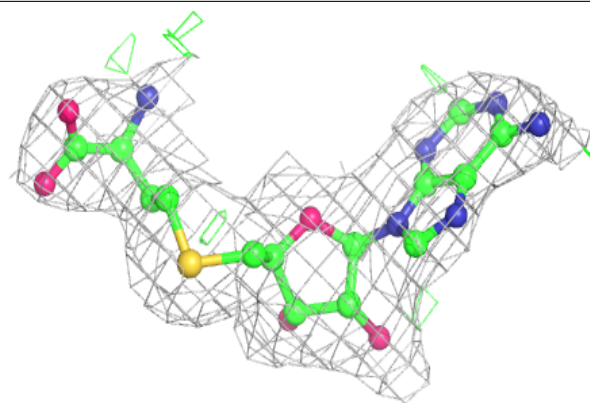
**Electron density around SAH Q 701:**

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

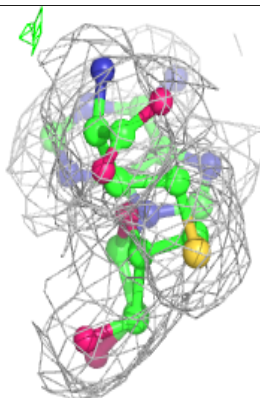
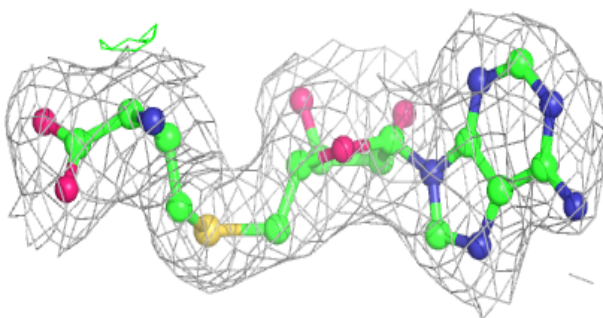
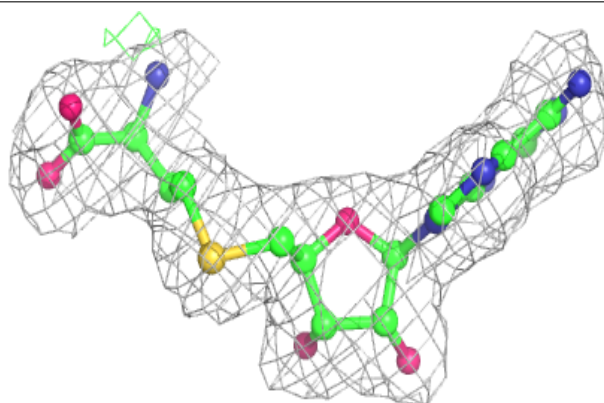


Electron density around SAH G 701:

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

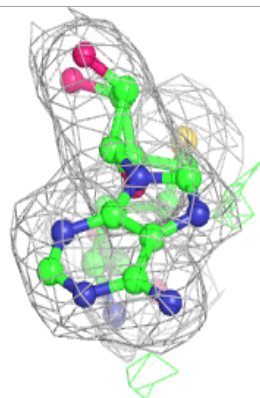
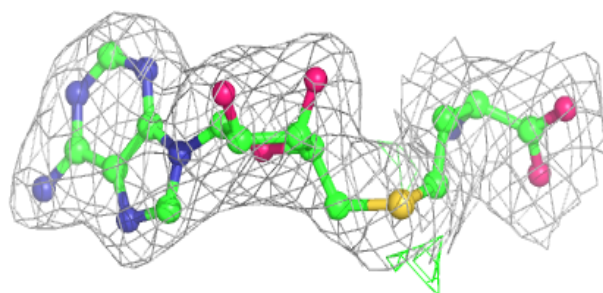
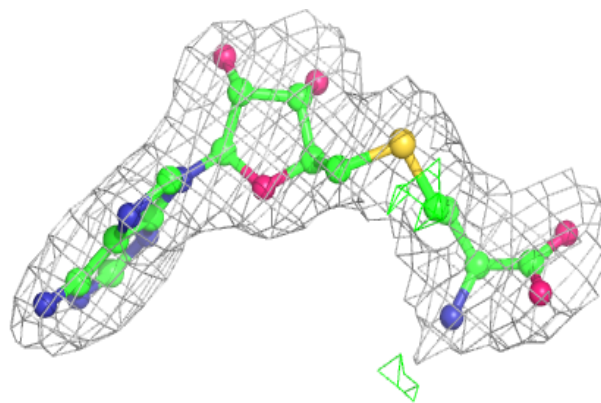
**Electron density around SAH P 701:**

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

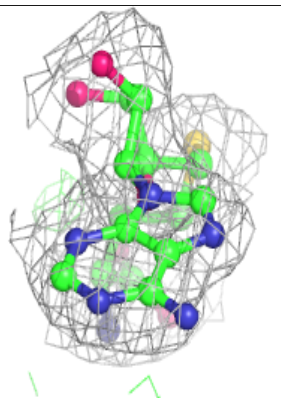
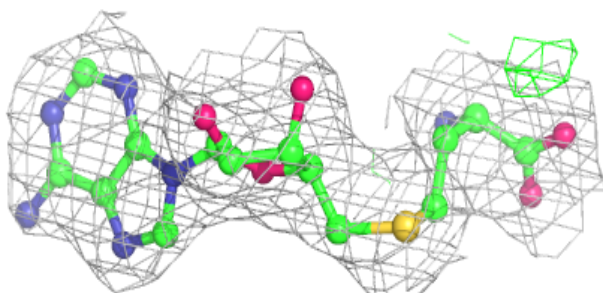
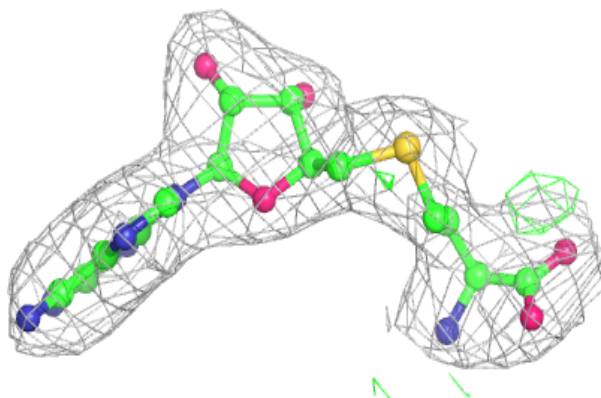


Electron density around SAH K 701:

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

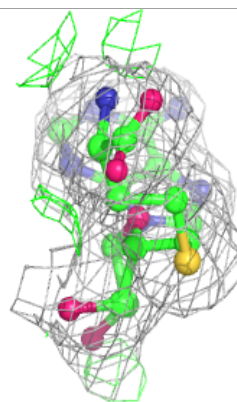
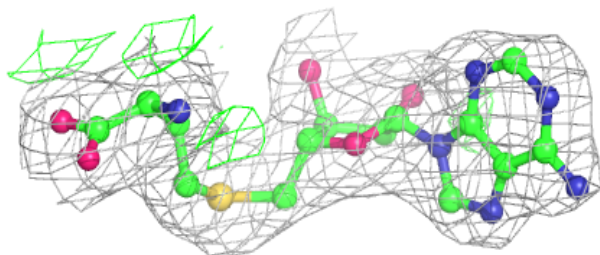
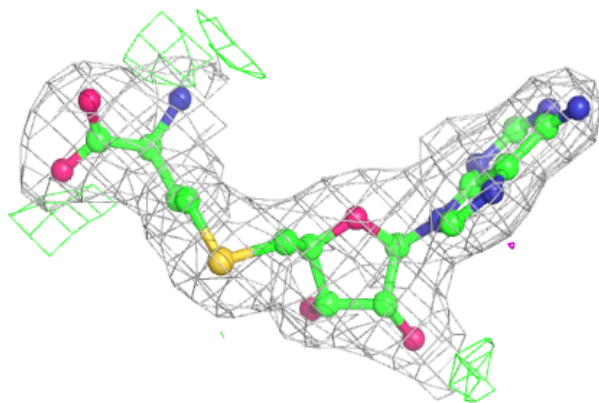
**Electron density around SAH C 701:**

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

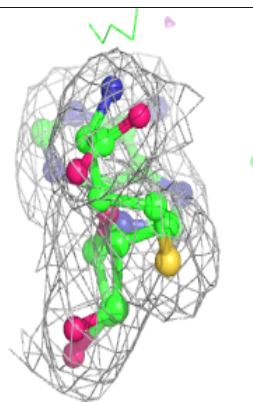
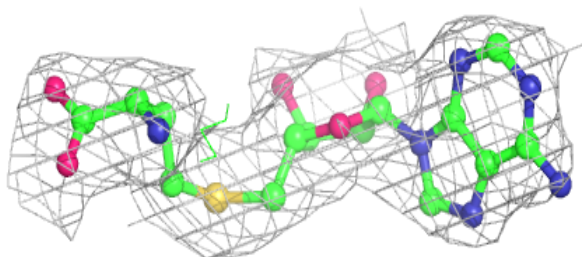
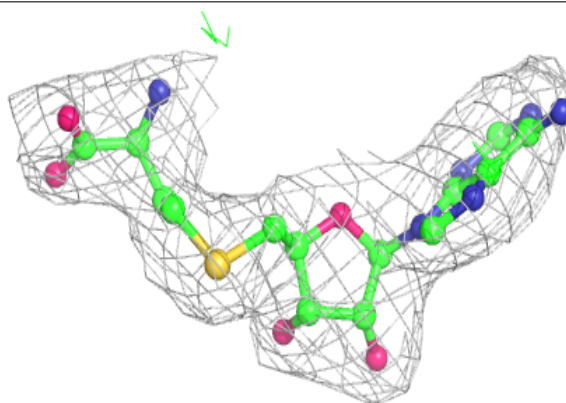


Electron density around SAH D 701:

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

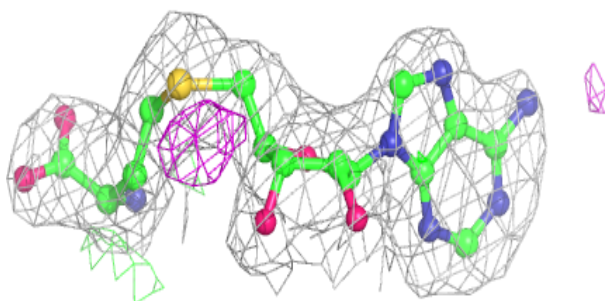
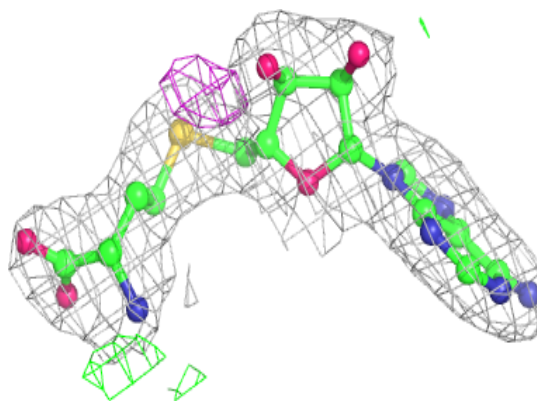
**Electron density around SAH E 701:**

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

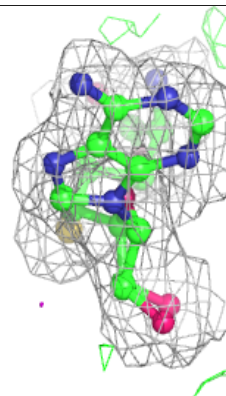
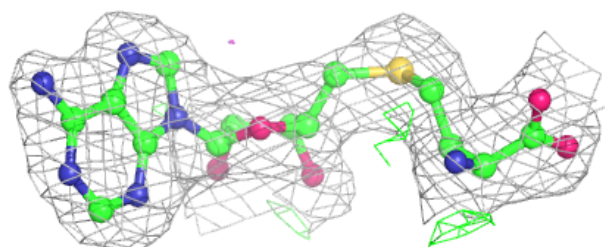
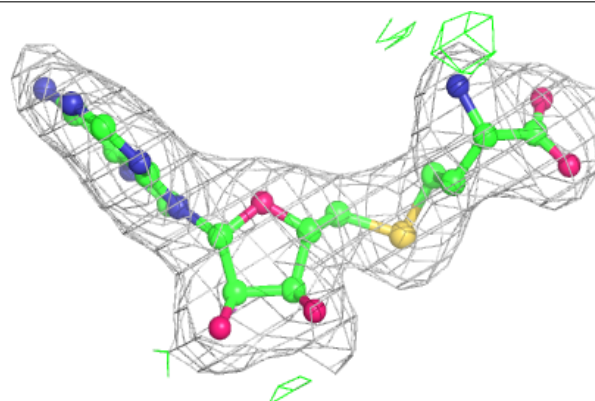


Electron density around SAH F 701:

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

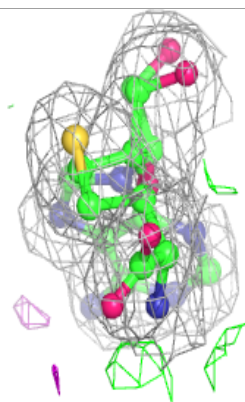
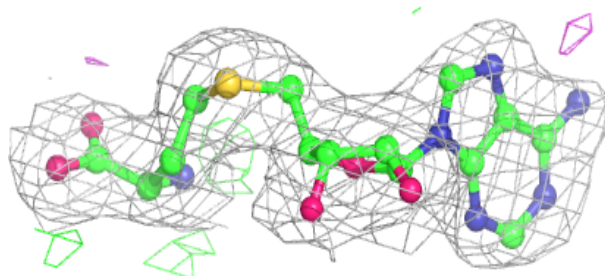
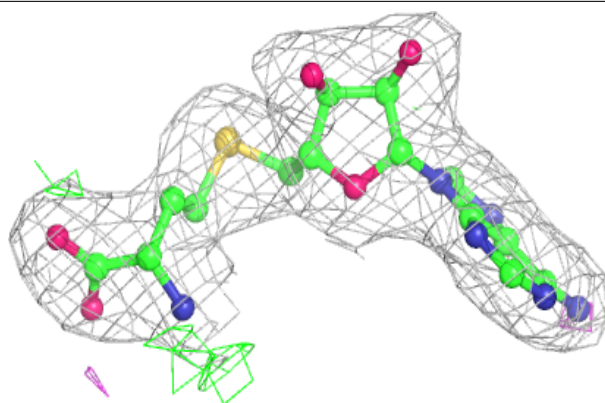
**Electron density around SAH O 701:**

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

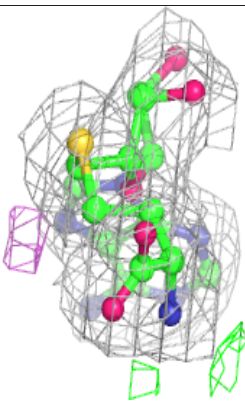
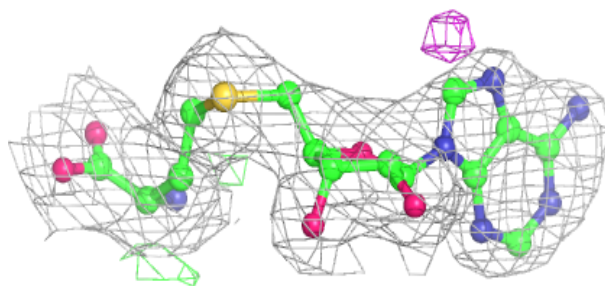
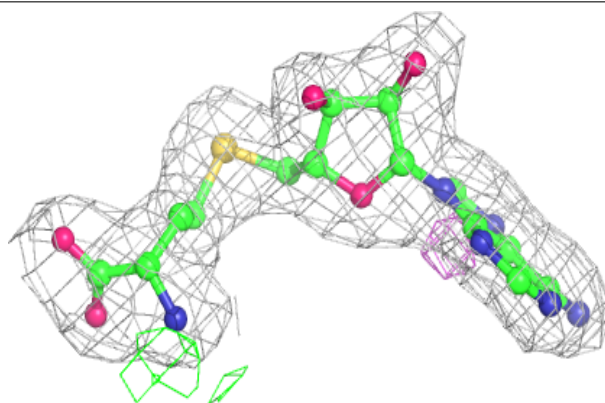


Electron density around SAH I 701:

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

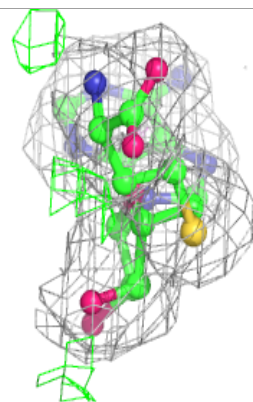
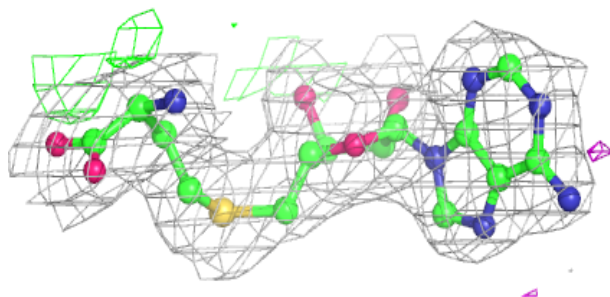
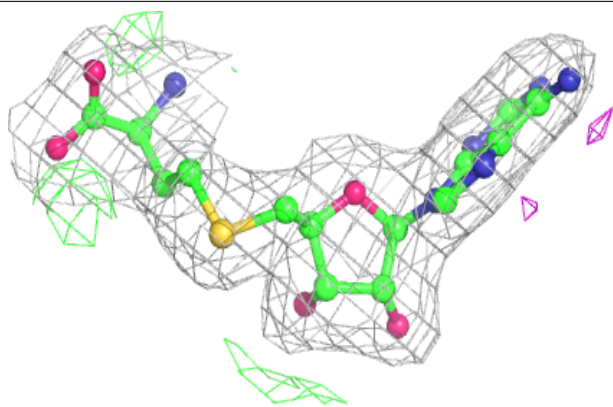
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and green (positive)

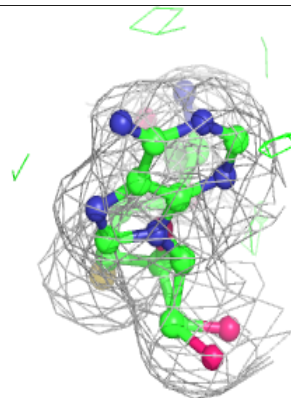
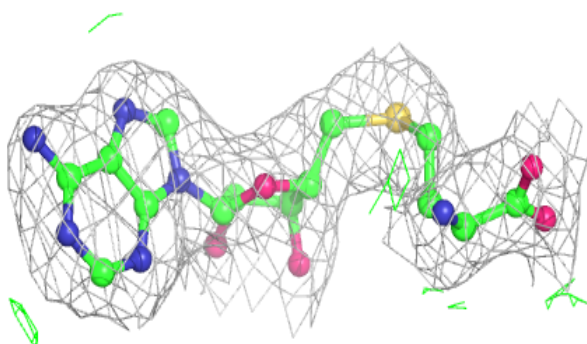
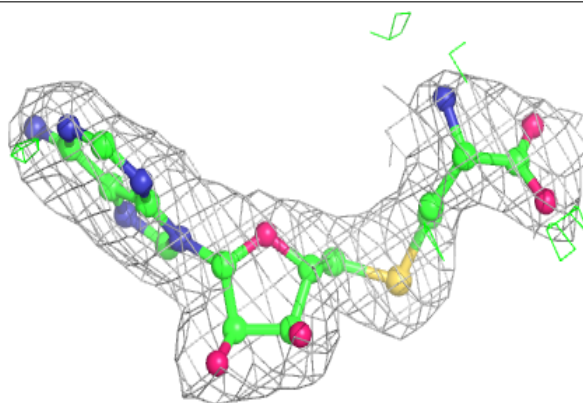


Electron density around SAH J 701:

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

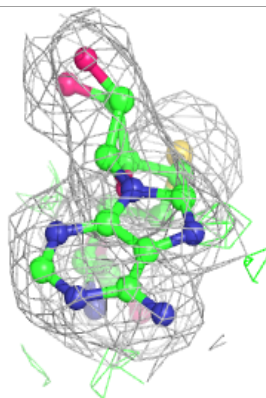
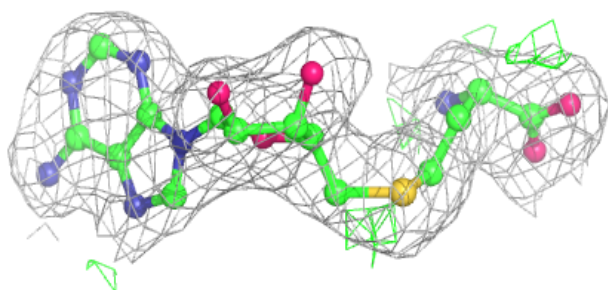
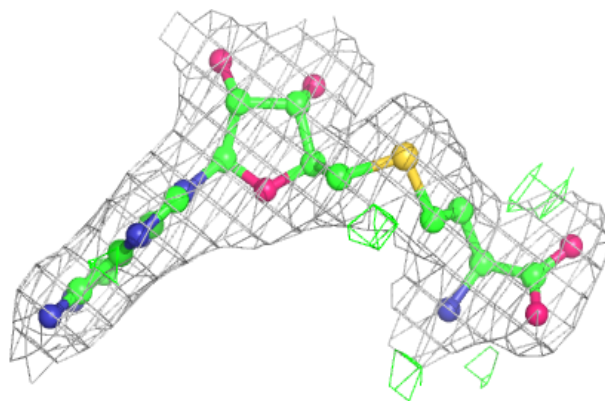
**Electron density around SAH B 701:**

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

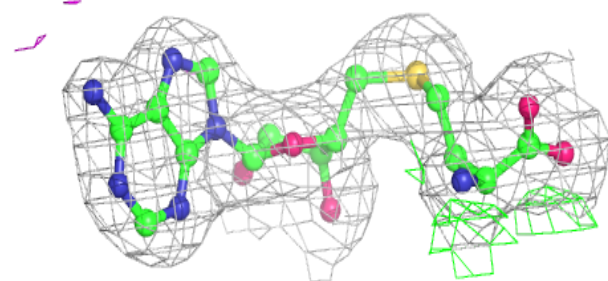
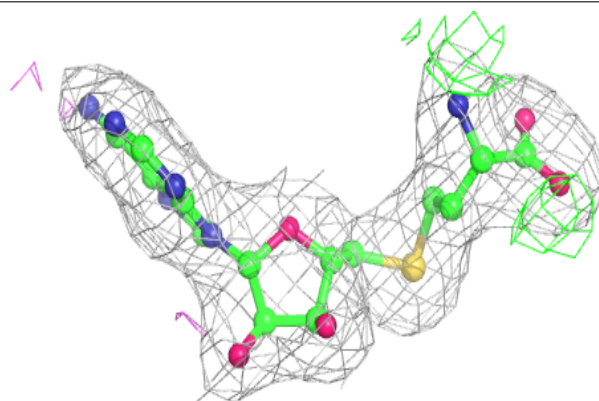


Electron density around SAH H 701:

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

**Electron density around SAH L 701:**

$2mF_o-DF_c$ (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.