



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:12 PM GMT

PDB ID : 4NZF
Title : Crystal structure of Abp-D197A (a GH27-b-L-arabinopyranosidase from *Geobacillus stearothermophilus*), in complex with arabinose
Authors : Lansky, S.; Solomon, H.V.; Salama, R.; Belrhali, H.; Shoham, Y.; Shoham, G.
Deposited on : 2013-12-12
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

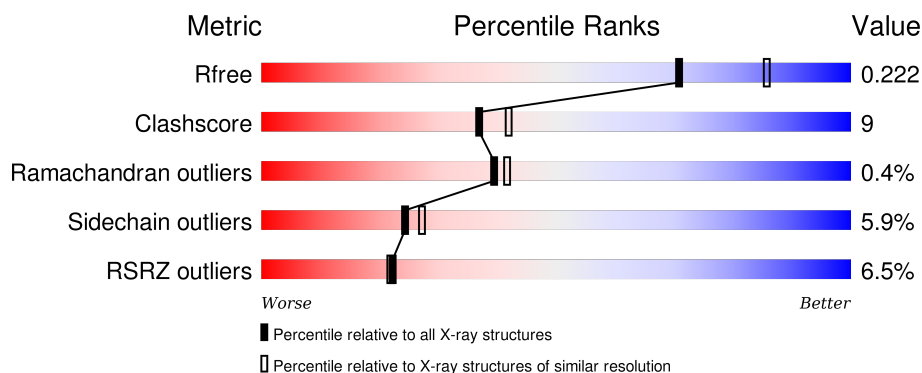
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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} | 91344 | 3774 (2.20-2.20) |
| Clashscore | 102246 | 4477 (2.20-2.20) |
| Ramachandran outliers | 100387 | 4404 (2.20-2.20) |
| Sidechain outliers | 100360 | 4405 (2.20-2.20) |
| RSRZ outliers | 91569 | 3781 (2.20-2.20) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 448 | <div> <div>83%</div> <div>11%</div> <div>...</div> </div> |
| 1 | B | 448 | <div> <div>82%</div> <div>12%</div> <div>..</div> </div> |
| 1 | C | 448 | <div> <div>3%</div> <div>82%</div> <div>13%</div> <div>..</div> </div> |
| 1 | D | 448 | <div> <div>2%</div> <div>81%</div> <div>15%</div> <div>..</div> </div> |
| 1 | E | 448 | <div> <div>5%</div> <div>85%</div> <div>11%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | F | 448 | |
| 1 | G | 448 | |
| 1 | H | 448 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2 | GOL | A | 501 | - | - | X | - |
| 2 | GOL | B | 502 | - | - | - | X |
| 2 | GOL | C | 505 | - | - | - | X |
| 2 | GOL | D | 503 | - | - | X | - |
| 2 | GOL | E | 501 | - | - | - | X |
| 2 | GOL | E | 504 | - | - | - | X |
| 2 | GOL | H | 501 | - | - | - | X |
| 2 | GOL | H | 502 | - | - | X | - |
| 4 | SO4 | A | 507 | - | - | - | X |
| 4 | SO4 | A | 509 | - | - | - | X |
| 4 | SO4 | A | 510 | - | - | - | X |
| 4 | SO4 | A | 514 | - | - | - | X |
| 4 | SO4 | B | 506 | - | - | - | X |
| 4 | SO4 | B | 509 | - | - | - | X |
| 4 | SO4 | C | 509 | - | - | - | X |
| 4 | SO4 | C | 511 | - | - | - | X |
| 4 | SO4 | C | 512 | - | - | - | X |
| 4 | SO4 | C | 514 | - | - | - | X |
| 4 | SO4 | D | 505 | - | - | - | X |
| 4 | SO4 | D | 506 | - | - | - | X |
| 4 | SO4 | D | 507 | - | - | - | X |
| 4 | SO4 | E | 508 | - | - | - | X |
| 4 | SO4 | E | 510 | - | - | - | X |
| 4 | SO4 | E | 512 | - | - | - | X |
| 4 | SO4 | E | 513 | - | - | - | X |
| 4 | SO4 | E | 515 | - | - | - | X |
| 4 | SO4 | F | 504 | - | - | - | X |
| 4 | SO4 | F | 505 | - | - | - | X |
| 4 | SO4 | F | 506 | - | - | - | X |
| 4 | SO4 | F | 513 | - | - | - | X |
| 4 | SO4 | G | 504 | - | - | - | X |
| 4 | SO4 | G | 507 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5 | CIT | A | 515 | - | - | X | X |
| 5 | CIT | B | 519 | - | - | X | X |
| 5 | CIT | C | 519 | - | - | X | X |
| 5 | CIT | D | 515 | - | - | X | X |
| 5 | CIT | E | 517 | - | - | X | X |
| 5 | CIT | G | 510 | - | - | - | X |

2 Entry composition

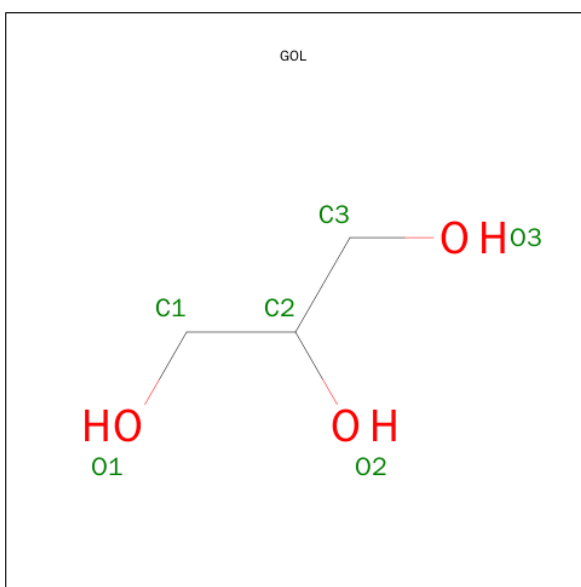
There are 6 unique types of molecules in this entry. The entry contains 31507 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Abp, a GH27 beta-L-arabinopyranosidase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 431 | Total | C | N | O | S | 0 | 3 | 0 |
| | | | 3489 | 2232 | 599 | 633 | 25 | | | |
| 1 | B | 430 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 3482 | 2227 | 598 | 632 | 25 | | | |
| 1 | C | 432 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 3492 | 2233 | 599 | 635 | 25 | | | |
| 1 | D | 435 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 3503 | 2242 | 603 | 633 | 25 | | | |
| 1 | E | 431 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 3477 | 2224 | 597 | 631 | 25 | | | |
| 1 | F | 430 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3467 | 2218 | 596 | 628 | 25 | | | |
| 1 | G | 431 | Total | C | N | O | S | 0 | 4 | 0 |
| | | | 3494 | 2235 | 599 | 635 | 25 | | | |
| 1 | H | 430 | Total | C | N | O | S | 0 | 3 | 0 |
| | | | 3483 | 2230 | 597 | 629 | 27 | | | |

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



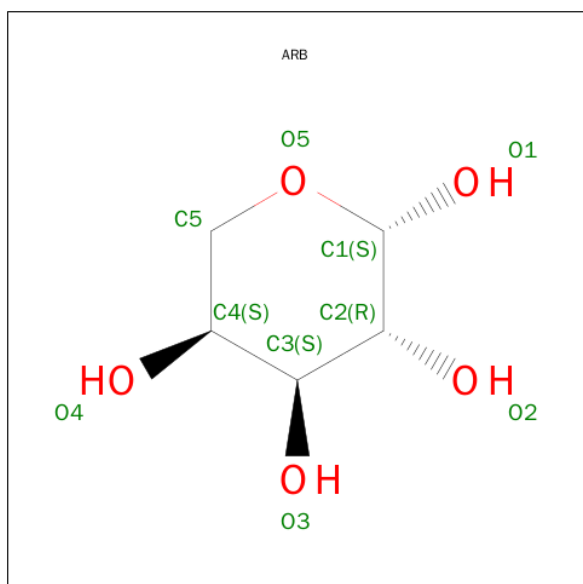
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | A | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | C | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | C | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | C | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | C | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | D | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | D | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | D | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | E | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | E | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | E | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | E | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | F | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | G | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | H | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 2 | H | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |

- Molecule 3 is SUGAR (BETA-L-ARABINOSE) (three-letter code: ARB) (formula: C₅H₁₀O₅).



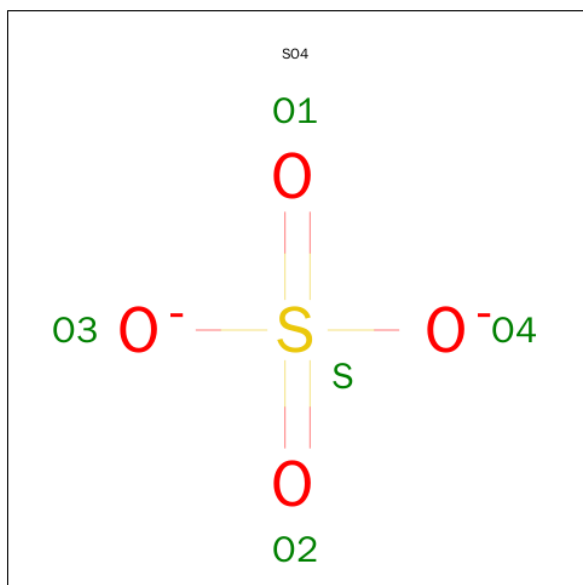
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3 | A | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 5 | 5 | | |
| 3 | B | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 5 | 5 | | |
| 3 | C | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 5 | 5 | | |
| 3 | D | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 5 | 5 | | |
| 3 | E | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 5 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3 | F | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 5 | 5 | | |
| 3 | G | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 5 | 5 | | |
| 3 | H | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 5 | 5 | | |

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

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

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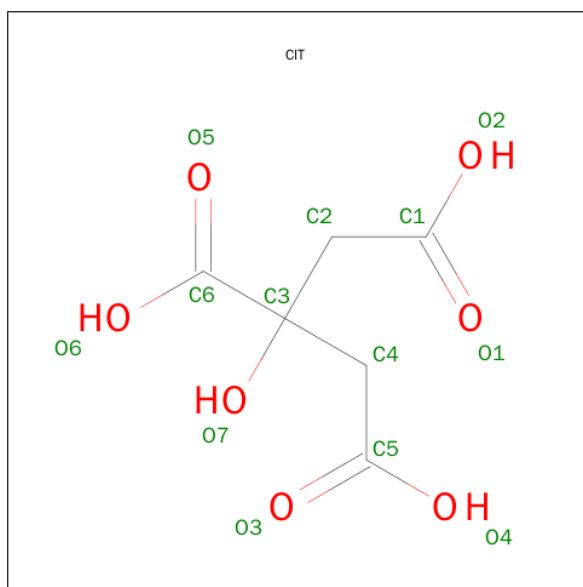
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | G | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4 | G | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | G | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | G | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | G | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | G | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | H | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | H | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | H | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 4 | H | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|---------------------|---------|---------|
| 5 | A | 1 | Total C O 13 6 7 | 0 | 0 |
| 5 | B | 1 | Total C O 13 6 7 | 0 | 0 |
| 5 | C | 1 | Total C O 13 6 7 | 0 | 0 |
| 5 | D | 1 | Total C O 13 6 7 | 0 | 0 |
| 5 | E | 1 | Total C O 13 6 7 | 0 | 0 |
| 5 | G | 1 | Total C O 13 6 7 | 0 | 0 |

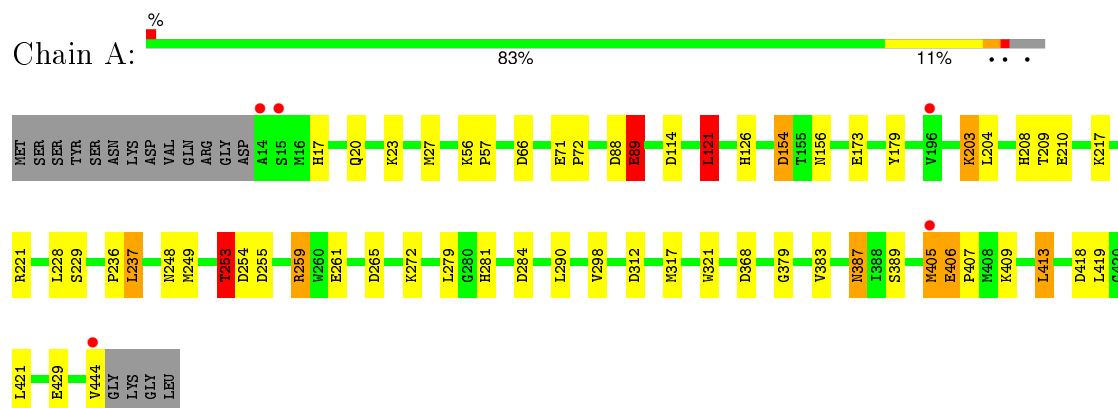
- Molecule 6 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 6 | A | 540 | Total O 540 540 | 0 | 0 |
| 6 | B | 465 | Total O 465 465 | 0 | 0 |
| 6 | C | 421 | Total O 421 421 | 0 | 0 |
| 6 | D | 380 | Total O 380 380 | 0 | 0 |
| 6 | E | 388 | Total O 388 388 | 0 | 0 |
| 6 | F | 298 | Total O 298 298 | 0 | 0 |
| 6 | G | 264 | Total O 264 264 | 0 | 0 |
| 6 | H | 176 | Total O 176 176 | 0 | 0 |

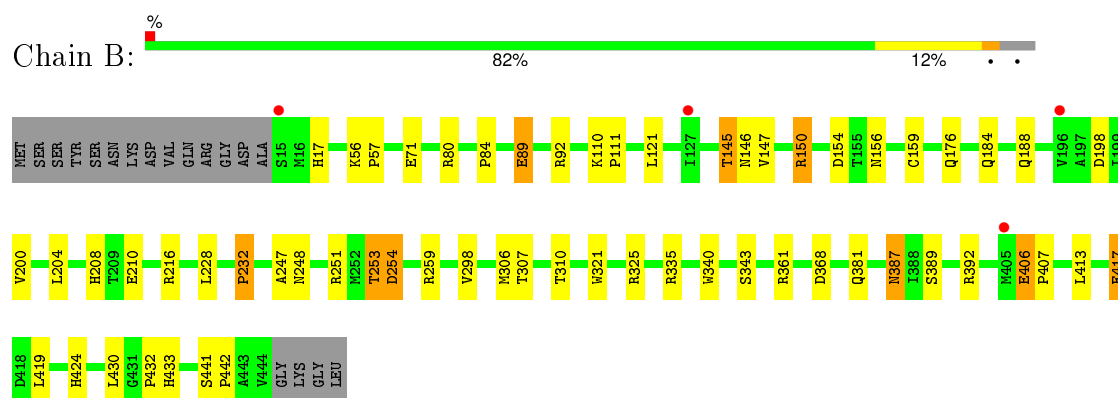
3 Residue-property plots [i](#)

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

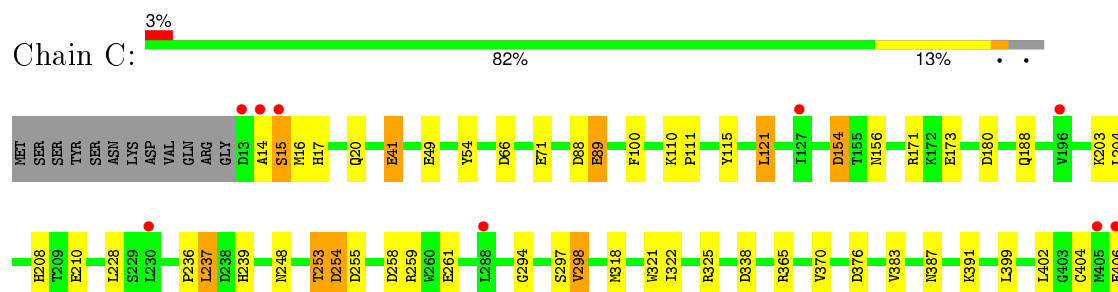
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

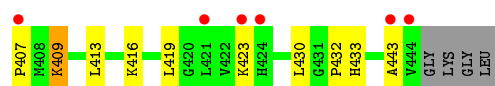


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

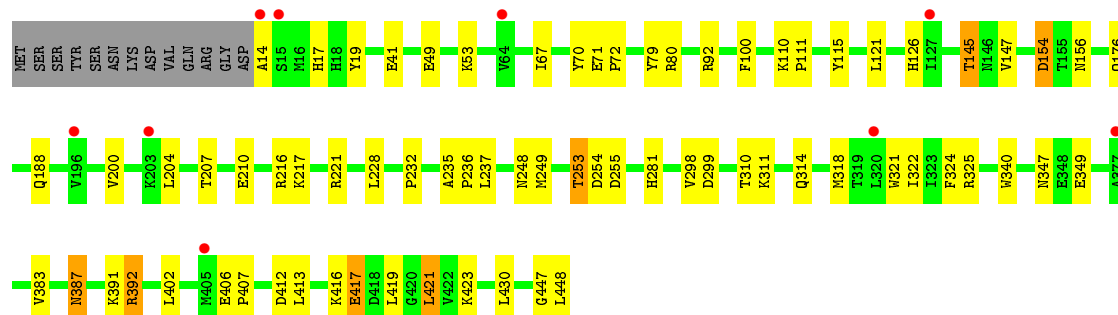
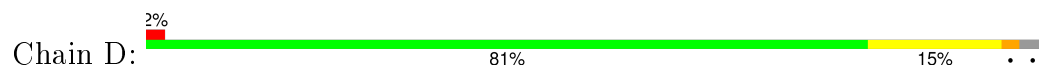


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

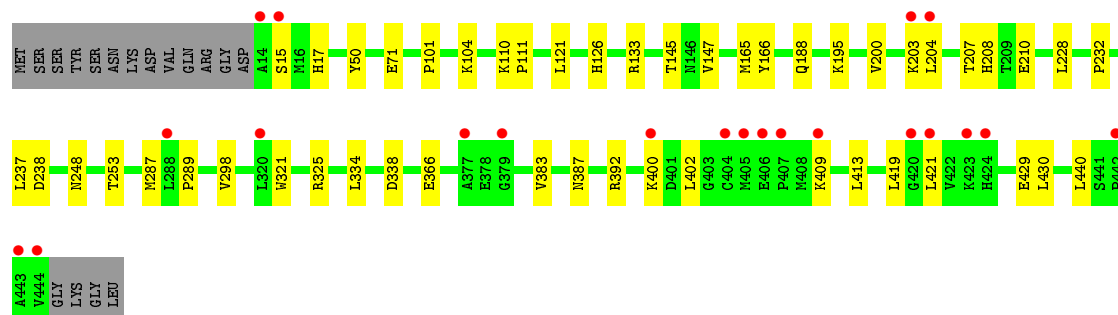
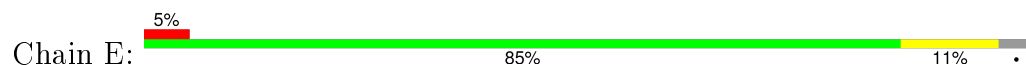




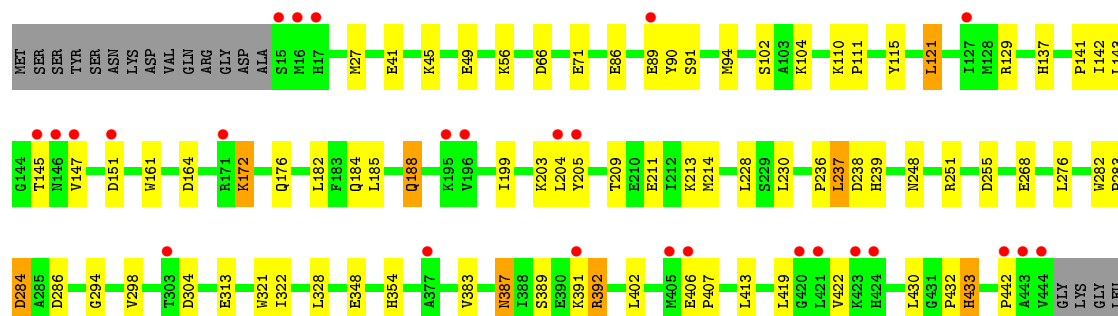
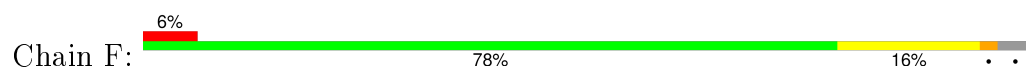
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

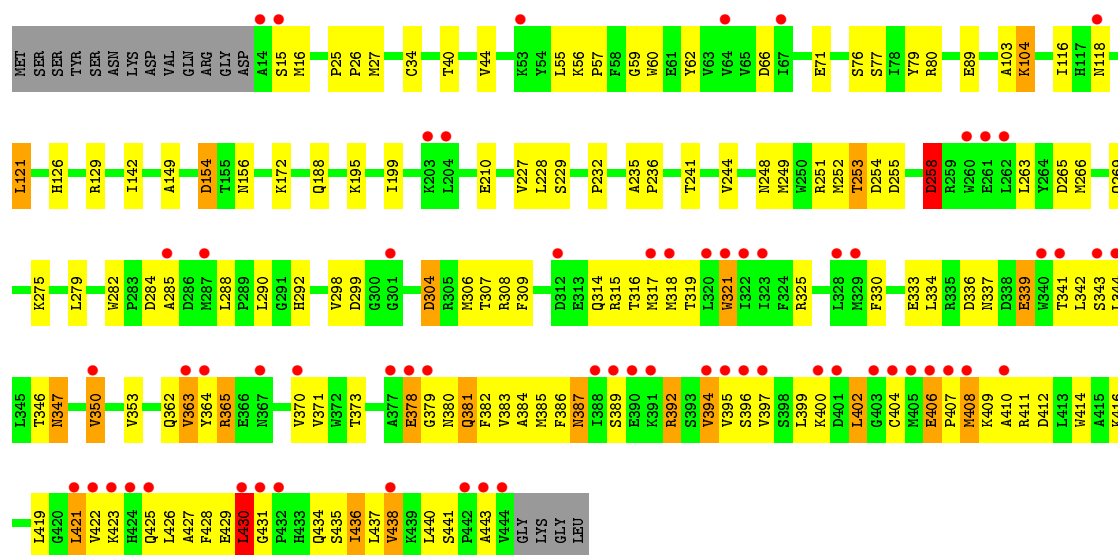


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

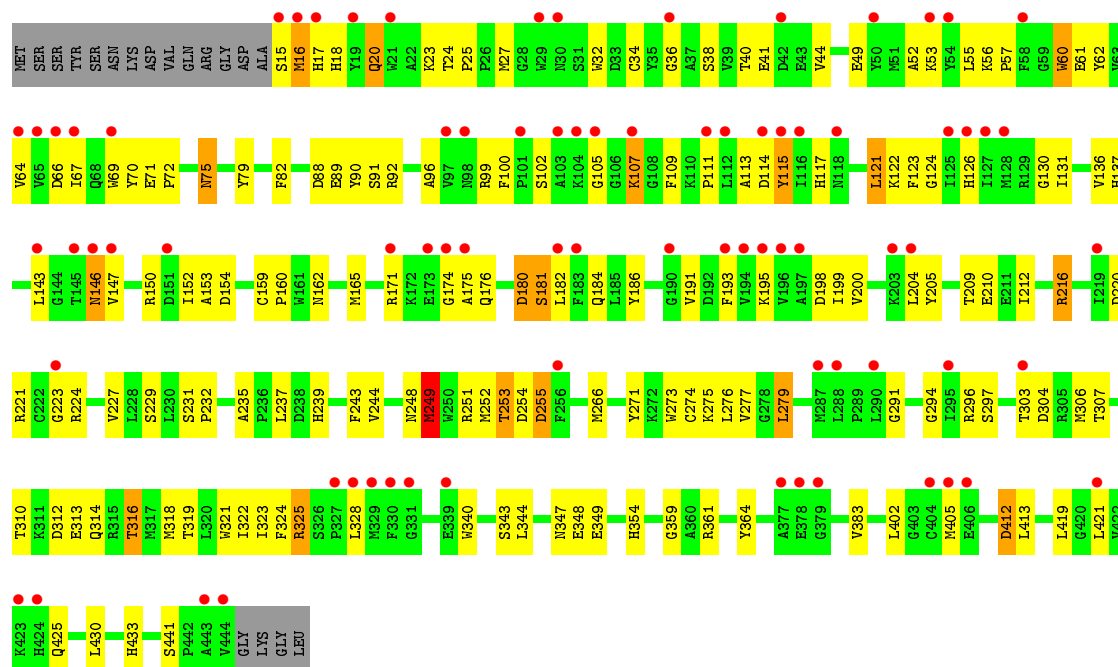


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase





• Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 107.60 Å 201.50 Å 286.91 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 34.71 – 2.19 34.68 – 2.19 | Depositor EDS |
| % Data completeness (in resolution range) | 89.0 (34.71-2.19) 89.1 (34.68-2.19) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.22 (at 2.20 Å) | Xtriage |
| Refinement program | REFMAC 5.7.0029 | Depositor |
| R, R_{free} | 0.168 , 0.219 0.176 , 0.222 | Depositor DCC |
| R_{free} test set | 14318 reflections (5.34%) | DCC |
| Wilson B-factor (Å ²) | 24.9 | Xtriage |
| Anisotropy | 0.800 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.35 , 50.3 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$ | Xtriage |
| Outliers | 0 of 282558 reflections | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 31507 | wwPDB-VP |
| Average B, all atoms (Å ²) | 35.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, ARB, SO4, CIT

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 1.10 | 3/3600 (0.1%) | 1.06 | 17/4887 (0.3%) |
| 1 | B | 1.02 | 1/3587 (0.0%) | 1.00 | 12/4869 (0.2%) |
| 1 | C | 0.93 | 1/3600 (0.0%) | 0.99 | 19/4887 (0.4%) |
| 1 | D | 0.98 | 0/3608 | 0.99 | 7/4895 (0.1%) |
| 1 | E | 0.87 | 0/3582 | 0.92 | 1/4863 (0.0%) |
| 1 | F | 0.85 | 0/3569 | 0.91 | 4/4845 (0.1%) |
| 1 | G | 0.96 | 1/3608 (0.0%) | 1.06 | 10/4898 (0.2%) |
| 1 | H | 0.86 | 0/3594 | 1.00 | 7/4877 (0.1%) |
| All | All | 0.95 | 6/28748 (0.0%) | 0.99 | 77/39021 (0.2%) |

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 | E | 0 | 1 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 253 | THR | CB-CG2 | -7.02 | 1.29 | 1.52 |
| 1 | G | 89 | GLU | CG-CD | 5.74 | 1.60 | 1.51 |
| 1 | A | 179 | TYR | CE1-CZ | -5.29 | 1.31 | 1.38 |
| 1 | C | 154 | ASP | CB-CG | -5.24 | 1.40 | 1.51 |
| 1 | B | 325 | ARG | CZ-NH2 | 5.02 | 1.39 | 1.33 |
| 1 | A | 89 | GLU | CG-CD | 5.01 | 1.59 | 1.51 |

All (77) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|--------|------|------------|--------|-------------|----------|
| 1 | D | 154 | ASP | CB-CG-OD2 | -10.11 | 109.20 | 118.30 |
| 1 | C | 154 | ASP | CB-CG-OD2 | -9.64 | 109.63 | 118.30 |
| 1 | C | 338 | ASP | CB-CG-OD1 | 8.30 | 125.78 | 118.30 |
| 1 | G | 251 | ARG | NE-CZ-NH2 | -8.16 | 116.22 | 120.30 |
| 1 | A | 368 | ASP | CB-CG-OD1 | 8.02 | 125.52 | 118.30 |
| 1 | A | 368 | ASP | CB-CG-OD2 | -7.95 | 111.15 | 118.30 |
| 1 | A | 259 | ARG | NE-CZ-NH2 | -7.76 | 116.42 | 120.30 |
| 1 | G | 430 | LEU | CA-CB-CG | 7.24 | 131.94 | 115.30 |
| 1 | H | 180 | ASP | CB-CG-OD2 | 7.24 | 124.81 | 118.30 |
| 1 | A | 154 | ASP | CB-CG-OD2 | -7.08 | 111.93 | 118.30 |
| 1 | A | 237 | LEU | CA-CB-CG | -7.05 | 99.08 | 115.30 |
| 1 | A | 121 | LEU | CB-CG-CD1 | 6.97 | 122.84 | 111.00 |
| 1 | G | 80 | ARG | NE-CZ-NH1 | 6.89 | 123.75 | 120.30 |
| 1 | C | 88 | ASP | CB-CG-OD1 | 6.88 | 124.50 | 118.30 |
| 1 | G | 154[A] | ASP | CB-CG-OD2 | -6.83 | 112.15 | 118.30 |
| 1 | G | 154[B] | ASP | CB-CG-OD2 | -6.83 | 112.15 | 118.30 |
| 1 | D | 80 | ARG | NE-CZ-NH1 | 6.83 | 123.71 | 120.30 |
| 1 | G | 251 | ARG | NE-CZ-NH1 | 6.68 | 123.64 | 120.30 |
| 1 | B | 216 | ARG | NE-CZ-NH2 | 6.63 | 123.61 | 120.30 |
| 1 | H | 249 | MET | CG-SD-CE | 6.53 | 110.64 | 100.20 |
| 1 | C | 338 | ASP | CB-CG-OD2 | -6.42 | 112.52 | 118.30 |
| 1 | H | 88 | ASP | CB-CG-OD1 | -6.35 | 112.58 | 118.30 |
| 1 | A | 284 | ASP | CB-CG-OD1 | 6.34 | 124.01 | 118.30 |
| 1 | G | 80 | ARG | NE-CZ-NH2 | -6.25 | 117.18 | 120.30 |
| 1 | B | 92 | ARG | NE-CZ-NH1 | 6.24 | 123.42 | 120.30 |
| 1 | H | 216 | ARG | NE-CZ-NH2 | 6.21 | 123.40 | 120.30 |
| 1 | C | 171 | ARG | NE-CZ-NH2 | 6.11 | 123.36 | 120.30 |
| 1 | B | 80 | ARG | NE-CZ-NH1 | 6.09 | 123.35 | 120.30 |
| 1 | C | 89 | GLU | CB-CA-C | -6.04 | 98.31 | 110.40 |
| 1 | C | 180 | ASP | CB-CG-OD2 | 6.02 | 123.72 | 118.30 |
| 1 | A | 284 | ASP | CB-CG-OD2 | -6.01 | 112.89 | 118.30 |
| 1 | A | 418 | ASP | CB-CG-OD1 | 5.96 | 123.66 | 118.30 |
| 1 | H | 255 | ASP | CB-CG-OD2 | -5.91 | 112.98 | 118.30 |
| 1 | C | 376 | ASP | CB-CG-OD1 | 5.88 | 123.59 | 118.30 |
| 1 | D | 92 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 1 | B | 325 | ARG | NE-CZ-NH1 | -5.85 | 117.38 | 120.30 |
| 1 | D | 421 | LEU | CA-CB-CG | 5.80 | 128.64 | 115.30 |
| 1 | C | 41 | GLU | OE1-CD-OE2 | -5.79 | 116.35 | 123.30 |
| 1 | C | 325 | ARG | NE-CZ-NH2 | -5.78 | 117.41 | 120.30 |
| 1 | B | 251 | ARG | NE-CZ-NH2 | -5.78 | 117.41 | 120.30 |
| 1 | C | 237 | LEU | CA-CB-CG | -5.74 | 102.10 | 115.30 |
| 1 | F | 284 | ASP | CB-CG-OD2 | -5.62 | 113.24 | 118.30 |
| 1 | B | 254 | ASP | CB-CG-OD1 | 5.54 | 123.29 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | H | 412 | ASP | CB-CG-OD2 | 5.54 | 123.29 | 118.30 |
| 1 | A | 88 | ASP | CB-CG-OD1 | 5.53 | 123.28 | 118.30 |
| 1 | F | 237 | LEU | CA-CB-CG | -5.50 | 102.65 | 115.30 |
| 1 | C | 121 | LEU | CB-CG-CD1 | 5.48 | 120.32 | 111.00 |
| 1 | C | 298 | VAL | N-CA-CB | -5.44 | 99.53 | 111.50 |
| 1 | D | 299 | ASP | CB-CG-OD2 | 5.41 | 123.17 | 118.30 |
| 1 | A | 221 | ARG | NE-CZ-NH1 | 5.41 | 123.00 | 120.30 |
| 1 | A | 312 | ASP | CB-CG-OD1 | 5.39 | 123.15 | 118.30 |
| 1 | B | 150 | ARG | NE-CZ-NH2 | -5.39 | 117.61 | 120.30 |
| 1 | G | 304 | ASP | CB-CG-OD2 | 5.35 | 123.11 | 118.30 |
| 1 | B | 368 | ASP | CB-CG-OD1 | 5.33 | 123.09 | 118.30 |
| 1 | A | 27 | MET | CG-SD-CE | 5.30 | 108.68 | 100.20 |
| 1 | B | 361 | ARG | NE-CZ-NH1 | -5.29 | 117.66 | 120.30 |
| 1 | B | 150 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 1 | H | 180 | ASP | CB-CG-OD1 | -5.22 | 113.60 | 118.30 |
| 1 | D | 80 | ARG | NE-CZ-NH2 | -5.22 | 117.69 | 120.30 |
| 1 | A | 405 | MET | CG-SD-CE | 5.21 | 108.53 | 100.20 |
| 1 | C | 171 | ARG | NE-CZ-NH1 | -5.17 | 117.72 | 120.30 |
| 1 | B | 259 | ARG | NE-CZ-NH2 | -5.16 | 117.72 | 120.30 |
| 1 | A | 253 | THR | N-CA-CB | -5.14 | 100.53 | 110.30 |
| 1 | C | 254 | ASP | CB-CG-OD1 | 5.14 | 122.92 | 118.30 |
| 1 | F | 164 | ASP | CB-CG-OD1 | 5.12 | 122.91 | 118.30 |
| 1 | G | 129 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 1 | A | 114 | ASP | CB-CG-OD1 | 5.10 | 122.89 | 118.30 |
| 1 | C | 88 | ASP | CB-CG-OD2 | -5.08 | 113.72 | 118.30 |
| 1 | G | 392 | ARG | NE-CZ-NH2 | -5.08 | 117.76 | 120.30 |
| 1 | E | 238 | ASP | CB-CG-OD2 | -5.08 | 113.73 | 118.30 |
| 1 | A | 413 | LEU | CB-CG-CD1 | 5.07 | 119.62 | 111.00 |
| 1 | D | 154 | ASP | OD1-CG-OD2 | 5.06 | 132.91 | 123.30 |
| 1 | F | 286 | ASP | CB-CG-OD2 | -5.03 | 113.78 | 118.30 |
| 1 | C | 255 | ASP | CB-CG-OD2 | -5.02 | 113.78 | 118.30 |
| 1 | C | 298 | VAL | CG1-CB-CG2 | 5.02 | 118.93 | 110.90 |
| 1 | B | 335 | ARG | NE-CZ-NH2 | 5.02 | 122.81 | 120.30 |
| 1 | C | 15 | SER | N-CA-C | 5.00 | 124.51 | 111.00 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | E | 165 | MET | 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 | 3489 | 0 | 3372 | 47 | 0 |
| 1 | B | 3482 | 0 | 3360 | 40 | 0 |
| 1 | C | 3492 | 0 | 3370 | 35 | 0 |
| 1 | D | 3503 | 0 | 3395 | 49 | 0 |
| 1 | E | 3477 | 0 | 3356 | 30 | 0 |
| 1 | F | 3467 | 0 | 3347 | 43 | 0 |
| 1 | G | 3494 | 0 | 3376 | 124 | 0 |
| 1 | H | 3483 | 0 | 3373 | 140 | 0 |
| 2 | A | 6 | 0 | 8 | 8 | 0 |
| 2 | B | 18 | 0 | 24 | 2 | 0 |
| 2 | C | 30 | 0 | 40 | 2 | 0 |
| 2 | D | 18 | 0 | 24 | 7 | 0 |
| 2 | E | 24 | 0 | 32 | 3 | 0 |
| 2 | F | 6 | 0 | 8 | 0 | 0 |
| 2 | G | 6 | 0 | 8 | 1 | 0 |
| 2 | H | 12 | 0 | 16 | 4 | 0 |
| 3 | A | 10 | 0 | 10 | 0 | 0 |
| 3 | B | 10 | 0 | 10 | 0 | 0 |
| 3 | C | 10 | 0 | 10 | 0 | 0 |
| 3 | D | 10 | 0 | 10 | 0 | 0 |
| 3 | E | 10 | 0 | 10 | 0 | 0 |
| 3 | F | 10 | 0 | 10 | 1 | 0 |
| 3 | G | 10 | 0 | 10 | 2 | 0 |
| 3 | H | 10 | 0 | 10 | 0 | 0 |
| 4 | A | 60 | 0 | 0 | 1 | 0 |
| 4 | B | 70 | 0 | 0 | 4 | 0 |
| 4 | C | 60 | 0 | 0 | 4 | 0 |
| 4 | D | 50 | 0 | 0 | 5 | 0 |
| 4 | E | 55 | 0 | 0 | 1 | 0 |
| 4 | F | 55 | 0 | 0 | 0 | 0 |
| 4 | G | 35 | 0 | 0 | 0 | 0 |
| 4 | H | 25 | 0 | 0 | 0 | 0 |
| 5 | A | 13 | 0 | 5 | 6 | 0 |
| 5 | B | 13 | 0 | 5 | 6 | 0 |
| 5 | C | 13 | 0 | 5 | 9 | 0 |
| 5 | D | 13 | 0 | 5 | 7 | 0 |
| 5 | E | 13 | 0 | 5 | 9 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | G | 13 | 0 | 5 | 3 | 0 |
| 6 | A | 540 | 0 | 0 | 21 | 1 |
| 6 | B | 465 | 0 | 0 | 13 | 1 |
| 6 | C | 421 | 0 | 0 | 10 | 0 |
| 6 | D | 380 | 0 | 0 | 11 | 0 |
| 6 | E | 388 | 0 | 0 | 8 | 0 |
| 6 | F | 298 | 0 | 0 | 10 | 0 |
| 6 | G | 264 | 0 | 0 | 35 | 0 |
| 6 | H | 176 | 0 | 0 | 37 | 0 |
| All | All | 31507 | 0 | 27219 | 522 | 1 |

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 9.

All (522) 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:G:347:ASN:HA | 6:G:785:HOH:O | 1.48 | 1.10 |
| 1:A:17:HIS:CE1 | 6:A:1094:HOH:O | 2.18 | 0.96 |
| 1:G:363:VAL:HG13 | 1:G:371:VAL:HG23 | 1.47 | 0.93 |
| 1:A:406:GLU:HB2 | 1:A:407:PRO:HD2 | 1.49 | 0.92 |
| 1:G:188[B]:GLN:HG3 | 6:G:731:HOH:O | 1.70 | 0.90 |
| 1:G:346:THR:HG21 | 6:G:846:HOH:O | 1.73 | 0.87 |
| 1:H:324:PHE:O | 6:H:761:HOH:O | 1.93 | 0.85 |
| 1:H:82:PHE:HA | 6:H:658:HOH:O | 1.76 | 0.85 |
| 1:G:431:GLY:HA3 | 6:G:666:HOH:O | 1.77 | 0.84 |
| 1:B:228:LEU:H | 1:B:248:ASN:HD22 | 1.22 | 0.83 |
| 1:F:228:LEU:H | 1:F:248:ASN:HD22 | 1.22 | 0.83 |
| 1:G:292:HIS:ND1 | 1:G:336:ASP:OD2 | 2.10 | 0.83 |
| 1:H:425[B]:GLN:NE2 | 6:H:766:HOH:O | 2.08 | 0.82 |
| 1:D:210:GLU:H | 5:D:515:CIT:H22 | 1.44 | 0.82 |
| 1:E:145:THR:HG23 | 6:E:841:HOH:O | 1.81 | 0.81 |
| 1:G:318:MET:HB3 | 6:G:835:HOH:O | 1.80 | 0.80 |
| 1:H:56:LYS:HB2 | 6:H:742:HOH:O | 1.82 | 0.80 |
| 1:A:228:LEU:H | 1:A:248:ASN:HD22 | 1.31 | 0.79 |
| 1:B:210:GLU:H | 5:B:519:CIT:H41 | 1.47 | 0.78 |
| 1:G:77:SER:OG | 1:G:299:ASP:OD1 | 2.01 | 0.77 |
| 1:A:154:ASP:HB2 | 6:A:744:HOH:O | 1.85 | 0.77 |
| 1:C:228:LEU:H | 1:C:248:ASN:HD22 | 1.32 | 0.77 |
| 1:E:208:HIS:HA | 5:E:517:CIT:O5 | 1.85 | 0.76 |
| 1:C:14:ALA:HB3 | 6:C:958:HOH:O | 1.85 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:417:GLU:CB | 6:D:810:HOH:O | 2.34 | 0.75 |
| 1:H:340:TRP:O | 1:H:343:SER:OG | 2.04 | 0.75 |
| 1:H:70:TYR:CE2 | 6:H:649:HOH:O | 2.40 | 0.75 |
| 1:H:92:ARG:HD3 | 1:H:181:SER:OG | 1.87 | 0.73 |
| 1:H:56:LYS:CB | 6:H:742:HOH:O | 2.35 | 0.73 |
| 1:H:159:CYS:SG | 1:H:198:ASP:OD1 | 2.45 | 0.73 |
| 1:E:228:LEU:H | 1:E:248:ASN:HD22 | 1.34 | 0.73 |
| 1:H:184:GLN:HA | 6:H:646:HOH:O | 1.89 | 0.73 |
| 1:H:223:GLY:N | 6:H:760:HOH:O | 2.17 | 0.72 |
| 1:D:17:HIS:CE1 | 6:D:782:HOH:O | 2.41 | 0.72 |
| 1:B:406:GLU:HB2 | 1:B:407:PRO:CD | 2.20 | 0.71 |
| 1:G:363:VAL:CG1 | 1:G:371:VAL:HG23 | 2.20 | 0.71 |
| 1:A:89:GLU:CD | 1:A:89:GLU:H | 1.94 | 0.71 |
| 1:A:406:GLU:HB2 | 1:A:407:PRO:CD | 2.21 | 0.70 |
| 1:H:318:MET:O | 1:H:322:ILE:HG12 | 1.91 | 0.70 |
| 1:C:188[B]:GLN:CD | 6:C:830:HOH:O | 2.30 | 0.70 |
| 1:C:253:THR:HG23 | 1:C:254:ASP:O | 1.91 | 0.70 |
| 1:F:41:GLU:OE2 | 1:F:102:SER:OG | 2.07 | 0.70 |
| 1:H:114:ASP:HA | 6:H:746:HOH:O | 1.92 | 0.69 |
| 1:G:342:LEU:O | 1:G:342:LEU:HD12 | 1.93 | 0.69 |
| 1:D:417:GLU:HB2 | 6:D:810:HOH:O | 1.93 | 0.68 |
| 1:B:210:GLU:HG2 | 5:B:519:CIT:H42 | 1.76 | 0.68 |
| 1:G:378:GLU:OE1 | 1:G:378:GLU:N | 2.27 | 0.67 |
| 1:G:304:ASP:OD1 | 1:G:304:ASP:C | 2.31 | 0.67 |
| 2:A:501:GOL:C1 | 6:A:1086:HOH:O | 2.42 | 0.67 |
| 1:F:129:ARG:NH1 | 1:F:211:GLU:OE2 | 2.22 | 0.67 |
| 1:D:228:LEU:H | 1:D:248:ASN:HD22 | 1.43 | 0.66 |
| 1:G:362:GLN:NE2 | 6:G:837:HOH:O | 2.28 | 0.65 |
| 1:G:275:LYS:HE3 | 1:H:244:VAL:HG11 | 1.78 | 0.65 |
| 1:G:412:ASP:OD2 | 1:G:436:ILE:HD11 | 1.95 | 0.65 |
| 1:C:14:ALA:CB | 6:C:958:HOH:O | 2.41 | 0.65 |
| 1:C:210:GLU:HB2 | 5:C:519:CIT:H41 | 1.76 | 0.65 |
| 1:B:145:THR:HG23 | 6:B:945:HOH:O | 1.96 | 0.65 |
| 4:D:510:SO4:O2 | 6:D:961:HOH:O | 2.13 | 0.65 |
| 1:H:75:ASN:HD22 | 1:H:75:ASN:N | 1.94 | 0.65 |
| 1:H:182:LEU:O | 1:H:186:TYR:CD2 | 2.50 | 0.65 |
| 1:A:265:ASP:HB3 | 6:A:975:HOH:O | 1.96 | 0.64 |
| 1:H:20:GLN:N | 1:H:20:GLN:HE21 | 1.95 | 0.64 |
| 1:A:210:GLU:HB2 | 5:A:515:CIT:H22 | 1.79 | 0.64 |
| 1:A:173:GLU:OE2 | 4:A:506:SO4:O4 | 2.14 | 0.64 |
| 1:D:448:LEU:C | 6:D:824:HOH:O | 2.34 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:G:266:MET:HE3 | 1:G:321:TRP:CH2 | 2.33 | 0.64 |
| 1:G:255:ASP:OD1 | 2:G:501:GOL:H11 | 1.98 | 0.64 |
| 2:A:501:GOL:C2 | 6:A:1086:HOH:O | 2.45 | 0.64 |
| 1:G:334:LEU:O | 1:G:337:ASN:ND2 | 2.30 | 0.64 |
| 1:D:210:GLU:HB2 | 5:D:515:CIT:H41 | 1.80 | 0.64 |
| 5:B:519:CIT:O1 | 6:B:1049:HOH:O | 2.16 | 0.63 |
| 5:G:510:CIT:H22 | 5:G:510:CIT:O3 | 1.97 | 0.63 |
| 1:H:210:GLU:HA | 1:H:210:GLU:OE1 | 1.99 | 0.63 |
| 1:B:253:THR:HG23 | 1:B:254:ASP:O | 1.98 | 0.62 |
| 1:H:66:ASP:HA | 1:H:126:HIS:HB2 | 1.82 | 0.62 |
| 1:D:255:ASP:OD2 | 2:D:501:GOL:H31 | 2.00 | 0.62 |
| 1:G:394:VAL:HA | 1:G:429:GLU:HA | 1.82 | 0.62 |
| 4:B:507:SO4:O3 | 6:B:1031:HOH:O | 2.15 | 0.62 |
| 1:G:342:LEU:HD12 | 1:G:342:LEU:C | 2.20 | 0.62 |
| 1:G:347:ASN:HD22 | 1:G:350:VAL:H | 1.47 | 0.62 |
| 1:F:110:LYS:HB3 | 1:F:111:PRO:HD3 | 1.82 | 0.61 |
| 1:D:188:GLN:NE2 | 6:D:820:HOH:O | 2.32 | 0.61 |
| 1:A:208:HIS:HA | 5:A:515:CIT:O6 | 2.00 | 0.61 |
| 1:G:428:PHE:O | 1:G:430:LEU:HD22 | 2.00 | 0.61 |
| 1:H:130:GLY:C | 6:H:634:HOH:O | 2.38 | 0.61 |
| 1:C:210:GLU:H | 5:C:519:CIT:H22 | 1.65 | 0.61 |
| 1:G:210:GLU:H | 5:G:510:CIT:H42 | 1.65 | 0.61 |
| 1:C:49:GLU:OE2 | 1:C:115:TYR:OH | 2.17 | 0.61 |
| 1:A:89:GLU:CG | 6:A:856:HOH:O | 2.49 | 0.60 |
| 1:B:253:THR:CG2 | 1:B:254:ASP:O | 2.49 | 0.60 |
| 1:A:203:LYS:HE3 | 6:A:1127:HOH:O | 2.02 | 0.60 |
| 1:A:208:HIS:C | 5:A:515:CIT:O6 | 2.39 | 0.60 |
| 1:G:346:THR:CG2 | 6:G:846:HOH:O | 2.38 | 0.60 |
| 1:F:45:LYS:NZ | 6:F:838:HOH:O | 2.23 | 0.60 |
| 1:E:325:ARG:HD2 | 6:E:984:HOH:O | 2.01 | 0.60 |
| 1:G:350:VAL:HG22 | 1:G:437:LEU:HD23 | 1.84 | 0.60 |
| 1:H:175:ALA:N | 2:H:502:GOL:H32 | 2.16 | 0.60 |
| 1:G:66:ASP:OD2 | 1:G:195:LYS:NZ | 2.35 | 0.60 |
| 1:G:350:VAL:HG22 | 1:G:437:LEU:CD2 | 2.32 | 0.60 |
| 1:A:208:HIS:CA | 5:A:515:CIT:O6 | 2.50 | 0.60 |
| 1:A:154:ASP:CB | 6:A:744:HOH:O | 2.43 | 0.60 |
| 1:G:172:LYS:NZ | 6:G:677:HOH:O | 2.34 | 0.60 |
| 1:G:154[B]:ASP:OD2 | 6:G:653:HOH:O | 2.16 | 0.59 |
| 1:G:378:GLU:CD | 1:G:378:GLU:H | 2.05 | 0.59 |
| 1:B:156:ASN:HD21 | 1:D:204:LEU:HD11 | 1.67 | 0.59 |
| 1:A:255:ASP:OD2 | 2:A:501:GOL:C1 | 2.50 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:G:365:ARG:HB2 | 1:G:370:VAL:HG22 | 1.85 | 0.59 |
| 1:D:253:THR:CG2 | 1:D:254:ASP:O | 2.50 | 0.59 |
| 1:E:188:GLN:HG2 | 6:E:831:HOH:O | 2.02 | 0.59 |
| 1:B:176:GLN:HB3 | 2:B:503:GOL:H31 | 1.84 | 0.59 |
| 1:G:347:ASN:HB3 | 1:G:350:VAL:HB | 1.83 | 0.59 |
| 1:H:252[A]:MET:HG2 | 1:H:273:TRP:CD1 | 2.37 | 0.59 |
| 1:G:344:LEU:HD21 | 6:G:804:HOH:O | 2.02 | 0.59 |
| 1:H:136:VAL:HG21 | 1:H:153:ALA:HB2 | 1.85 | 0.59 |
| 1:G:228:LEU:H | 1:G:248:ASN:HD22 | 1.51 | 0.59 |
| 1:F:161:TRP:O | 6:F:674:HOH:O | 2.17 | 0.58 |
| 1:H:254:ASP:O | 1:H:255:ASP:C | 2.42 | 0.58 |
| 1:B:210:GLU:CG | 5:B:519:CIT:H42 | 2.33 | 0.58 |
| 1:G:252:MET:O | 6:G:842:HOH:O | 2.17 | 0.58 |
| 1:H:102:SER:OG | 1:H:111:PRO:HB2 | 2.04 | 0.58 |
| 1:H:159:CYS:CB | 1:H:198:ASP:OD1 | 2.52 | 0.58 |
| 1:G:330:PHE:CE2 | 1:G:334:LEU:HD23 | 2.39 | 0.58 |
| 1:A:156:ASN:HD21 | 1:C:204:LEU:HD11 | 1.69 | 0.58 |
| 1:G:315:ARG:N | 6:G:804:HOH:O | 2.37 | 0.58 |
| 1:G:308:ARG:CB | 6:G:830:HOH:O | 2.52 | 0.58 |
| 1:G:314:GLN:HB3 | 6:G:804:HOH:O | 2.03 | 0.57 |
| 1:F:184:GLN:O | 1:F:188:GLN:HG2 | 2.04 | 0.57 |
| 1:H:17:HIS:HB2 | 6:H:670:HOH:O | 2.04 | 0.57 |
| 1:D:176:GLN:HB3 | 2:D:503:GOL:H32 | 1.86 | 0.57 |
| 2:C:505:GOL:H2 | 4:C:510:SO4:O3 | 2.05 | 0.57 |
| 1:G:339:GLU:N | 1:G:339:GLU:OE2 | 2.37 | 0.57 |
| 1:H:107:LYS:O | 6:H:659:HOH:O | 2.17 | 0.57 |
| 1:G:421:LEU:HD12 | 1:G:422:VAL:N | 2.18 | 0.57 |
| 1:H:107:LYS:HA | 1:H:107:LYS:CE | 2.34 | 0.57 |
| 1:H:70:TYR:HE2 | 6:H:649:HOH:O | 1.81 | 0.57 |
| 2:A:501:GOL:H11 | 6:A:1086:HOH:O | 2.05 | 0.57 |
| 1:H:105:GLY:O | 6:H:710:HOH:O | 2.18 | 0.57 |
| 1:G:306:MET:O | 1:G:307:THR:C | 2.40 | 0.57 |
| 1:D:255:ASP:CG | 2:D:501:GOL:H31 | 2.25 | 0.57 |
| 1:D:49:GLU:OE1 | 1:D:115:TYR:OH | 2.21 | 0.57 |
| 1:G:266:MET:O | 1:G:269:GLN:N | 2.37 | 0.57 |
| 6:A:845:HOH:O | 2:E:504:GOL:H12 | 2.05 | 0.57 |
| 1:B:204:LEU:HD11 | 1:D:156:ASN:HD21 | 1.69 | 0.57 |
| 1:A:253:THR:HG23 | 1:A:254:ASP:O | 2.04 | 0.56 |
| 2:A:501:GOL:O2 | 6:A:1086:HOH:O | 2.18 | 0.56 |
| 1:E:366:GLU:HB2 | 6:E:953:HOH:O | 2.04 | 0.56 |
| 1:G:380:ASN:ND2 | 6:G:730:HOH:O | 2.19 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:G:253:THR:HG23 | 1:G:254:ASP:O | 2.06 | 0.56 |
| 1:C:208:HIS:ND1 | 5:C:519:CIT:O5 | 2.31 | 0.56 |
| 1:H:38:SER:O | 1:H:296:ARG:NH2 | 2.33 | 0.56 |
| 1:H:252[B]:MET:SD | 1:H:266[B]:MET:CE | 2.93 | 0.56 |
| 1:H:49:GLU:OE2 | 1:H:115:TYR:OH | 2.24 | 0.56 |
| 1:D:253:THR:HG22 | 1:D:254:ASP:O | 2.06 | 0.55 |
| 1:F:188:GLN:HG3 | 6:F:791:HOH:O | 2.05 | 0.55 |
| 1:H:313:GLU:OE2 | 6:H:667:HOH:O | 2.18 | 0.55 |
| 1:H:252[B]:MET:HE1 | 1:H:273:TRP:HB2 | 1.87 | 0.55 |
| 1:D:67:ILE:HD13 | 1:D:79:TYR:CE1 | 2.41 | 0.55 |
| 1:F:392:ARG:NH1 | 6:F:640:HOH:O | 2.39 | 0.55 |
| 1:H:248:ASN:ND2 | 6:H:739:HOH:O | 2.39 | 0.55 |
| 1:H:239:HIS:HA | 6:H:664:HOH:O | 2.06 | 0.55 |
| 1:H:113:ALA:O | 1:H:117:HIS:ND1 | 2.40 | 0.55 |
| 1:C:253:THR:CG2 | 1:C:254:ASP:O | 2.55 | 0.55 |
| 1:H:67:ILE:CG1 | 1:H:126:HIS:CE1 | 2.89 | 0.55 |
| 1:H:200:VAL:HB | 1:H:232:PRO:O | 2.07 | 0.54 |
| 1:F:151:ASP:O | 1:F:172:LYS:HG2 | 2.08 | 0.54 |
| 1:H:130:GLY:O | 1:H:165:MET:CE | 2.56 | 0.54 |
| 1:G:279:LEU:C | 1:G:279:LEU:HD23 | 2.28 | 0.54 |
| 1:G:396:SER:CB | 1:G:427:ALA:HB2 | 2.37 | 0.54 |
| 1:H:67:ILE:HG13 | 1:H:126:HIS:CE1 | 2.42 | 0.54 |
| 1:G:395:VAL:HB | 1:G:430:LEU:HD23 | 1.90 | 0.54 |
| 1:H:312:ASP:O | 1:H:316:THR:HG23 | 2.08 | 0.54 |
| 5:E:517:CIT:H22 | 6:E:670:HOH:O | 2.08 | 0.54 |
| 1:H:198:ASP:OD2 | 1:H:198:ASP:O | 2.26 | 0.54 |
| 1:B:154:ASP:OD2 | 6:B:782:HOH:O | 2.18 | 0.54 |
| 1:G:421:LEU:HD11 | 1:G:423:LYS:HE3 | 1.90 | 0.54 |
| 1:H:27:MET:HA | 1:H:328:LEU:O | 2.07 | 0.53 |
| 1:H:56:LYS:N | 1:H:57:PRO:CD | 2.71 | 0.53 |
| 1:H:253:THR:HB | 6:H:606:HOH:O | 2.08 | 0.53 |
| 1:H:150:ARG:HD2 | 6:H:627:HOH:O | 2.08 | 0.53 |
| 1:B:150:ARG:HD2 | 6:B:725:HOH:O | 2.07 | 0.53 |
| 5:C:519:CIT:C6 | 5:C:519:CIT:O1 | 2.57 | 0.53 |
| 1:F:49:GLU:OE2 | 1:F:115:TYR:OH | 2.23 | 0.53 |
| 1:F:387:ASN:ND2 | 1:F:389:SER:H | 2.07 | 0.53 |
| 1:H:131:ILE:CD1 | 1:H:152:ILE:HD11 | 2.39 | 0.53 |
| 1:G:341:THR:O | 1:G:344:LEU:HB2 | 2.09 | 0.53 |
| 1:G:381:GLN:NE2 | 1:G:404:CYS:SG | 2.82 | 0.53 |
| 1:G:266:MET:HE3 | 1:G:285:ALA:HB1 | 1.90 | 0.53 |
| 1:H:115:TYR:CG | 1:H:115:TYR:O | 2.62 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:210:GLU:H | 5:B:519:CIT:C4 | 2.20 | 0.52 |
| 1:D:325:ARG:HD2 | 6:D:979:HOH:O | 2.07 | 0.52 |
| 1:D:176:GLN:H | 2:D:503:GOL:C3 | 2.22 | 0.52 |
| 1:G:346:THR:CB | 6:G:846:HOH:O | 2.57 | 0.52 |
| 1:B:406:GLU:HB2 | 1:B:407:PRO:HD2 | 1.90 | 0.52 |
| 1:E:101:PRO:O | 1:E:104:LYS:HB2 | 2.09 | 0.52 |
| 1:H:297:SER:CB | 6:H:615:HOH:O | 2.57 | 0.52 |
| 1:H:123:PHE:CD2 | 1:H:191:VAL:HG22 | 2.45 | 0.52 |
| 1:H:70:TYR:O | 1:H:72:PRO:HD3 | 2.09 | 0.52 |
| 1:H:273:TRP:CE3 | 1:H:276:LEU:HD23 | 2.45 | 0.52 |
| 4:C:508:SO4:O3 | 6:C:1007:HOH:O | 2.18 | 0.52 |
| 1:C:17:HIS:CE1 | 6:C:779:HOH:O | 2.62 | 0.52 |
| 1:H:324:PHE:O | 1:H:325:ARG:HB2 | 2.10 | 0.52 |
| 1:E:210:GLU:HB2 | 5:E:517:CIT:H22 | 1.91 | 0.52 |
| 1:F:406:GLU:HB2 | 1:F:407:PRO:HD2 | 1.92 | 0.52 |
| 1:C:318:MET:O | 1:C:322:ILE:HG12 | 2.10 | 0.52 |
| 1:A:387:ASN:HD22 | 1:A:389:SER:H | 1.58 | 0.52 |
| 1:G:103:ALA:O | 1:G:104:LYS:C | 2.47 | 0.52 |
| 6:A:1140:HOH:O | 2:E:504:GOL:H32 | 2.11 | 0.51 |
| 1:F:204:LEU:HB2 | 1:F:205:TYR:CD2 | 2.44 | 0.51 |
| 1:G:406:GLU:HG3 | 1:G:407:PRO:O | 2.10 | 0.51 |
| 1:G:363:VAL:HG13 | 1:G:371:VAL:O | 2.10 | 0.51 |
| 1:G:337:ASN:CG | 6:G:843:HOH:O | 2.48 | 0.51 |
| 1:H:316:THR:HG21 | 1:H:433:HIS:O | 2.10 | 0.51 |
| 1:G:410:ALA:HB2 | 1:G:440:LEU:HD23 | 1.92 | 0.51 |
| 1:G:318:MET:CB | 6:G:835:HOH:O | 2.48 | 0.51 |
| 1:D:281:HIS:O | 1:D:281:HIS:ND1 | 2.43 | 0.51 |
| 1:H:412:ASP:OD1 | 1:H:412:ASP:C | 2.49 | 0.51 |
| 1:G:319:THR:OG1 | 1:G:414:TRP:NE1 | 2.34 | 0.51 |
| 1:D:417:GLU:HB3 | 6:D:810:HOH:O | 2.06 | 0.51 |
| 1:G:290:LEU:HD21 | 1:G:317:MET:HE1 | 1.92 | 0.51 |
| 1:H:23:LYS:HA | 1:H:279:LEU:CD2 | 2.40 | 0.51 |
| 1:D:392:ARG:NH1 | 4:D:512:SO4:O4 | 2.44 | 0.51 |
| 1:D:423:LYS:HE3 | 2:D:502:GOL:H2 | 1.93 | 0.51 |
| 1:D:318:MET:O | 1:D:322:ILE:HG12 | 2.11 | 0.51 |
| 1:G:353:VAL:HG12 | 1:G:353:VAL:O | 2.10 | 0.51 |
| 1:B:306:MET:CE | 6:B:674:HOH:O | 2.58 | 0.51 |
| 1:G:308:ARG:HB2 | 6:G:830:HOH:O | 2.09 | 0.51 |
| 1:H:107:LYS:HE2 | 1:H:107:LYS:HA | 1.93 | 0.51 |
| 1:B:306:MET:HE1 | 6:B:674:HOH:O | 2.11 | 0.51 |
| 1:D:406:GLU:HB2 | 1:D:407:PRO:CD | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:G:27:MET:HE2 | 1:G:59:GLY:C | 2.31 | 0.51 |
| 1:H:52:ALA:HA | 6:H:742:HOH:O | 2.09 | 0.51 |
| 1:A:259:ARG:NH2 | 1:A:261:GLU:OE2 | 2.44 | 0.51 |
| 1:H:64:VAL:HG22 | 1:H:124:GLY:HA3 | 1.93 | 0.51 |
| 1:G:314:GLN:CB | 6:G:804:HOH:O | 2.59 | 0.50 |
| 1:H:90:TYR:CE1 | 1:H:143:LEU:HD12 | 2.45 | 0.50 |
| 1:D:210:GLU:CG | 5:D:515:CIT:H21 | 2.41 | 0.50 |
| 1:A:154:ASP:OD1 | 6:A:1101:HOH:O | 2.18 | 0.50 |
| 1:A:279:LEU:C | 1:A:279:LEU:HD23 | 2.31 | 0.50 |
| 1:H:89:GLU:HB3 | 1:H:90:TYR:CE2 | 2.47 | 0.50 |
| 1:B:145:THR:HG21 | 1:B:147:VAL:HG22 | 1.93 | 0.50 |
| 1:F:176:GLN:OE1 | 1:F:214:MET:HG2 | 2.12 | 0.50 |
| 1:H:252[B]:MET:HE3 | 1:H:324:PHE:CE2 | 2.46 | 0.50 |
| 1:A:89:GLU:HG3 | 6:A:856:HOH:O | 2.11 | 0.50 |
| 1:G:275:LYS:CE | 1:H:244:VAL:HG11 | 2.41 | 0.50 |
| 1:H:100:PHE:CD1 | 1:H:109:PHE:HE1 | 2.30 | 0.50 |
| 1:D:412:ASP:OD1 | 1:D:412:ASP:C | 2.49 | 0.50 |
| 1:H:297:SER:HB2 | 6:H:615:HOH:O | 2.11 | 0.50 |
| 1:G:290:LEU:HD21 | 1:G:317:MET:CE | 2.41 | 0.50 |
| 1:E:204:LEU:HD11 | 1:G:156:ASN:HD21 | 1.75 | 0.50 |
| 1:D:200:VAL:HB | 1:D:232:PRO:O | 2.12 | 0.50 |
| 1:D:67:ILE:HG13 | 1:D:126:HIS:CE1 | 2.47 | 0.49 |
| 1:G:373:THR:OG1 | 1:G:382:PHE:O | 2.18 | 0.49 |
| 1:G:421:LEU:HD12 | 1:G:422:VAL:CA | 2.42 | 0.49 |
| 1:C:416:LYS:HD2 | 6:C:948:HOH:O | 2.12 | 0.49 |
| 1:F:56:LYS:HD3 | 1:F:121:LEU:HD13 | 1.93 | 0.49 |
| 1:H:310:THR:O | 1:H:314:GLN:HG3 | 2.12 | 0.49 |
| 1:D:207:THR:N | 4:D:506:SO4:O1 | 2.45 | 0.49 |
| 1:G:333:GLU:OE2 | 1:G:334:LEU:N | 2.45 | 0.49 |
| 1:H:319:THR:O | 1:H:323:ILE:HG22 | 2.13 | 0.49 |
| 1:A:387:ASN:ND2 | 1:A:389:SER:H | 2.11 | 0.49 |
| 1:H:253:THR:HG22 | 1:H:254:ASP:O | 2.12 | 0.49 |
| 1:G:25:PRO:HG3 | 1:G:282:TRP:CE3 | 2.48 | 0.49 |
| 1:G:364:TYR:O | 1:G:370:VAL:HA | 2.12 | 0.48 |
| 1:B:146:ASN:CB | 6:B:801:HOH:O | 2.60 | 0.48 |
| 1:F:145:THR:O | 6:F:881:HOH:O | 2.19 | 0.48 |
| 1:H:231:SER:HB2 | 1:H:232:PRO:HA | 1.95 | 0.48 |
| 1:H:62:TYR:N | 6:H:744:HOH:O | 2.46 | 0.48 |
| 1:D:210:GLU:H | 5:D:515:CIT:C2 | 2.19 | 0.48 |
| 1:E:145:THR:HG22 | 1:E:147:VAL:HG13 | 1.94 | 0.48 |
| 1:H:124:GLY:HA2 | 1:H:193:PHE:O | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:387:ASN:C | 1:D:387:ASN:HD22 | 2.15 | 0.48 |
| 1:F:348:GLU:HG2 | 6:F:647:HOH:O | 2.13 | 0.48 |
| 1:H:252[B]:MET:CE | 1:H:273:TRP:HB2 | 2.43 | 0.48 |
| 5:D:515:CIT:H41 | 6:D:634:HOH:O | 2.13 | 0.48 |
| 1:F:387:ASN:HD22 | 1:F:389:SER:H | 1.62 | 0.48 |
| 1:G:284:ASP:OD1 | 6:G:777:HOH:O | 2.20 | 0.48 |
| 1:G:56:LYS:HB3 | 1:G:57:PRO:HD3 | 1.94 | 0.48 |
| 1:B:432:PRO:O | 1:B:433:HIS:HB2 | 2.14 | 0.48 |
| 1:G:347:ASN:CG | 6:G:785:HOH:O | 2.52 | 0.48 |
| 1:G:384:ALA:HA | 1:G:436:ILE:O | 2.13 | 0.48 |
| 1:H:67:ILE:HB | 1:H:126:HIS:CE1 | 2.48 | 0.48 |
| 1:H:291:GLY:O | 1:H:306:MET:HA | 2.13 | 0.48 |
| 1:E:208:HIS:HE1 | 6:E:610:HOH:O | 1.96 | 0.47 |
| 1:H:159:CYS:HB3 | 1:H:162:ASN:O | 2.14 | 0.47 |
| 1:H:229:SER:HA | 1:H:249:MET:O | 2.14 | 0.47 |
| 1:H:75:ASN:ND2 | 1:H:75:ASN:N | 2.61 | 0.47 |
| 1:D:176:GLN:CB | 2:D:503:GOL:H32 | 2.44 | 0.47 |
| 1:C:423:LYS:N | 4:C:516:SO4:O3 | 2.32 | 0.47 |
| 1:G:142:ILE:HD11 | 1:G:149:ALA:HA | 1.95 | 0.47 |
| 1:G:76:SER:OG | 1:G:77:SER:N | 2.47 | 0.47 |
| 1:G:66:ASP:HA | 1:G:126:HIS:HB2 | 1.96 | 0.47 |
| 1:H:131:ILE:HD13 | 1:H:152:ILE:HD11 | 1.96 | 0.47 |
| 1:E:210:GLU:HG2 | 5:E:517:CIT:H41 | 1.94 | 0.47 |
| 1:G:434:GLN:NE2 | 6:G:784:HOH:O | 2.48 | 0.47 |
| 1:D:310:THR:O | 1:D:314:GLN:HG3 | 2.14 | 0.47 |
| 1:F:209:THR:O | 1:F:213:LYS:HG3 | 2.15 | 0.47 |
| 1:G:241:THR:HG21 | 1:H:271:TYR:CE1 | 2.50 | 0.47 |
| 1:F:86:GLU:HB3 | 1:F:94:MET:O | 2.14 | 0.47 |
| 1:G:387:ASN:ND2 | 1:G:389:SER:OG | 2.46 | 0.47 |
| 1:E:210:GLU:CG | 5:E:517:CIT:H41 | 2.45 | 0.47 |
| 1:A:255:ASP:OD1 | 2:A:501:GOL:H12 | 2.14 | 0.47 |
| 1:H:67:ILE:HD12 | 1:H:126:HIS:CE1 | 2.50 | 0.47 |
| 1:H:69:TRP:HA | 1:H:99:ARG:HH22 | 1.79 | 0.47 |
| 1:D:110:LYS:HB3 | 1:D:111:PRO:HD3 | 1.97 | 0.47 |
| 1:G:399:LEU:HA | 1:G:402:LEU:HB2 | 1.95 | 0.47 |
| 1:C:399:LEU:HB3 | 1:C:404:CYS:HB2 | 1.97 | 0.47 |
| 1:G:253:THR:N | 6:G:828:HOH:O | 2.45 | 0.47 |
| 1:E:133:ARG:HD3 | 1:E:166:TYR:CZ | 2.50 | 0.47 |
| 1:A:253:THR:CG2 | 1:A:254:ASP:O | 2.63 | 0.47 |
| 1:B:310:THR:HB | 4:B:516:SO4:O3 | 2.15 | 0.47 |
| 1:F:91:SER:OG | 1:F:141:PRO:O | 2.22 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:56:LYS:HD3 | 1:A:121:LEU:HD13 | 1.97 | 0.47 |
| 1:H:306:MET:O | 1:H:307:THR:C | 2.53 | 0.47 |
| 1:F:182:LEU:O | 1:F:185:LEU:HB3 | 2.15 | 0.47 |
| 1:C:41:GLU:HB2 | 1:C:100:PHE:HA | 1.96 | 0.47 |
| 1:B:208:HIS:ND1 | 5:B:519:CIT:O5 | 2.46 | 0.46 |
| 1:H:41:GLU:OE2 | 1:H:102:SER:HB3 | 2.15 | 0.46 |
| 1:H:24:THR:O | 1:H:25:PRO:C | 2.49 | 0.46 |
| 1:A:281:HIS:O | 1:A:281:HIS:ND1 | 2.49 | 0.46 |
| 1:F:129:ARG:HD2 | 1:F:211:GLU:OE2 | 2.14 | 0.46 |
| 1:D:253:THR:HG23 | 1:D:254:ASP:O | 2.15 | 0.46 |
| 1:C:239:HIS:ND1 | 4:C:512:SO4:O4 | 2.32 | 0.46 |
| 1:H:274:CYS:SG | 1:H:275:LYS:HE2 | 2.56 | 0.46 |
| 1:H:224:ARG:HG3 | 1:H:224:ARG:HH11 | 1.80 | 0.46 |
| 1:G:342:LEU:HG | 6:G:737:HOH:O | 2.15 | 0.46 |
| 1:B:387:ASN:HD22 | 1:B:389:SER:H | 1.62 | 0.46 |
| 1:H:67:ILE:HD13 | 1:H:79:TYR:OH | 2.16 | 0.46 |
| 1:F:322:ILE:HG23 | 1:F:354:HIS:HB2 | 1.98 | 0.46 |
| 1:G:288:LEU:HD21 | 1:G:321:TRP:CD1 | 2.50 | 0.46 |
| 1:F:282:TRP:O | 1:F:283:PRO:C | 2.54 | 0.46 |
| 1:G:318:MET:CA | 6:G:835:HOH:O | 2.64 | 0.46 |
| 1:D:253:THR:HB | 6:D:610:HOH:O | 2.16 | 0.46 |
| 1:B:110:LYS:HB3 | 1:B:111:PRO:HD3 | 1.98 | 0.46 |
| 1:B:387:ASN:ND2 | 1:B:389:SER:H | 2.14 | 0.46 |
| 1:A:72:PRO:HG2 | 6:A:1054:HOH:O | 2.16 | 0.46 |
| 1:G:232:PRO:HB3 | 3:G:502:ARB:O2 | 2.16 | 0.45 |
| 1:B:247:ALA:O | 6:B:697:HOH:O | 2.21 | 0.45 |
| 1:H:221:ARG:HA | 6:H:637:HOH:O | 2.16 | 0.45 |
| 1:H:146:ASN:OD1 | 1:H:146:ASN:N | 2.43 | 0.45 |
| 5:D:515:CIT:O5 | 5:D:515:CIT:C1 | 2.64 | 0.45 |
| 1:H:130:GLY:CA | 6:H:634:HOH:O | 2.64 | 0.45 |
| 1:G:40:THR:O | 1:G:44:VAL:HG23 | 2.16 | 0.45 |
| 1:G:392:ARG:HB2 | 1:G:431:GLY:HA2 | 1.98 | 0.45 |
| 1:H:55:LEU:HB3 | 1:H:60:TRP:HB2 | 1.98 | 0.45 |
| 1:H:322:ILE:HG23 | 1:H:354:HIS:HB2 | 1.99 | 0.45 |
| 1:G:26:PRO:HB3 | 1:G:62:TYR:CE2 | 2.51 | 0.45 |
| 1:H:32:TRP:CE3 | 1:H:36:GLY:HA2 | 2.51 | 0.45 |
| 1:C:294:GLY:HA2 | 1:C:297:SER:HB3 | 1.97 | 0.45 |
| 1:H:224:ARG:NH1 | 1:H:224:ARG:HG3 | 2.31 | 0.45 |
| 2:D:503:GOL:O2 | 4:D:513:SO4:O1 | 2.23 | 0.45 |
| 1:H:344:LEU:O | 6:H:724:HOH:O | 2.21 | 0.45 |
| 1:H:16:MET:HB3 | 1:H:18:HIS:CD2 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:441:SER:HB2 | 1:B:442:PRO:HD2 | 1.98 | 0.45 |
| 2:A:501:GOL:C3 | 6:A:1086:HOH:O | 2.63 | 0.45 |
| 1:A:255:ASP:CG | 2:A:501:GOL:H12 | 2.36 | 0.45 |
| 1:H:126:HIS:CD2 | 6:H:737:HOH:O | 2.69 | 0.45 |
| 1:C:259:ARG:NH2 | 1:C:261:GLU:OE2 | 2.50 | 0.45 |
| 1:B:424:HIS:HB2 | 6:B:764:HOH:O | 2.16 | 0.45 |
| 1:B:146:ASN:N | 1:B:146:ASN:OD1 | 2.37 | 0.45 |
| 1:F:27:MET:HA | 1:F:328:LEU:O | 2.16 | 0.45 |
| 1:C:110:LYS:HB3 | 1:C:111:PRO:HD3 | 1.99 | 0.45 |
| 1:E:200:VAL:O | 1:E:207:THR:HA | 2.17 | 0.45 |
| 1:B:406:GLU:CB | 1:B:407:PRO:CD | 2.91 | 0.44 |
| 1:D:349:GLU:OE2 | 1:D:416:LYS:HG2 | 2.16 | 0.44 |
| 1:F:255:ASP:OD1 | 3:F:502:ARB:O2 | 2.26 | 0.44 |
| 1:G:378:GLU:O | 1:G:380:ASN:N | 2.51 | 0.44 |
| 1:G:244:VAL:HG11 | 1:H:275:LYS:HD2 | 1.99 | 0.44 |
| 1:F:137:HIS:CE1 | 1:H:137:HIS:CE1 | 3.05 | 0.44 |
| 1:A:208:HIS:HE1 | 6:A:611:HOH:O | 2.00 | 0.44 |
| 1:H:220:ASP:C | 6:H:776:HOH:O | 2.56 | 0.44 |
| 1:H:16:MET:HB3 | 1:H:18:HIS:HD2 | 1.82 | 0.44 |
| 1:A:379:GLY:N | 6:A:1021:HOH:O | 2.37 | 0.44 |
| 1:H:193:PHE:CD1 | 1:H:227:VAL:CG1 | 3.01 | 0.44 |
| 1:H:61:GLU:C | 6:H:744:HOH:O | 2.56 | 0.44 |
| 1:H:195:LYS:NZ | 6:H:737:HOH:O | 2.51 | 0.44 |
| 1:C:236:PRO:HG2 | 1:C:239:HIS:HD2 | 1.83 | 0.44 |
| 1:D:221:ARG:NH2 | 4:D:514:SO4:O3 | 2.42 | 0.44 |
| 1:H:160:PRO:HG3 | 1:H:204:LEU:HG | 1.98 | 0.44 |
| 1:H:239:HIS:O | 1:H:243:PHE:CD2 | 2.70 | 0.44 |
| 1:B:306:MET:O | 1:B:307:THR:C | 2.56 | 0.44 |
| 1:A:409:LYS:HD2 | 1:A:444:VAL:HG23 | 2.00 | 0.44 |
| 1:B:392:ARG:HE | 1:E:338:ASP:HA | 1.83 | 0.44 |
| 1:A:290:LEU:HD21 | 1:A:317:MET:CE | 2.48 | 0.44 |
| 1:A:89:GLU:CD | 1:A:89:GLU:N | 2.68 | 0.43 |
| 1:G:66:ASP:OD1 | 3:G:502:ARB:O4 | 2.33 | 0.43 |
| 1:H:253:THR:CG2 | 1:H:254:ASP:O | 2.65 | 0.43 |
| 6:A:1139:HOH:O | 2:E:504:GOL:H31 | 2.18 | 0.43 |
| 1:E:17:HIS:NE2 | 4:E:506:SO4:O4 | 2.50 | 0.43 |
| 1:G:55:LEU:HB3 | 1:G:60:TRP:CD1 | 2.53 | 0.43 |
| 1:G:258:ASP:OD1 | 1:G:258:ASP:N | 2.50 | 0.43 |
| 5:C:519:CIT:H41 | 6:C:666:HOH:O | 2.17 | 0.43 |
| 5:C:519:CIT:O1 | 5:C:519:CIT:O6 | 2.37 | 0.43 |
| 1:A:379:GLY:CA | 6:A:1021:HOH:O | 2.66 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:145:THR:HB | 1:D:147:VAL:H | 1.83 | 0.43 |
| 1:C:365:ARG:HG3 | 1:C:370:VAL:HG22 | 1.99 | 0.43 |
| 1:F:432:PRO:O | 1:F:433:HIS:HB2 | 2.17 | 0.43 |
| 1:G:426:LEU:HD12 | 6:G:714:HOH:O | 2.17 | 0.43 |
| 1:A:209:THR:N | 5:A:515:CIT:O6 | 2.50 | 0.43 |
| 1:F:313:GLU:OE2 | 1:F:433:HIS:HD2 | 2.00 | 0.43 |
| 1:F:294:GLY:O | 1:F:304:ASP:HA | 2.19 | 0.43 |
| 1:H:348:GLU:CD | 1:H:348:GLU:O | 2.56 | 0.43 |
| 1:H:55:LEU:C | 1:H:57:PRO:HD2 | 2.39 | 0.43 |
| 1:H:193:PHE:CD1 | 1:H:227:VAL:HG12 | 2.54 | 0.43 |
| 1:H:180:ASP:OD2 | 1:H:221:ARG:NH1 | 2.42 | 0.43 |
| 1:E:126:HIS:HA | 1:E:195:LYS:O | 2.19 | 0.43 |
| 1:B:340:TRP:O | 1:B:343:SER:OG | 2.26 | 0.43 |
| 1:B:56:LYS:N | 1:B:57:PRO:CD | 2.82 | 0.43 |
| 1:E:145:THR:CG2 | 1:E:147:VAL:HG13 | 2.48 | 0.43 |
| 1:E:210:GLU:HB2 | 5:E:517:CIT:H41 | 2.00 | 0.43 |
| 1:E:248:ASN:ND2 | 6:E:733:HOH:O | 2.51 | 0.43 |
| 1:H:235:ALA:HB2 | 1:H:251:ARG:O | 2.17 | 0.43 |
| 1:B:17:HIS:HE1 | 4:B:505:SO4:O2 | 2.01 | 0.43 |
| 1:E:110:LYS:HB3 | 1:E:111:PRO:HD3 | 2.01 | 0.43 |
| 1:C:432:PRO:O | 1:C:433:HIS:HB2 | 2.19 | 0.43 |
| 1:H:23:LYS:HA | 1:H:279:LEU:HD23 | 2.00 | 0.43 |
| 1:F:199:ILE:HG21 | 1:F:230:LEU:HD22 | 2.00 | 0.43 |
| 1:A:210:GLU:H | 5:A:515:CIT:H41 | 1.84 | 0.43 |
| 1:H:113:ALA:O | 1:H:117:HIS:CE1 | 2.72 | 0.43 |
| 1:H:294:GLY:O | 1:H:304:ASP:HA | 2.18 | 0.43 |
| 1:H:89:GLU:HA | 1:H:89:GLU:OE2 | 2.19 | 0.43 |
| 1:A:56:LYS:N | 1:A:57:PRO:CD | 2.82 | 0.43 |
| 1:F:142:ILE:HG22 | 1:F:143:LEU:O | 2.18 | 0.43 |
| 1:G:118:ASN:HB3 | 6:G:779:HOH:O | 2.19 | 0.43 |
| 1:H:216:ARG:NE | 6:H:743:HOH:O | 2.51 | 0.43 |
| 1:A:290:LEU:HD21 | 1:A:317:MET:HE2 | 2.00 | 0.42 |
| 1:C:406:GLU:HB2 | 1:C:407:PRO:HD2 | 2.01 | 0.42 |
| 1:C:409:LYS:HD2 | 1:C:443:ALA:HA | 2.00 | 0.42 |
| 1:H:92:ARG:CD | 1:H:181:SER:OG | 2.63 | 0.42 |
| 1:H:67:ILE:HA | 1:H:126:HIS:ND1 | 2.34 | 0.42 |
| 1:B:417[B]:GLU:CD | 6:B:860:HOH:O | 2.57 | 0.42 |
| 1:D:14:ALA:HA | 1:D:19:TYR:HD2 | 1.83 | 0.42 |
| 1:C:258:ASP:N | 1:C:258:ASP:OD1 | 2.52 | 0.42 |
| 1:F:89:GLU:C | 6:F:690:HOH:O | 2.57 | 0.42 |
| 1:F:442:PRO:HA | 6:F:714:HOH:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:174:GLY:N | 2:H:502:GOL:C3 | 2.83 | 0.42 |
| 1:F:387:ASN:C | 1:F:387:ASN:HD22 | 2.22 | 0.42 |
| 1:C:406:GLU:HB2 | 1:C:407:PRO:CD | 2.49 | 0.42 |
| 1:H:277:VAL:HG21 | 1:H:324:PHE:CZ | 2.55 | 0.42 |
| 1:B:200:VAL:HB | 1:B:232:PRO:O | 2.20 | 0.42 |
| 1:D:70:TYR:O | 1:D:72:PRO:HD3 | 2.20 | 0.42 |
| 1:B:89:GLU:HG3 | 6:B:892:HOH:O | 2.19 | 0.42 |
| 1:G:266:MET:CE | 1:G:285:ALA:HB1 | 2.50 | 0.42 |
| 1:D:311:LYS:HG2 | 1:D:340:TRP:CE2 | 2.55 | 0.42 |
| 1:E:409:LYS:O | 1:E:440:LEU:HA | 2.20 | 0.42 |
| 5:E:517:CIT:C2 | 6:E:670:HOH:O | 2.66 | 0.42 |
| 1:G:396:SER:HB3 | 1:G:427:ALA:HB2 | 2.01 | 0.42 |
| 1:E:200:VAL:HB | 1:E:232:PRO:O | 2.19 | 0.42 |
| 1:B:159:CYS:HB2 | 1:B:198:ASP:CG | 2.40 | 0.42 |
| 1:G:411:ARG:O | 1:G:438:VAL:HA | 2.20 | 0.42 |
| 1:E:210:GLU:CB | 5:E:517:CIT:H41 | 2.49 | 0.42 |
| 1:D:324:PHE:O | 1:D:325:ARG:HB2 | 2.20 | 0.42 |
| 1:G:409:LYS:HG2 | 6:G:648:HOH:O | 2.20 | 0.42 |
| 1:C:54:TYR:OH | 2:C:504:GOL:H2 | 2.19 | 0.42 |
| 1:C:173:GLU:HG3 | 6:C:970:HOH:O | 2.19 | 0.42 |
| 1:A:66:ASP:HA | 1:A:126:HIS:HB2 | 2.01 | 0.42 |
| 1:H:216:ARG:CD | 6:H:743:HOH:O | 2.67 | 0.42 |
| 1:G:79:TYR:O | 6:G:762:HOH:O | 2.22 | 0.42 |
| 1:G:347:ASN:ND2 | 1:G:350:VAL:H | 2.13 | 0.41 |
| 1:H:277:VAL:HG11 | 6:H:761:HOH:O | 2.20 | 0.41 |
| 1:D:210:GLU:HG2 | 5:D:515:CIT:H21 | 2.02 | 0.41 |
| 1:G:253:THR:C | 1:G:254:ASP:O | 2.57 | 0.41 |
| 1:H:180:ASP:N | 1:H:180:ASP:OD1 | 2.51 | 0.41 |
| 1:H:347:ASN:OD1 | 1:H:349:GLU:N | 2.52 | 0.41 |
| 1:F:251:ARG:HA | 1:F:284:ASP:HB3 | 2.02 | 0.41 |
| 1:H:159:CYS:HA | 1:H:160:PRO:HD3 | 1.86 | 0.41 |
| 1:C:208:HIS:HD1 | 5:C:519:CIT:C6 | 2.30 | 0.41 |
| 1:E:50:TYR:CD2 | 1:E:334:LEU:HB3 | 2.55 | 0.41 |
| 1:E:237:LEU:HD13 | 1:F:238:ASP:HA | 2.02 | 0.41 |
| 1:C:16:MET:HE2 | 6:C:892:HOH:O | 2.19 | 0.41 |
| 1:F:268:GLU:HG3 | 6:F:852:HOH:O | 2.21 | 0.41 |
| 1:H:122:LYS:HB2 | 6:H:744:HOH:O | 2.20 | 0.41 |
| 1:G:55:LEU:HB3 | 1:G:60:TRP:HB2 | 2.01 | 0.41 |
| 1:H:364:TYR:C | 1:H:364:TYR:CD1 | 2.93 | 0.41 |
| 1:D:347:ASN:OD1 | 1:D:347:ASN:C | 2.58 | 0.41 |
| 1:E:287:MET:O | 1:E:289:PRO:HD3 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:H:252[B]:MET:SD | 1:H:266[B]:MET:HE2 | 2.59 | 0.41 |
| 1:G:318:MET:HG3 | 1:G:344:LEU:HD22 | 2.02 | 0.41 |
| 1:E:210:GLU:HG2 | 5:E:517:CIT:C4 | 2.51 | 0.41 |
| 1:G:343:SER:N | 6:G:737:HOH:O | 2.52 | 0.41 |
| 1:G:330:PHE:CD2 | 1:G:334:LEU:CD2 | 3.03 | 0.41 |
| 1:A:204:LEU:HD11 | 1:C:156:ASN:HD21 | 1.85 | 0.41 |
| 1:B:184:GLN:O | 1:B:188[A]:GLN:HG3 | 2.21 | 0.41 |
| 1:G:378:GLU:CD | 1:G:378:GLU:N | 2.70 | 0.41 |
| 1:C:210:GLU:HG2 | 5:C:519:CIT:H21 | 2.02 | 0.41 |
| 1:G:406:GLU:CG | 1:G:407:PRO:O | 2.68 | 0.41 |
| 1:D:416:LYS:HE2 | 6:D:935:HOH:O | 2.20 | 0.41 |
| 1:H:199:ILE:HD11 | 1:H:212:ILE:HG13 | 2.03 | 0.41 |
| 1:G:195:LYS:HA | 1:G:229:SER:HB3 | 2.02 | 0.41 |
| 1:A:387:ASN:HD22 | 1:A:387:ASN:C | 2.23 | 0.41 |
| 1:G:385:MET:O | 1:G:435:SER:HA | 2.20 | 0.41 |
| 1:F:236:PRO:HG2 | 1:F:239:HIS:HD2 | 1.86 | 0.41 |
| 2:B:503:GOL:H2 | 4:B:514:SO4:O2 | 2.20 | 0.41 |
| 1:H:40:THR:O | 1:H:44:VAL:HG23 | 2.21 | 0.41 |
| 1:G:116:ILE:O | 1:G:121:LEU:HB2 | 2.20 | 0.41 |
| 1:G:408:MET:CA | 6:G:713:HOH:O | 2.67 | 0.41 |
| 1:A:229:SER:HB2 | 1:A:249:MET:HG3 | 2.01 | 0.41 |
| 1:G:227:VAL:HA | 1:G:248:ASN:HD22 | 1.86 | 0.41 |
| 1:G:265:ASP:HB3 | 6:G:765:HOH:O | 2.21 | 0.41 |
| 1:A:20:GLN:HE21 | 1:A:23:LYS:HE3 | 1.85 | 0.41 |
| 5:G:510:CIT:C2 | 5:G:510:CIT:O3 | 2.65 | 0.41 |
| 1:G:253:THR:HB | 6:G:828:HOH:O | 2.20 | 0.41 |
| 1:D:235:ALA:HA | 1:D:236:PRO:HD3 | 1.92 | 0.41 |
| 1:G:325:ARG:HD3 | 6:G:824:HOH:O | 2.20 | 0.41 |
| 1:G:315:ARG:O | 1:G:316:THR:C | 2.58 | 0.41 |
| 1:H:204:LEU:HB2 | 1:H:205:TYR:CD2 | 2.56 | 0.41 |
| 5:C:519:CIT:C1 | 5:C:519:CIT:O6 | 2.69 | 0.41 |
| 1:G:386:PHE:CE1 | 1:G:435:SER:HB2 | 2.56 | 0.41 |
| 1:A:217:LYS:HE3 | 6:A:1106:HOH:O | 2.21 | 0.41 |
| 1:H:273:TRP:HE3 | 1:H:276:LEU:HD23 | 1.86 | 0.40 |
| 1:H:174:GLY:N | 2:H:502:GOL:H31 | 2.36 | 0.40 |
| 1:G:387:ASN:HB3 | 1:G:431:GLY:O | 2.21 | 0.40 |
| 1:H:176:GLN:HB3 | 2:H:502:GOL:H2 | 2.02 | 0.40 |
| 1:A:272:LYS:CD | 6:B:774:HOH:O | 2.70 | 0.40 |
| 1:H:61:GLU:HB2 | 6:H:744:HOH:O | 2.21 | 0.40 |
| 1:H:359:GLY:O | 6:H:764:HOH:O | 2.22 | 0.40 |
| 1:G:235:ALA:HA | 1:G:236:PRO:HD3 | 1.93 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:90:TYR:N | 6:F:690:HOH:O | 2.53 | 0.40 |
| 1:F:276:LEU:HD22 | 1:F:276:LEU:N | 2.37 | 0.40 |
| 1:D:41:GLU:HB2 | 1:D:100:PHE:HA | 2.03 | 0.40 |
| 1:C:20:GLN:HG3 | 6:C:779:HOH:O | 2.21 | 0.40 |
| 1:E:392:ARG:HD3 | 1:E:429:GLU:OE1 | 2.21 | 0.40 |

All (1) 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) |
|---------------|-----------------------|--------------------------|-------------------|
| 6:A:836:HOH:O | 6:B:1011:HOH:O[4_445] | 2.02 | 0.18 |

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 432/448 (96%) | 417 (96%) | 15 (4%) | 0 | 100 | 100 |
| 1 | B | 430/448 (96%) | 412 (96%) | 18 (4%) | 0 | 100 | 100 |
| 1 | C | 432/448 (96%) | 419 (97%) | 13 (3%) | 0 | 100 | 100 |
| 1 | D | 434/448 (97%) | 415 (96%) | 18 (4%) | 1 (0%) | 52 | 59 |
| 1 | E | 430/448 (96%) | 411 (96%) | 19 (4%) | 0 | 100 | 100 |
| 1 | F | 428/448 (96%) | 406 (95%) | 21 (5%) | 1 (0%) | 52 | 59 |
| 1 | G | 433/448 (97%) | 393 (91%) | 35 (8%) | 5 (1%) | 16 | 12 |
| 1 | H | 431/448 (96%) | 384 (89%) | 41 (10%) | 6 (1%) | 14 | 10 |
| All | All | 3450/3584 (96%) | 3257 (94%) | 180 (5%) | 13 (0%) | 39 | 42 |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 379 | GLY |
| 1 | H | 121 | LEU |
| 1 | H | 325 | ARG |
| 1 | G | 104 | LYS |
| 1 | G | 258 | ASP |
| 1 | G | 443 | ALA |
| 1 | H | 53 | LYS |
| 1 | H | 96 | ALA |
| 1 | H | 60 | TRP |
| 1 | H | 115 | TYR |
| 1 | F | 66 | ASP |
| 1 | D | 447 | GLY |
| 1 | G | 397 | VAL |

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 | 371/382 (97%) | 354 (95%) | 17 (5%) | 33 | 40 |
| 1 | B | 370/382 (97%) | 353 (95%) | 17 (5%) | 33 | 40 |
| 1 | C | 371/382 (97%) | 352 (95%) | 19 (5%) | 29 | 34 |
| 1 | D | 371/382 (97%) | 349 (94%) | 22 (6%) | 24 | 27 |
| 1 | E | 369/382 (97%) | 354 (96%) | 15 (4%) | 37 | 45 |
| 1 | F | 368/382 (96%) | 348 (95%) | 20 (5%) | 27 | 31 |
| 1 | G | 372/382 (97%) | 337 (91%) | 35 (9%) | 11 | 10 |
| 1 | H | 371/382 (97%) | 340 (92%) | 31 (8%) | 14 | 13 |
| All | All | 2963/3056 (97%) | 2787 (94%) | 176 (6%) | 24 | 27 |

All (176) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 71 | GLU |
| 1 | A | 89 | GLU |
| 1 | A | 121 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|--------|------|
| 1 | A | 203 | LYS |
| 1 | A | 236 | PRO |
| 1 | A | 237 | LEU |
| 1 | A | 253 | THR |
| 1 | A | 298 | VAL |
| 1 | A | 321 | TRP |
| 1 | A | 383 | VAL |
| 1 | A | 387 | ASN |
| 1 | A | 405 | MET |
| 1 | A | 406 | GLU |
| 1 | A | 413 | LEU |
| 1 | A | 419 | LEU |
| 1 | A | 421 | LEU |
| 1 | A | 429 | GLU |
| 1 | B | 71 | GLU |
| 1 | B | 84 | PRO |
| 1 | B | 89 | GLU |
| 1 | B | 121 | LEU |
| 1 | B | 145 | THR |
| 1 | B | 232 | PRO |
| 1 | B | 253 | THR |
| 1 | B | 298 | VAL |
| 1 | B | 321 | TRP |
| 1 | B | 381 | GLN |
| 1 | B | 387 | ASN |
| 1 | B | 406 | GLU |
| 1 | B | 413 | LEU |
| 1 | B | 417[A] | GLU |
| 1 | B | 417[B] | GLU |
| 1 | B | 419 | LEU |
| 1 | B | 430 | LEU |
| 1 | C | 15 | SER |
| 1 | C | 66 | ASP |
| 1 | C | 71 | GLU |
| 1 | C | 89 | GLU |
| 1 | C | 121 | LEU |
| 1 | C | 154 | ASP |
| 1 | C | 203 | LYS |
| 1 | C | 237 | LEU |
| 1 | C | 253 | THR |
| 1 | C | 298 | VAL |
| 1 | C | 321 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 383 | VAL |
| 1 | C | 387 | ASN |
| 1 | C | 391 | LYS |
| 1 | C | 402 | LEU |
| 1 | C | 409 | LYS |
| 1 | C | 413 | LEU |
| 1 | C | 419 | LEU |
| 1 | C | 430 | LEU |
| 1 | D | 53 | LYS |
| 1 | D | 71 | GLU |
| 1 | D | 121 | LEU |
| 1 | D | 145 | THR |
| 1 | D | 154 | ASP |
| 1 | D | 216 | ARG |
| 1 | D | 217 | LYS |
| 1 | D | 237 | LEU |
| 1 | D | 249 | MET |
| 1 | D | 253 | THR |
| 1 | D | 298 | VAL |
| 1 | D | 321 | TRP |
| 1 | D | 383 | VAL |
| 1 | D | 387 | ASN |
| 1 | D | 391 | LYS |
| 1 | D | 392 | ARG |
| 1 | D | 402 | LEU |
| 1 | D | 413 | LEU |
| 1 | D | 417 | GLU |
| 1 | D | 419 | LEU |
| 1 | D | 421 | LEU |
| 1 | D | 430 | LEU |
| 1 | E | 15 | SER |
| 1 | E | 71 | GLU |
| 1 | E | 121 | LEU |
| 1 | E | 203 | LYS |
| 1 | E | 253 | THR |
| 1 | E | 298 | VAL |
| 1 | E | 321 | TRP |
| 1 | E | 383 | VAL |
| 1 | E | 387 | ASN |
| 1 | E | 400 | LYS |
| 1 | E | 402 | LEU |
| 1 | E | 413 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 419 | LEU |
| 1 | E | 421 | LEU |
| 1 | E | 430 | LEU |
| 1 | F | 71 | GLU |
| 1 | F | 104 | LYS |
| 1 | F | 121 | LEU |
| 1 | F | 147 | VAL |
| 1 | F | 172 | LYS |
| 1 | F | 188 | GLN |
| 1 | F | 203 | LYS |
| 1 | F | 237 | LEU |
| 1 | F | 298 | VAL |
| 1 | F | 321 | TRP |
| 1 | F | 383 | VAL |
| 1 | F | 387 | ASN |
| 1 | F | 391 | LYS |
| 1 | F | 392 | ARG |
| 1 | F | 402 | LEU |
| 1 | F | 413 | LEU |
| 1 | F | 419 | LEU |
| 1 | F | 422 | VAL |
| 1 | F | 430 | LEU |
| 1 | F | 433 | HIS |
| 1 | G | 15 | SER |
| 1 | G | 16 | MET |
| 1 | G | 34 | CYS |
| 1 | G | 71 | GLU |
| 1 | G | 121 | LEU |
| 1 | G | 199 | ILE |
| 1 | G | 249 | MET |
| 1 | G | 253 | THR |
| 1 | G | 258 | ASP |
| 1 | G | 263 | LEU |
| 1 | G | 298 | VAL |
| 1 | G | 309 | PHE |
| 1 | G | 321 | TRP |
| 1 | G | 339 | GLU |
| 1 | G | 347 | ASN |
| 1 | G | 350 | VAL |
| 1 | G | 363 | VAL |
| 1 | G | 365 | ARG |
| 1 | G | 378 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 381 | GLN |
| 1 | G | 383 | VAL |
| 1 | G | 387 | ASN |
| 1 | G | 394 | VAL |
| 1 | G | 400 | LYS |
| 1 | G | 402 | LEU |
| 1 | G | 406 | GLU |
| 1 | G | 408 | MET |
| 1 | G | 416 | LYS |
| 1 | G | 419 | LEU |
| 1 | G | 421 | LEU |
| 1 | G | 425 | GLN |
| 1 | G | 430 | LEU |
| 1 | G | 436 | ILE |
| 1 | G | 438 | VAL |
| 1 | G | 441 | SER |
| 1 | H | 15 | SER |
| 1 | H | 16 | MET |
| 1 | H | 20 | GLN |
| 1 | H | 34 | CYS |
| 1 | H | 71 | GLU |
| 1 | H | 75 | ASN |
| 1 | H | 91 | SER |
| 1 | H | 107 | LYS |
| 1 | H | 121 | LEU |
| 1 | H | 146 | ASN |
| 1 | H | 147 | VAL |
| 1 | H | 154 | ASP |
| 1 | H | 171 | ARG |
| 1 | H | 181 | SER |
| 1 | H | 209 | THR |
| 1 | H | 237 | LEU |
| 1 | H | 249 | MET |
| 1 | H | 253 | THR |
| 1 | H | 279 | LEU |
| 1 | H | 303 | THR |
| 1 | H | 316 | THR |
| 1 | H | 321 | TRP |
| 1 | H | 361 | ARG |
| 1 | H | 383 | VAL |
| 1 | H | 402 | LEU |
| 1 | H | 405 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 413 | LEU |
| 1 | H | 419 | LEU |
| 1 | H | 421 | LEU |
| 1 | H | 430 | LEU |
| 1 | H | 441 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 20 | GLN |
| 1 | A | 156 | ASN |
| 1 | A | 208 | HIS |
| 1 | A | 248 | ASN |
| 1 | A | 381 | GLN |
| 1 | A | 387 | ASN |
| 1 | B | 17 | HIS |
| 1 | B | 20 | GLN |
| 1 | B | 156 | ASN |
| 1 | B | 248 | ASN |
| 1 | B | 356 | ASN |
| 1 | B | 387 | ASN |
| 1 | C | 156 | ASN |
| 1 | C | 248 | ASN |
| 1 | C | 356 | ASN |
| 1 | C | 387 | ASN |
| 1 | D | 156 | ASN |
| 1 | D | 248 | ASN |
| 1 | D | 356 | ASN |
| 1 | D | 387 | ASN |
| 1 | E | 18 | HIS |
| 1 | E | 156 | ASN |
| 1 | E | 208 | HIS |
| 1 | E | 248 | ASN |
| 1 | E | 356 | ASN |
| 1 | E | 387 | ASN |
| 1 | F | 134 | GLN |
| 1 | F | 137 | HIS |
| 1 | F | 248 | ASN |
| 1 | F | 356 | ASN |
| 1 | F | 387 | ASN |
| 1 | F | 433 | HIS |
| 1 | G | 118 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 156 | ASN |
| 1 | G | 208 | HIS |
| 1 | G | 248 | ASN |
| 1 | G | 314 | GLN |
| 1 | G | 337 | ASN |
| 1 | G | 347 | ASN |
| 1 | G | 356 | ASN |
| 1 | G | 387 | ASN |
| 1 | H | 17 | HIS |
| 1 | H | 18 | HIS |
| 1 | H | 20 | GLN |
| 1 | H | 75 | ASN |
| 1 | H | 126 | HIS |
| 1 | H | 137 | HIS |
| 1 | H | 246 | ASN |
| 1 | H | 248 | ASN |
| 1 | H | 356 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

116 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | GOL | A | 501 | - | 5,5,5 | 0.39 | 0 | 5,5,5 | 0.58 | 0 |
| 3 | ARB | A | 502 | - | 10,10,10 | 1.24 | 2 (20%) | 12,14,14 | 2.38 | 7 (58%) |
| 4 | SO4 | A | 503 | - | 4,4,4 | 0.94 | 0 | 6,6,6 | 0.34 | 0 |
| 4 | SO4 | A | 504 | - | 4,4,4 | 0.50 | 0 | 6,6,6 | 1.04 | 1 (16%) |
| 4 | SO4 | A | 505 | - | 4,4,4 | 0.70 | 0 | 6,6,6 | 0.43 | 0 |
| 4 | SO4 | A | 506 | - | 4,4,4 | 1.02 | 0 | 6,6,6 | 0.61 | 0 |
| 4 | SO4 | A | 507 | - | 4,4,4 | 0.78 | 0 | 6,6,6 | 0.56 | 0 |
| 4 | SO4 | A | 508 | - | 4,4,4 | 0.65 | 0 | 6,6,6 | 0.27 | 0 |
| 4 | SO4 | A | 509 | - | 4,4,4 | 0.79 | 0 | 6,6,6 | 0.72 | 0 |
| 4 | SO4 | A | 510 | - | 4,4,4 | 1.43 | 0 | 6,6,6 | 1.16 | 1 (16%) |
| 4 | SO4 | A | 511 | - | 4,4,4 | 0.38 | 0 | 6,6,6 | 0.35 | 0 |
| 4 | SO4 | A | 512 | - | 4,4,4 | 0.97 | 0 | 6,6,6 | 0.44 | 0 |
| 4 | SO4 | A | 513 | - | 4,4,4 | 1.47 | 1 (25%) | 6,6,6 | 1.27 | 1 (16%) |
| 4 | SO4 | A | 514 | - | 4,4,4 | 0.91 | 0 | 6,6,6 | 0.42 | 0 |
| 5 | CIT | A | 515 | - | 3,12,12 | 1.88 | 1 (33%) | 3,17,17 | 2.66 | 1 (33%) |
| 2 | GOL | B | 501 | - | 5,5,5 | 0.66 | 0 | 5,5,5 | 1.39 | 0 |
| 2 | GOL | B | 502 | - | 5,5,5 | 0.54 | 0 | 5,5,5 | 0.71 | 0 |
| 2 | GOL | B | 503 | - | 5,5,5 | 0.78 | 0 | 5,5,5 | 1.08 | 0 |
| 3 | ARB | B | 504 | - | 10,10,10 | 1.14 | 1 (10%) | 12,14,14 | 2.07 | 5 (41%) |
| 4 | SO4 | B | 505 | - | 4,4,4 | 0.81 | 0 | 6,6,6 | 0.60 | 0 |
| 4 | SO4 | B | 506 | - | 4,4,4 | 0.98 | 0 | 6,6,6 | 0.92 | 1 (16%) |
| 4 | SO4 | B | 507 | - | 4,4,4 | 0.60 | 0 | 6,6,6 | 0.70 | 0 |
| 4 | SO4 | B | 508 | - | 4,4,4 | 0.49 | 0 | 6,6,6 | 0.86 | 0 |
| 4 | SO4 | B | 509 | - | 4,4,4 | 1.04 | 0 | 6,6,6 | 0.62 | 0 |
| 4 | SO4 | B | 510 | - | 4,4,4 | 0.72 | 0 | 6,6,6 | 0.29 | 0 |
| 4 | SO4 | B | 511 | - | 4,4,4 | 0.64 | 0 | 6,6,6 | 0.41 | 0 |
| 4 | SO4 | B | 512 | - | 4,4,4 | 0.55 | 0 | 6,6,6 | 0.55 | 0 |
| 4 | SO4 | B | 513 | - | 4,4,4 | 0.74 | 0 | 6,6,6 | 0.41 | 0 |
| 4 | SO4 | B | 514 | - | 4,4,4 | 0.67 | 0 | 6,6,6 | 0.47 | 0 |
| 4 | SO4 | B | 515 | - | 4,4,4 | 0.68 | 0 | 6,6,6 | 0.53 | 0 |
| 4 | SO4 | B | 516 | - | 4,4,4 | 0.90 | 0 | 6,6,6 | 0.54 | 0 |
| 4 | SO4 | B | 517 | - | 4,4,4 | 0.75 | 0 | 6,6,6 | 0.46 | 0 |
| 4 | SO4 | B | 518 | - | 4,4,4 | 0.42 | 0 | 6,6,6 | 0.30 | 0 |
| 5 | CIT | B | 519 | - | 3,12,12 | 2.80 | 1 (33%) | 3,17,17 | 4.32 | 3 (100%) |
| 2 | GOL | C | 501 | - | 5,5,5 | 0.43 | 0 | 5,5,5 | 0.80 | 0 |
| 2 | GOL | C | 502 | - | 5,5,5 | 0.44 | 0 | 5,5,5 | 0.42 | 0 |
| 2 | GOL | C | 503 | - | 5,5,5 | 0.37 | 0 | 5,5,5 | 0.61 | 0 |
| 2 | GOL | C | 504 | - | 5,5,5 | 0.78 | 0 | 5,5,5 | 2.48 | 2 (40%) |
| 2 | GOL | C | 505 | - | 5,5,5 | 1.10 | 0 | 5,5,5 | 1.24 | 0 |
| 3 | ARB | C | 506 | - | 10,10,10 | 0.96 | 1 (10%) | 12,14,14 | 2.28 | 4 (33%) |
| 4 | SO4 | C | 507 | - | 4,4,4 | 0.85 | 0 | 6,6,6 | 0.68 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | SO4 | C | 508 | - | 4,4,4 | 0.82 | 0 | 6,6,6 | 0.29 | 0 |
| 4 | SO4 | C | 509 | - | 4,4,4 | 1.14 | 0 | 6,6,6 | 2.49 | 1 (16%) |
| 4 | SO4 | C | 510 | - | 4,4,4 | 0.64 | 0 | 6,6,6 | 0.69 | 0 |
| 4 | SO4 | C | 511 | - | 4,4,4 | 0.62 | 0 | 6,6,6 | 0.66 | 0 |
| 4 | SO4 | C | 512 | - | 4,4,4 | 0.80 | 0 | 6,6,6 | 1.09 | 0 |
| 4 | SO4 | C | 513 | - | 4,4,4 | 0.93 | 0 | 6,6,6 | 1.15 | 1 (16%) |
| 4 | SO4 | C | 514 | - | 4,4,4 | 0.57 | 0 | 6,6,6 | 0.69 | 0 |
| 4 | SO4 | C | 515 | - | 4,4,4 | 0.56 | 0 | 6,6,6 | 0.20 | 0 |
| 4 | SO4 | C | 516 | - | 4,4,4 | 0.46 | 0 | 6,6,6 | 0.45 | 0 |
| 4 | SO4 | C | 517 | - | 4,4,4 | 0.74 | 0 | 6,6,6 | 0.39 | 0 |
| 4 | SO4 | C | 518 | - | 4,4,4 | 0.55 | 0 | 6,6,6 | 0.41 | 0 |
| 5 | CIT | C | 519 | - | 3,12,12 | 2.47 | 1 (33%) | 3,17,17 | 6.21 | 2 (66%) |
| 2 | GOL | D | 501 | - | 5,5,5 | 0.36 | 0 | 5,5,5 | 0.97 | 0 |
| 2 | GOL | D | 502 | - | 5,5,5 | 0.37 | 0 | 5,5,5 | 0.55 | 0 |
| 2 | GOL | D | 503 | - | 5,5,5 | 0.49 | 0 | 5,5,5 | 1.69 | 2 (40%) |
| 3 | ARB | D | 504 | - | 10,10,10 | 1.13 | 1 (10%) | 12,14,14 | 1.67 | 4 (33%) |
| 4 | SO4 | D | 505 | - | 4,4,4 | 0.80 | 0 | 6,6,6 | 0.72 | 0 |
| 4 | SO4 | D | 506 | - | 4,4,4 | 0.75 | 0 | 6,6,6 | 0.68 | 0 |
| 4 | SO4 | D | 507 | - | 4,4,4 | 1.01 | 0 | 6,6,6 | 0.42 | 0 |
| 4 | SO4 | D | 508 | - | 4,4,4 | 0.54 | 0 | 6,6,6 | 0.36 | 0 |
| 4 | SO4 | D | 509 | - | 4,4,4 | 0.62 | 0 | 6,6,6 | 0.57 | 0 |
| 4 | SO4 | D | 510 | - | 4,4,4 | 0.54 | 0 | 6,6,6 | 0.65 | 0 |
| 4 | SO4 | D | 511 | - | 4,4,4 | 0.68 | 0 | 6,6,6 | 0.45 | 0 |
| 4 | SO4 | D | 512 | - | 4,4,4 | 0.52 | 0 | 6,6,6 | 0.43 | 0 |
| 4 | SO4 | D | 513 | - | 4,4,4 | 0.55 | 0 | 6,6,6 | 0.49 | 0 |
| 4 | SO4 | D | 514 | - | 4,4,4 | 0.56 | 0 | 6,6,6 | 0.43 | 0 |
| 5 | CIT | D | 515 | - | 3,12,12 | 2.24 | 1 (33%) | 3,17,17 | 4.06 | 2 (66%) |
| 2 | GOL | E | 501 | - | 5,5,5 | 0.24 | 0 | 5,5,5 | 0.56 | 0 |
| 2 | GOL | E | 502 | - | 5,5,5 | 0.38 | 0 | 5,5,5 | 0.25 | 0 |
| 2 | GOL | E | 503 | - | 5,5,5 | 0.45 | 0 | 5,5,5 | 1.08 | 0 |
| 2 | GOL | E | 504 | - | 5,5,5 | 0.33 | 0 | 5,5,5 | 0.68 | 0 |
| 3 | ARB | E | 505 | - | 10,10,10 | 0.60 | 0 | 12,14,14 | 2.50 | 6 (50%) |
| 4 | SO4 | E | 506 | - | 4,4,4 | 0.56 | 0 | 6,6,6 | 0.20 | 0 |
| 4 | SO4 | E | 507 | - | 4,4,4 | 0.59 | 0 | 6,6,6 | 0.48 | 0 |
| 4 | SO4 | E | 508 | - | 4,4,4 | 0.85 | 0 | 6,6,6 | 0.41 | 0 |
| 4 | SO4 | E | 509 | - | 4,4,4 | 0.91 | 0 | 6,6,6 | 0.33 | 0 |
| 4 | SO4 | E | 510 | - | 4,4,4 | 1.31 | 1 (25%) | 6,6,6 | 0.55 | 0 |
| 4 | SO4 | E | 511 | - | 4,4,4 | 0.72 | 0 | 6,6,6 | 0.28 | 0 |
| 4 | SO4 | E | 512 | - | 4,4,4 | 0.79 | 0 | 6,6,6 | 0.67 | 0 |
| 4 | SO4 | E | 513 | - | 4,4,4 | 0.81 | 0 | 6,6,6 | 0.51 | 0 |
| 4 | SO4 | E | 514 | - | 4,4,4 | 0.43 | 0 | 6,6,6 | 0.25 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | SO4 | E | 515 | - | 4,4,4 | 0.74 | 0 | 6,6,6 | 0.34 | 0 |
| 4 | SO4 | E | 516 | - | 4,4,4 | 0.53 | 0 | 6,6,6 | 0.42 | 0 |
| 5 | CIT | E | 517 | - | 3,12,12 | 0.83 | 0 | 3,17,17 | 3.23 | 1 (33%) |
| 2 | GOL | F | 501 | - | 5,5,5 | 0.33 | 0 | 5,5,5 | 0.62 | 0 |
| 3 | ARB | F | 502 | - | 10,10,10 | 0.95 | 0 | 12,14,14 | 2.37 | 5 (41%) |
| 4 | SO4 | F | 503 | - | 4,4,4 | 0.53 | 0 | 6,6,6 | 0.30 | 0 |
| 4 | SO4 | F | 504 | - | 4,4,4 | 0.75 | 0 | 6,6,6 | 0.44 | 0 |
| 4 | SO4 | F | 505 | - | 4,4,4 | 0.62 | 0 | 6,6,6 | 0.66 | 0 |
| 4 | SO4 | F | 506 | - | 4,4,4 | 0.76 | 0 | 6,6,6 | 0.30 | 0 |
| 4 | SO4 | F | 507 | - | 4,4,4 | 0.50 | 0 | 6,6,6 | 0.20 | 0 |
| 4 | SO4 | F | 508 | - | 4,4,4 | 0.75 | 0 | 6,6,6 | 0.32 | 0 |
| 4 | SO4 | F | 509 | - | 4,4,4 | 0.54 | 0 | 6,6,6 | 0.15 | 0 |
| 4 | SO4 | F | 510 | - | 4,4,4 | 0.78 | 0 | 6,6,6 | 0.63 | 0 |
| 4 | SO4 | F | 511 | - | 4,4,4 | 0.39 | 0 | 6,6,6 | 0.31 | 0 |
| 4 | SO4 | F | 512 | - | 4,4,4 | 0.57 | 0 | 6,6,6 | 0.45 | 0 |
| 4 | SO4 | F | 513 | - | 4,4,4 | 0.67 | 0 | 6,6,6 | 0.59 | 0 |
| 2 | GOL | G | 501 | - | 5,5,5 | 0.45 | 0 | 5,5,5 | 1.13 | 0 |
| 3 | ARB | G | 502 | - | 10,10,10 | 1.21 | 1 (10%) | 12,14,14 | 2.53 | 8 (66%) |
| 4 | SO4 | G | 503 | - | 4,4,4 | 0.66 | 0 | 6,6,6 | 1.40 | 2 (33%) |
| 4 | SO4 | G | 504 | - | 4,4,4 | 0.87 | 0 | 6,6,6 | 0.23 | 0 |
| 4 | SO4 | G | 505 | - | 4,4,4 | 0.51 | 0 | 6,6,6 | 0.25 | 0 |
| 4 | SO4 | G | 506 | - | 4,4,4 | 0.51 | 0 | 6,6,6 | 0.26 | 0 |
| 4 | SO4 | G | 507 | - | 4,4,4 | 0.63 | 0 | 6,6,6 | 0.22 | 0 |
| 4 | SO4 | G | 508 | - | 4,4,4 | 0.56 | 0 | 6,6,6 | 0.51 | 0 |
| 4 | SO4 | G | 509 | - | 4,4,4 | 0.83 | 0 | 6,6,6 | 0.58 | 0 |
| 5 | CIT | G | 510 | - | 3,12,12 | 3.03 | 2 (66%) | 3,17,17 | 4.69 | 1 (33%) |
| 2 | GOL | H | 501 | - | 5,5,5 | 0.28 | 0 | 5,5,5 | 1.32 | 1 (20%) |
| 2 | GOL | H | 502 | - | 5,5,5 | 0.31 | 0 | 5,5,5 | 0.97 | 0 |
| 3 | ARB | H | 503 | - | 10,10,10 | 1.13 | 1 (10%) | 12,14,14 | 1.89 | 3 (25%) |
| 4 | SO4 | H | 504 | - | 4,4,4 | 0.57 | 0 | 6,6,6 | 0.23 | 0 |
| 4 | SO4 | H | 505 | - | 4,4,4 | 0.63 | 0 | 6,6,6 | 0.66 | 0 |
| 4 | SO4 | H | 506 | - | 4,4,4 | 0.80 | 0 | 6,6,6 | 0.71 | 0 |
| 4 | SO4 | H | 507 | - | 4,4,4 | 0.52 | 0 | 6,6,6 | 0.27 | 0 |
| 4 | SO4 | H | 508 | - | 4,4,4 | 0.55 | 0 | 6,6,6 | 0.45 | 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 | GOL | A | 501 | - | - | 0/4/4/4 | 0/0/0/0 |
| 3 | ARB | A | 502 | - | - | 0/0/17/17 | 0/1/1/1 |
| 4 | SO4 | A | 503 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | A | 504 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | A | 505 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | A | 506 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | A | 507 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | A | 508 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | A | 509 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | A | 510 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | A | 511 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | A | 512 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | A | 513 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | A | 514 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | CIT | A | 515 | - | - | 0/6/16/16 | 0/0/0/0 |
| 2 | GOL | B | 501 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | GOL | B | 502 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | GOL | B | 503 | - | - | 0/4/4/4 | 0/0/0/0 |
| 3 | ARB | B | 504 | - | - | 0/0/17/17 | 0/1/1/1 |
| 4 | SO4 | B | 505 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | B | 506 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | B | 507 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | B | 508 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | B | 509 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | B | 510 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | B | 511 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | B | 512 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | B | 513 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | B | 514 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | B | 515 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | B | 516 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | B | 517 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | B | 518 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | CIT | B | 519 | - | - | 0/6/16/16 | 0/0/0/0 |
| 2 | GOL | C | 501 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | GOL | C | 502 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | GOL | C | 503 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | GOL | C | 504 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | GOL | C | 505 | - | - | 0/4/4/4 | 0/0/0/0 |
| 3 | ARB | C | 506 | - | - | 0/0/17/17 | 0/1/1/1 |
| 4 | SO4 | C | 507 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | C | 508 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | C | 509 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4 | SO4 | C | 510 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | C | 511 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | C | 512 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | C | 513 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | C | 514 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | C | 515 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | C | 516 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | C | 517 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | C | 518 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | CIT | C | 519 | - | - | 0/6/16/16 | 0/0/0/0 |
| 2 | GOL | D | 501 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | GOL | D | 502 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | GOL | D | 503 | - | - | 0/4/4/4 | 0/0/0/0 |
| 3 | ARB | D | 504 | - | - | 0/0/17/17 | 0/1/1/1 |
| 4 | SO4 | D | 505 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | D | 506 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | D | 507 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | D | 508 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | D | 509 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | D | 510 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | D | 511 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | D | 512 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | D | 513 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | D | 514 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | CIT | D | 515 | - | - | 0/6/16/16 | 0/0/0/0 |
| 2 | GOL | E | 501 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | GOL | E | 502 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | GOL | E | 503 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | GOL | E | 504 | - | - | 0/4/4/4 | 0/0/0/0 |
| 3 | ARB | E | 505 | - | - | 0/0/17/17 | 0/1/1/1 |
| 4 | SO4 | E | 506 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | E | 507 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | E | 508 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | E | 509 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | E | 510 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | E | 511 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | E | 512 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | E | 513 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | E | 514 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | E | 515 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | E | 516 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | CIT | E | 517 | - | - | 0/6/16/16 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2 | GOL | F | 501 | - | - | 0/4/4/4 | 0/0/0/0 |
| 3 | ARB | F | 502 | - | - | 0/0/17/17 | 0/1/1/1 |
| 4 | SO4 | F | 503 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | F | 504 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | F | 505 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | F | 506 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | F | 507 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | F | 508 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | F | 509 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | F | 510 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | F | 511 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | F | 512 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | F | 513 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | GOL | G | 501 | - | - | 0/4/4/4 | 0/0/0/0 |
| 3 | ARB | G | 502 | - | - | 0/0/17/17 | 0/1/1/1 |
| 4 | SO4 | G | 503 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | G | 504 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | G | 505 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | G | 506 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | G | 507 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | G | 508 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | G | 509 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | CIT | G | 510 | - | - | 0/6/16/16 | 0/0/0/0 |
| 2 | GOL | H | 501 | - | - | 0/4/4/4 | 0/0/0/0 |
| 2 | GOL | H | 502 | - | - | 0/4/4/4 | 0/0/0/0 |
| 3 | ARB | H | 503 | - | - | 0/0/17/17 | 0/1/1/1 |
| 4 | SO4 | H | 504 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | H | 505 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | H | 506 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | H | 507 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | SO4 | H | 508 | - | - | 0/0/0/0 | 0/0/0/0 |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5 | B | 519 | CIT | C4-C3 | -4.73 | 1.47 | 1.54 |
| 5 | C | 519 | CIT | C2-C3 | -3.85 | 1.48 | 1.54 |
| 5 | D | 515 | CIT | C2-C3 | -3.81 | 1.48 | 1.54 |
| 5 | G | 510 | CIT | C4-C3 | -3.75 | 1.49 | 1.54 |
| 5 | A | 515 | CIT | C4-C3 | -2.46 | 1.51 | 1.54 |
| 3 | B | 504 | ARB | O5-C5 | -2.29 | 1.39 | 1.43 |
| 3 | C | 506 | ARB | C3-C2 | -2.15 | 1.46 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4 | E | 510 | SO4 | O4-S | 2.06 | 1.54 | 1.47 |
| 4 | A | 513 | SO4 | O2-S | 2.18 | 1.54 | 1.47 |
| 3 | A | 502 | ARB | O5-C1 | 2.18 | 1.46 | 1.43 |
| 3 | G | 502 | ARB | O1-C1 | 2.23 | 1.47 | 1.39 |
| 3 | A | 502 | ARB | O1-C1 | 2.25 | 1.47 | 1.39 |
| 3 | D | 504 | ARB | C1-C2 | 2.38 | 1.57 | 1.52 |
| 3 | H | 503 | ARB | C4-C3 | 2.42 | 1.55 | 1.52 |
| 5 | G | 510 | CIT | C2-C3 | 3.53 | 1.60 | 1.54 |

All (65) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4 | C | 509 | SO4 | O2-S-O1 | -5.77 | 91.20 | 109.50 |
| 3 | G | 502 | ARB | O3-C3-C4 | -4.68 | 101.54 | 110.00 |
| 2 | C | 504 | GOL | O2-C2-C3 | -4.31 | 88.89 | 108.65 |
| 3 | B | 504 | ARB | O4-C4-C5 | -4.30 | 100.58 | 109.21 |
| 3 | F | 502 | ARB | O3-C3-C2 | -3.09 | 103.38 | 110.34 |
| 5 | B | 519 | CIT | C3-C4-C5 | -3.06 | 110.06 | 114.96 |
| 2 | C | 504 | GOL | O3-C3-C2 | -3.06 | 95.37 | 110.18 |
| 3 | D | 504 | ARB | O3-C3-C4 | -3.01 | 104.56 | 110.00 |
| 3 | E | 505 | ARB | C5-C4-C3 | -2.97 | 106.03 | 109.54 |
| 3 | E | 505 | ARB | O4-C4-C5 | -2.95 | 103.30 | 109.21 |
| 3 | G | 502 | ARB | O4-C4-C5 | -2.91 | 103.38 | 109.21 |
| 3 | C | 506 | ARB | O3-C3-C2 | -2.90 | 103.80 | 110.34 |
| 3 | C | 506 | ARB | O4-C4-C5 | -2.85 | 103.48 | 109.21 |
| 3 | F | 502 | ARB | C5-C4-C3 | -2.83 | 106.19 | 109.54 |
| 3 | A | 502 | ARB | C5-C4-C3 | -2.75 | 106.28 | 109.54 |
| 2 | D | 503 | GOL | C3-C2-C1 | -2.75 | 100.34 | 111.12 |
| 3 | A | 502 | ARB | O3-C3-C2 | -2.74 | 104.17 | 110.34 |
| 3 | A | 502 | ARB | O4-C4-C5 | -2.73 | 103.73 | 109.21 |
| 3 | B | 504 | ARB | O3-C3-C2 | -2.49 | 104.72 | 110.34 |
| 2 | H | 501 | GOL | C3-C2-C1 | -2.22 | 102.40 | 111.12 |
| 4 | A | 504 | SO4 | O2-S-O1 | -2.14 | 102.73 | 109.50 |
| 3 | G | 502 | ARB | O3-C3-C2 | -2.13 | 105.54 | 110.34 |
| 4 | A | 510 | SO4 | O2-S-O1 | -2.05 | 103.00 | 109.50 |
| 2 | D | 503 | GOL | O1-C1-C2 | -2.04 | 100.28 | 110.18 |
| 4 | B | 506 | SO4 | O2-S-O1 | -2.01 | 103.13 | 109.50 |
| 3 | D | 504 | ARB | O5-C5-C4 | 2.03 | 114.15 | 110.86 |
| 3 | G | 502 | ARB | O2-C2-C3 | 2.13 | 115.13 | 110.34 |
| 3 | E | 505 | ARB | O5-C5-C4 | 2.15 | 114.34 | 110.86 |
| 4 | G | 503 | SO4 | O4-S-O3 | 2.15 | 117.72 | 108.98 |
| 3 | D | 504 | ARB | O2-C2-C3 | 2.18 | 115.25 | 110.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4 | A | 513 | SO4 | O4-S-O3 | 2.25 | 118.13 | 108.98 |
| 3 | B | 504 | ARB | C5-C4-C3 | 2.33 | 112.29 | 109.54 |
| 4 | G | 503 | SO4 | O2-S-O1 | 2.40 | 117.09 | 109.50 |
| 3 | G | 502 | ARB | O1-C1-C2 | 2.47 | 115.83 | 109.21 |
| 3 | D | 504 | ARB | O1-C1-C2 | 2.49 | 115.88 | 109.21 |
| 3 | A | 502 | ARB | O2-C2-C1 | 2.53 | 115.39 | 109.82 |
| 3 | G | 502 | ARB | O4-C4-C3 | 2.54 | 115.22 | 110.12 |
| 4 | C | 513 | SO4 | O2-S-O1 | 2.66 | 117.93 | 109.50 |
| 3 | B | 504 | ARB | O2-C2-C1 | 2.73 | 115.83 | 109.82 |
| 3 | B | 504 | ARB | O4-C4-C3 | 2.87 | 115.89 | 110.12 |
| 5 | C | 519 | CIT | C4-C3-C2 | 2.88 | 116.68 | 109.81 |
| 3 | G | 502 | ARB | C5-C4-C3 | 2.88 | 112.95 | 109.54 |
| 3 | C | 506 | ARB | O2-C2-C3 | 2.97 | 117.03 | 110.34 |
| 3 | F | 502 | ARB | O4-C4-C3 | 2.99 | 116.12 | 110.12 |
| 5 | D | 515 | CIT | C3-C4-C5 | 3.00 | 119.75 | 114.96 |
| 3 | E | 505 | ARB | C1-C2-C3 | 3.09 | 115.02 | 110.43 |
| 3 | H | 503 | ARB | C1-C2-C3 | 3.09 | 115.03 | 110.43 |
| 3 | A | 502 | ARB | O4-C4-C3 | 3.13 | 116.41 | 110.12 |
| 3 | H | 503 | ARB | C4-C3-C2 | 3.24 | 116.55 | 111.04 |
| 3 | A | 502 | ARB | O5-C5-C4 | 3.40 | 116.37 | 110.86 |
| 3 | A | 502 | ARB | C1-C2-C3 | 3.44 | 115.55 | 110.43 |
| 3 | E | 505 | ARB | O3-C3-C4 | 3.52 | 116.35 | 110.00 |
| 3 | G | 502 | ARB | C4-C3-C2 | 3.68 | 117.29 | 111.04 |
| 3 | F | 502 | ARB | O2-C2-C1 | 3.78 | 118.14 | 109.82 |
| 3 | H | 503 | ARB | C5-C4-C3 | 4.37 | 114.71 | 109.54 |
| 5 | B | 519 | CIT | C4-C3-C2 | 4.40 | 120.33 | 109.81 |
| 5 | A | 515 | CIT | C3-C2-C1 | 4.40 | 122.00 | 114.96 |
| 3 | F | 502 | ARB | O3-C3-C4 | 4.56 | 118.23 | 110.00 |
| 3 | E | 505 | ARB | O4-C4-C3 | 5.11 | 120.39 | 110.12 |
| 3 | C | 506 | ARB | C5-C4-C3 | 5.14 | 115.62 | 109.54 |
| 5 | B | 519 | CIT | C3-C2-C1 | 5.21 | 123.29 | 114.96 |
| 5 | E | 517 | CIT | C3-C4-C5 | 5.31 | 123.45 | 114.96 |
| 5 | D | 515 | CIT | C3-C2-C1 | 6.35 | 125.12 | 114.96 |
| 5 | G | 510 | CIT | C3-C2-C1 | 8.01 | 127.77 | 114.96 |
| 5 | C | 519 | CIT | C3-C4-C5 | 10.36 | 131.52 | 114.96 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 82 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | A | 501 | GOL | 8 | 0 |
| 4 | A | 506 | SO4 | 1 | 0 |
| 5 | A | 515 | CIT | 6 | 0 |
| 2 | B | 503 | GOL | 2 | 0 |
| 4 | B | 505 | SO4 | 1 | 0 |
| 4 | B | 507 | SO4 | 1 | 0 |
| 4 | B | 514 | SO4 | 1 | 0 |
| 4 | B | 516 | SO4 | 1 | 0 |
| 5 | B | 519 | CIT | 6 | 0 |
| 2 | C | 504 | GOL | 1 | 0 |
| 2 | C | 505 | GOL | 1 | 0 |
| 4 | C | 508 | SO4 | 1 | 0 |
| 4 | C | 510 | SO4 | 1 | 0 |
| 4 | C | 512 | SO4 | 1 | 0 |
| 4 | C | 516 | SO4 | 1 | 0 |
| 5 | C | 519 | CIT | 9 | 0 |
| 2 | D | 501 | GOL | 2 | 0 |
| 2 | D | 502 | GOL | 1 | 0 |
| 2 | D | 503 | GOL | 4 | 0 |
| 4 | D | 506 | SO4 | 1 | 0 |
| 4 | D | 510 | SO4 | 1 | 0 |
| 4 | D | 512 | SO4 | 1 | 0 |
| 4 | D | 513 | SO4 | 1 | 0 |
| 4 | D | 514 | SO4 | 1 | 0 |
| 5 | D | 515 | CIT | 7 | 0 |
| 2 | E | 504 | GOL | 3 | 0 |
| 4 | E | 506 | SO4 | 1 | 0 |
| 5 | E | 517 | CIT | 9 | 0 |
| 3 | F | 502 | ARB | 1 | 0 |
| 2 | G | 501 | GOL | 1 | 0 |
| 3 | G | 502 | ARB | 2 | 0 |
| 5 | G | 510 | CIT | 3 | 0 |
| 2 | H | 502 | GOL | 4 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|--------|
| 1 | A | 431/448 (96%) | -0.39 | 5 (1%) 81 80 | 11, 17, 35, 83 | 0 |
| 1 | B | 430/448 (95%) | -0.37 | 4 (0%) 85 85 | 14, 23, 38, 74 | 0 |
| 1 | C | 432/448 (96%) | -0.18 | 15 (3%) 48 46 | 12, 24, 55, 99 | 0 |
| 1 | D | 435/448 (97%) | -0.29 | 9 (2%) 67 65 | 18, 26, 47, 97 | 0 |
| 1 | E | 431/448 (96%) | -0.04 | 21 (4%) 33 33 | 18, 29, 63, 110 | 0 |
| 1 | F | 430/448 (95%) | 0.15 | 26 (6%) 25 25 | 19, 37, 61, 98 | 0 |
| 1 | G | 431/448 (96%) | 0.65 | 64 (14%) 3 3 | 19, 43, 76, 134 | 1 (0%) |
| 1 | H | 430/448 (95%) | 1.00 | 79 (18%) 2 2 | 32, 55, 77, 116 | 0 |
| All | All | 3450/3584 (96%) | 0.07 | 223 (6%) 22 22 | 11, 29, 66, 134 | 1 (0%) |

All (223) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | G | 14 | ALA | 14.8 |
| 1 | E | 444 | VAL | 14.3 |
| 1 | F | 444 | VAL | 10.6 |
| 1 | G | 444 | VAL | 10.2 |
| 1 | H | 444 | VAL | 10.1 |
| 1 | C | 444 | VAL | 9.2 |
| 1 | H | 127 | ILE | 7.5 |
| 1 | G | 405 | MET | 7.4 |
| 1 | H | 405 | MET | 6.5 |
| 1 | F | 15 | SER | 6.2 |
| 1 | A | 14 | ALA | 6.0 |
| 1 | C | 405 | MET | 5.9 |
| 1 | G | 391 | LYS | 5.8 |
| 1 | H | 443 | ALA | 5.6 |
| 1 | H | 288 | LEU | 5.5 |
| 1 | E | 406 | GLU | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 405 | MET | 5.4 |
| 1 | C | 14 | ALA | 5.4 |
| 1 | F | 405 | MET | 5.3 |
| 1 | A | 444 | VAL | 5.3 |
| 1 | H | 15 | SER | 5.3 |
| 1 | G | 15 | SER | 5.0 |
| 1 | H | 103 | ALA | 4.7 |
| 1 | H | 146 | ASN | 4.6 |
| 1 | G | 403 | GLY | 4.6 |
| 1 | H | 196 | VAL | 4.6 |
| 1 | E | 14 | ALA | 4.6 |
| 1 | H | 104 | LYS | 4.6 |
| 1 | H | 406 | GLU | 4.5 |
| 1 | F | 443 | ALA | 4.5 |
| 1 | G | 404 | CYS | 4.5 |
| 1 | G | 442 | PRO | 4.4 |
| 1 | B | 405 | MET | 4.3 |
| 1 | G | 377 | ALA | 4.2 |
| 1 | G | 430 | LEU | 4.2 |
| 1 | H | 64 | VAL | 4.2 |
| 1 | G | 443 | ALA | 4.2 |
| 1 | H | 118 | ASN | 4.1 |
| 1 | D | 14 | ALA | 4.1 |
| 1 | G | 328 | LEU | 4.1 |
| 1 | E | 421 | LEU | 4.0 |
| 1 | H | 101 | PRO | 3.9 |
| 1 | H | 125 | ILE | 3.9 |
| 1 | B | 15 | SER | 3.9 |
| 1 | G | 388 | ILE | 3.9 |
| 1 | G | 341 | THR | 3.9 |
| 1 | H | 328 | LEU | 3.9 |
| 1 | G | 321 | TRP | 3.8 |
| 1 | F | 127 | ILE | 3.8 |
| 1 | H | 107 | LYS | 3.8 |
| 1 | G | 401 | ASP | 3.7 |
| 1 | H | 190 | GLY | 3.6 |
| 1 | E | 424 | HIS | 3.6 |
| 1 | H | 204 | LEU | 3.5 |
| 1 | G | 389 | SER | 3.5 |
| 1 | H | 183 | PHE | 3.5 |
| 1 | H | 287 | MET | 3.4 |
| 1 | F | 146 | ASN | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | H | 126 | HIS | 3.4 |
| 1 | F | 171 | ARG | 3.4 |
| 1 | H | 331 | GLY | 3.4 |
| 1 | G | 379 | GLY | 3.3 |
| 1 | F | 196 | VAL | 3.3 |
| 1 | E | 443 | ALA | 3.3 |
| 1 | G | 424 | HIS | 3.3 |
| 1 | G | 363 | VAL | 3.3 |
| 1 | E | 442 | PRO | 3.3 |
| 1 | G | 406 | GLU | 3.3 |
| 1 | H | 424 | HIS | 3.2 |
| 1 | G | 203 | LYS | 3.2 |
| 1 | H | 329 | MET | 3.2 |
| 1 | E | 420 | GLY | 3.2 |
| 1 | G | 410 | ALA | 3.2 |
| 1 | H | 173 | GLU | 3.2 |
| 1 | C | 423 | LYS | 3.2 |
| 1 | F | 406 | GLU | 3.2 |
| 1 | F | 303 | THR | 3.1 |
| 1 | H | 50 | TYR | 3.1 |
| 1 | E | 204 | LEU | 3.0 |
| 1 | H | 203 | LYS | 3.0 |
| 1 | G | 322 | ILE | 3.0 |
| 1 | H | 147 | VAL | 3.0 |
| 1 | C | 443 | ALA | 3.0 |
| 1 | B | 127 | ILE | 3.0 |
| 1 | H | 114 | ASP | 3.0 |
| 1 | G | 370 | VAL | 2.9 |
| 1 | H | 112 | LEU | 2.9 |
| 1 | G | 438 | VAL | 2.9 |
| 1 | C | 424 | HIS | 2.9 |
| 1 | H | 145 | THR | 2.9 |
| 1 | C | 127 | ILE | 2.9 |
| 1 | G | 287 | MET | 2.9 |
| 1 | H | 66 | ASP | 2.9 |
| 1 | F | 442 | PRO | 2.9 |
| 1 | E | 400 | LYS | 2.9 |
| 1 | H | 195 | LYS | 2.9 |
| 1 | H | 128 | MET | 2.8 |
| 1 | G | 407 | PRO | 2.8 |
| 1 | G | 378 | GLU | 2.8 |
| 1 | H | 379 | GLY | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 423 | LYS | 2.8 |
| 1 | G | 431 | GLY | 2.8 |
| 1 | H | 98 | ASN | 2.8 |
| 1 | D | 377 | ALA | 2.8 |
| 1 | H | 197 | ALA | 2.8 |
| 1 | H | 54 | TYR | 2.7 |
| 1 | H | 378 | GLU | 2.7 |
| 1 | E | 377 | ALA | 2.7 |
| 1 | F | 145 | THR | 2.7 |
| 1 | G | 204 | LEU | 2.7 |
| 1 | E | 203 | LYS | 2.7 |
| 1 | E | 407 | PRO | 2.7 |
| 1 | C | 421 | LEU | 2.7 |
| 1 | G | 422 | VAL | 2.7 |
| 1 | F | 424 | HIS | 2.7 |
| 1 | C | 406 | GLU | 2.7 |
| 1 | H | 105 | GLY | 2.7 |
| 1 | H | 175 | ALA | 2.7 |
| 1 | H | 30 | ASN | 2.7 |
| 1 | H | 16 | MET | 2.7 |
| 1 | H | 303 | THR | 2.6 |
| 1 | F | 423 | LYS | 2.6 |
| 1 | D | 127 | ILE | 2.6 |
| 1 | G | 323 | ILE | 2.6 |
| 1 | C | 196 | VAL | 2.6 |
| 1 | H | 42 | ASP | 2.6 |
| 1 | E | 379 | GLY | 2.5 |
| 1 | C | 288 | LEU | 2.5 |
| 1 | F | 421 | LEU | 2.5 |
| 1 | G | 64 | VAL | 2.5 |
| 1 | F | 195 | LYS | 2.5 |
| 1 | H | 97 | VAL | 2.5 |
| 1 | G | 301 | GLY | 2.5 |
| 1 | A | 405 | MET | 2.5 |
| 1 | G | 367 | ASN | 2.5 |
| 1 | H | 17 | HIS | 2.5 |
| 1 | E | 288 | LEU | 2.5 |
| 1 | G | 395 | VAL | 2.5 |
| 1 | C | 407 | PRO | 2.4 |
| 1 | H | 219 | ILE | 2.4 |
| 1 | G | 400 | LYS | 2.4 |
| 1 | G | 343 | SER | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | G | 262 | LEU | 2.4 |
| 1 | H | 193 | PHE | 2.4 |
| 1 | F | 147 | VAL | 2.4 |
| 1 | H | 256 | PHE | 2.4 |
| 1 | H | 295 | ILE | 2.4 |
| 1 | H | 423 | LYS | 2.4 |
| 1 | H | 327 | PRO | 2.3 |
| 1 | H | 65 | VAL | 2.3 |
| 1 | D | 405 | MET | 2.3 |
| 1 | H | 174 | GLY | 2.3 |
| 1 | G | 320 | LEU | 2.3 |
| 1 | G | 340 | TRP | 2.3 |
| 1 | G | 394 | VAL | 2.3 |
| 1 | G | 397 | VAL | 2.3 |
| 1 | D | 203 | LYS | 2.3 |
| 1 | E | 15 | SER | 2.3 |
| 1 | F | 391 | LYS | 2.3 |
| 1 | G | 396 | SER | 2.3 |
| 1 | G | 344 | LEU | 2.3 |
| 1 | G | 421 | LEU | 2.3 |
| 1 | D | 64 | VAL | 2.3 |
| 1 | F | 89 | GLU | 2.3 |
| 1 | H | 194 | VAL | 2.3 |
| 1 | H | 116 | ILE | 2.3 |
| 1 | H | 182 | LEU | 2.3 |
| 1 | C | 13 | ASP | 2.3 |
| 1 | G | 318 | MET | 2.3 |
| 1 | H | 111 | PRO | 2.3 |
| 1 | H | 171 | ARG | 2.3 |
| 1 | F | 204 | LEU | 2.3 |
| 1 | H | 290 | LEU | 2.3 |
| 1 | H | 19 | TYR | 2.2 |
| 1 | G | 408 | MET | 2.2 |
| 1 | G | 67 | ILE | 2.2 |
| 1 | G | 317 | MET | 2.2 |
| 1 | F | 151 | ASP | 2.2 |
| 1 | G | 312 | ASP | 2.2 |
| 1 | H | 339 | GLU | 2.2 |
| 1 | C | 230 | LEU | 2.2 |
| 1 | F | 205 | TYR | 2.2 |
| 1 | H | 58 | PHE | 2.2 |
| 1 | H | 67 | ILE | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | G | 260 | TRP | 2.2 |
| 1 | E | 320 | LEU | 2.2 |
| 1 | H | 69 | TRP | 2.2 |
| 1 | D | 15 | SER | 2.2 |
| 1 | H | 223 | GLY | 2.2 |
| 1 | H | 330 | PHE | 2.2 |
| 1 | H | 151 | ASP | 2.2 |
| 1 | G | 390 | GLU | 2.2 |
| 1 | G | 423 | LYS | 2.2 |
| 1 | G | 425 | GLN | 2.1 |
| 1 | F | 420 | GLY | 2.1 |
| 1 | G | 285 | ALA | 2.1 |
| 1 | G | 350 | VAL | 2.1 |
| 1 | G | 432 | PRO | 2.1 |
| 1 | G | 364 | TYR | 2.1 |
| 1 | H | 21 | TRP | 2.1 |
| 1 | B | 196 | VAL | 2.1 |
| 1 | G | 329 | MET | 2.1 |
| 1 | A | 15 | SER | 2.1 |
| 1 | G | 118 | ASN | 2.1 |
| 1 | G | 53 | LYS | 2.1 |
| 1 | D | 320 | LEU | 2.1 |
| 1 | D | 196 | VAL | 2.1 |
| 1 | E | 404 | CYS | 2.1 |
| 1 | F | 17 | HIS | 2.0 |
| 1 | H | 53 | LYS | 2.0 |
| 1 | H | 143 | LEU | 2.0 |
| 1 | F | 377 | ALA | 2.0 |
| 1 | H | 377 | ALA | 2.0 |
| 1 | F | 16 | MET | 2.0 |
| 1 | G | 261 | GLU | 2.0 |
| 1 | H | 115 | TYR | 2.0 |
| 1 | H | 29 | TRP | 2.0 |
| 1 | H | 36 | GLY | 2.0 |
| 1 | H | 421 | LEU | 2.0 |
| 1 | A | 196 | VAL | 2.0 |
| 1 | H | 404 | CYS | 2.0 |
| 1 | C | 15 | SER | 2.0 |
| 1 | E | 409 | LYS | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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 | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 4 | SO4 | F | 504 | 5/5 | 0.89 | 0.30 | 15.62 | 87,90,100,100 | 0 |
| 4 | SO4 | C | 511 | 5/5 | 0.91 | 0.27 | 14.15 | 63,77,82,89 | 0 |
| 4 | SO4 | E | 515 | 5/5 | 0.66 | 0.34 | 13.79 | 86,91,115,116 | 0 |
| 4 | SO4 | A | 509 | 5/5 | 0.95 | 0.29 | 10.48 | 53,59,70,74 | 0 |
| 4 | SO4 | C | 514 | 5/5 | 0.81 | 0.26 | 9.24 | 73,86,97,108 | 0 |
| 4 | SO4 | A | 514 | 5/5 | 0.81 | 0.27 | 7.14 | 76,91,105,108 | 0 |
| 4 | SO4 | B | 506 | 5/5 | 0.93 | 0.19 | 6.95 | 35,44,51,56 | 5 |
| 4 | SO4 | D | 507 | 5/5 | 0.93 | 0.22 | 6.93 | 46,55,60,71 | 0 |
| 4 | SO4 | E | 513 | 5/5 | 0.90 | 0.23 | 6.88 | 73,95,101,108 | 0 |
| 4 | SO4 | G | 504 | 5/5 | 0.92 | 0.29 | 6.81 | 66,80,88,90 | 0 |
| 4 | SO4 | C | 512 | 5/5 | 0.95 | 0.17 | 6.63 | 55,58,63,71 | 0 |
| 5 | CIT | E | 517 | 13/13 | 0.85 | 0.24 | 5.95 | 39,62,77,81 | 0 |
| 4 | SO4 | B | 509 | 5/5 | 0.95 | 0.20 | 4.93 | 50,60,63,75 | 0 |
| 2 | GOL | E | 504 | 6/6 | 0.93 | 0.16 | 4.76 | 49,51,55,64 | 0 |
| 4 | SO4 | F | 513 | 5/5 | 0.90 | 0.28 | 4.58 | 74,77,87,96 | 0 |
| 2 | GOL | C | 505 | 6/6 | 0.94 | 0.16 | 4.46 | 23,31,37,43 | 0 |
| 4 | SO4 | E | 512 | 5/5 | 0.90 | 0.24 | 4.31 | 77,78,87,92 | 0 |
| 5 | CIT | A | 515 | 13/13 | 0.89 | 0.20 | 4.20 | 31,43,56,58 | 0 |
| 5 | CIT | C | 519 | 13/13 | 0.89 | 0.20 | 4.19 | 26,43,64,66 | 0 |
| 5 | CIT | D | 515 | 13/13 | 0.89 | 0.26 | 3.96 | 32,55,69,86 | 0 |
| 5 | CIT | G | 510 | 13/13 | 0.88 | 0.23 | 3.95 | 36,59,73,76 | 0 |
| 4 | SO4 | E | 508 | 5/5 | 0.94 | 0.22 | 3.87 | 53,63,76,84 | 0 |
| 4 | SO4 | G | 507 | 5/5 | 0.88 | 0.25 | 3.81 | 75,84,96,105 | 0 |
| 4 | SO4 | D | 506 | 5/5 | 0.92 | 0.24 | 3.78 | 54,69,81,86 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 2 | GOL | B | 502 | 6/6 | 0.78 | 0.19 | 3.50 | 65,74,76,81 | 0 |
| 5 | CIT | B | 519 | 13/13 | 0.90 | 0.24 | 3.49 | 41,53,72,75 | 0 |
| 4 | SO4 | F | 505 | 5/5 | 0.88 | 0.28 | 3.36 | 79,91,98,108 | 0 |
| 4 | SO4 | C | 509 | 5/5 | 0.88 | 0.18 | 2.94 | 41,46,57,63 | 5 |
| 4 | SO4 | A | 510 | 5/5 | 0.96 | 0.14 | 2.62 | 31,37,42,62 | 0 |
| 2 | GOL | E | 501 | 6/6 | 0.92 | 0.14 | 2.39 | 37,45,50,61 | 0 |
| 4 | SO4 | A | 507 | 5/5 | 0.98 | 0.13 | 2.34 | 34,43,45,47 | 0 |
| 2 | GOL | H | 501 | 6/6 | 0.80 | 0.20 | 2.29 | 55,57,63,68 | 0 |
| 4 | SO4 | E | 510 | 5/5 | 0.95 | 0.23 | 2.26 | 52,58,73,73 | 0 |
| 4 | SO4 | F | 506 | 5/5 | 0.87 | 0.18 | 2.19 | 70,70,87,88 | 0 |
| 4 | SO4 | D | 505 | 5/5 | 0.96 | 0.14 | 2.09 | 49,60,66,67 | 0 |
| 2 | GOL | C | 501 | 6/6 | 0.95 | 0.14 | 2.00 | 28,33,40,44 | 0 |
| 2 | GOL | B | 501 | 6/6 | 0.92 | 0.15 | 1.97 | 29,35,40,43 | 0 |
| 4 | SO4 | A | 513 | 5/5 | 0.96 | 0.20 | 1.90 | 43,47,49,55 | 0 |
| 4 | SO4 | H | 507 | 5/5 | 0.81 | 0.33 | 1.83 | 86,101,114,127 | 0 |
| 4 | SO4 | F | 509 | 5/5 | 0.88 | 0.29 | 1.56 | 94,96,105,113 | 0 |
| 2 | GOL | D | 503 | 6/6 | 0.94 | 0.17 | 1.31 | 37,41,42,48 | 0 |
| 2 | GOL | B | 503 | 6/6 | 0.94 | 0.13 | 1.26 | 32,35,41,47 | 0 |
| 2 | GOL | F | 501 | 6/6 | 0.84 | 0.21 | 1.13 | 51,61,68,74 | 0 |
| 4 | SO4 | G | 508 | 5/5 | 0.95 | 0.15 | 1.09 | 59,72,82,86 | 0 |
| 3 | ARB | G | 502 | 10/10 | 0.92 | 0.21 | 0.78 | 32,39,44,50 | 0 |
| 4 | SO4 | C | 508 | 5/5 | 0.96 | 0.16 | 0.76 | 45,56,57,70 | 0 |
| 2 | GOL | C | 504 | 6/6 | 0.96 | 0.13 | 0.65 | 34,42,47,47 | 0 |
| 3 | ARB | C | 506 | 10/10 | 0.97 | 0.17 | 0.29 | 19,25,35,36 | 0 |
| 3 | ARB | A | 502 | 10/10 | 0.98 | 0.17 | 0.21 | 15,20,26,29 | 0 |
| 3 | ARB | F | 502 | 10/10 | 0.95 | 0.17 | 0.20 | 32,43,48,55 | 0 |
| 2 | GOL | C | 503 | 6/6 | 0.89 | 0.15 | 0.14 | 50,60,63,66 | 0 |
| 3 | ARB | B | 504 | 10/10 | 0.96 | 0.17 | 0.11 | 19,22,30,32 | 0 |
| 4 | SO4 | G | 503 | 5/5 | 1.00 | 0.07 | 0.05 | 28,29,36,39 | 0 |
| 3 | ARB | E | 505 | 10/10 | 0.97 | 0.14 | 0.02 | 24,28,36,40 | 0 |
| 3 | ARB | D | 504 | 10/10 | 0.95 | 0.14 | -0.04 | 19,25,28,32 | 0 |
| 3 | ARB | H | 503 | 10/10 | 0.91 | 0.21 | -0.08 | 52,62,67,67 | 0 |
| 2 | GOL | G | 501 | 6/6 | 0.92 | 0.12 | -0.09 | 40,47,52,54 | 0 |
| 2 | GOL | A | 501 | 6/6 | 0.94 | 0.12 | -0.11 | 25,32,38,41 | 0 |
| 4 | SO4 | A | 506 | 5/5 | 1.00 | 0.07 | -0.34 | 24,27,28,31 | 0 |
| 2 | GOL | H | 502 | 6/6 | 0.87 | 0.18 | -0.55 | 54,56,62,63 | 0 |
| 4 | SO4 | H | 506 | 5/5 | 0.94 | 0.11 | -2.49 | 59,72,79,80 | 0 |
| 4 | SO4 | D | 508 | 5/5 | 0.94 | 0.23 | - | 67,84,93,94 | 0 |
| 4 | SO4 | F | 511 | 5/5 | 0.95 | 0.28 | - | 89,98,104,104 | 0 |
| 4 | SO4 | A | 503 | 5/5 | 0.90 | 0.31 | - | 44,57,70,74 | 0 |
| 4 | SO4 | B | 508 | 5/5 | 0.94 | 0.28 | - | 59,67,76,91 | 0 |
| 4 | SO4 | D | 513 | 5/5 | 0.89 | 0.29 | - | 75,91,102,109 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 4 | SO4 | D | 510 | 5/5 | 0.92 | 0.20 | - | 62,64,72,76 | 0 |
| 4 | SO4 | C | 515 | 5/5 | 0.84 | 0.32 | - | 97,102,106,109 | 0 |
| 4 | SO4 | G | 505 | 5/5 | 0.93 | 0.32 | - | 73,73,76,76 | 5 |
| 4 | SO4 | B | 516 | 5/5 | 0.89 | 0.34 | - | 67,73,74,94 | 0 |
| 2 | GOL | D | 501 | 6/6 | 0.91 | 0.16 | - | 33,35,37,39 | 0 |
| 4 | SO4 | D | 509 | 5/5 | 0.90 | 0.30 | - | 63,82,90,102 | 0 |
| 4 | SO4 | B | 517 | 5/5 | 0.94 | 0.34 | - | 65,76,82,86 | 0 |
| 4 | SO4 | G | 506 | 5/5 | 0.91 | 0.36 | - | 85,87,103,110 | 0 |
| 4 | SO4 | A | 512 | 5/5 | 0.80 | 0.25 | - | 71,78,105,108 | 0 |
| 4 | SO4 | E | 516 | 5/5 | 0.90 | 0.29 | - | 92,99,110,113 | 0 |
| 2 | GOL | E | 503 | 6/6 | 0.89 | 0.24 | - | 49,57,62,65 | 0 |
| 4 | SO4 | B | 511 | 5/5 | 0.93 | 0.34 | - | 73,76,88,99 | 0 |
| 4 | SO4 | B | 512 | 5/5 | 0.78 | 0.25 | - | 94,106,111,116 | 0 |
| 4 | SO4 | E | 514 | 5/5 | 0.94 | 0.25 | - | 77,82,93,94 | 0 |
| 4 | SO4 | C | 510 | 5/5 | 0.98 | 0.17 | - | 44,52,62,68 | 0 |
| 4 | SO4 | B | 514 | 5/5 | 0.91 | 0.28 | - | 68,74,85,99 | 0 |
| 4 | SO4 | C | 518 | 5/5 | 0.93 | 0.31 | - | 86,87,96,100 | 0 |
| 4 | SO4 | B | 507 | 5/5 | 0.97 | 0.25 | - | 62,68,74,82 | 0 |
| 4 | SO4 | F | 512 | 5/5 | 0.84 | 0.36 | - | 82,88,100,103 | 0 |
| 4 | SO4 | H | 508 | 5/5 | 0.88 | 0.28 | - | 90,96,107,110 | 0 |
| 4 | SO4 | E | 507 | 5/5 | 0.98 | 0.11 | - | 45,47,54,58 | 0 |
| 4 | SO4 | F | 510 | 5/5 | 0.94 | 0.20 | - | 60,61,72,86 | 0 |
| 4 | SO4 | F | 503 | 5/5 | 0.79 | 0.28 | - | 97,105,115,117 | 0 |
| 4 | SO4 | A | 508 | 5/5 | 0.94 | 0.28 | - | 75,77,84,91 | 0 |
| 4 | SO4 | A | 511 | 5/5 | 0.93 | 0.31 | - | 65,73,84,89 | 0 |
| 4 | SO4 | A | 504 | 5/5 | 0.98 | 0.17 | - | 42,49,59,62 | 0 |
| 4 | SO4 | H | 504 | 5/5 | 0.86 | 0.31 | - | 86,96,99,111 | 0 |
| 4 | SO4 | A | 505 | 5/5 | 0.94 | 0.35 | - | 71,72,81,82 | 0 |
| 4 | SO4 | D | 512 | 5/5 | 0.88 | 0.36 | - | 94,95,103,107 | 0 |
| 4 | SO4 | C | 517 | 5/5 | 0.85 | 0.31 | - | 68,76,103,106 | 0 |
| 4 | SO4 | B | 518 | 5/5 | 0.76 | 0.39 | - | 99,101,110,114 | 0 |
| 4 | SO4 | F | 508 | 5/5 | 0.93 | 0.30 | - | 66,73,90,92 | 0 |
| 4 | SO4 | H | 505 | 5/5 | 0.65 | 0.38 | - | 92,113,123,129 | 0 |
| 2 | GOL | E | 502 | 6/6 | 0.77 | 0.20 | - | 63,67,70,78 | 0 |
| 2 | GOL | C | 502 | 6/6 | 0.92 | 0.11 | - | 48,53,54,57 | 0 |
| 4 | SO4 | D | 511 | 5/5 | 0.93 | 0.27 | - | 70,75,87,97 | 0 |
| 4 | SO4 | F | 507 | 5/5 | 0.65 | 0.45 | - | 122,124,130,137 | 0 |
| 4 | SO4 | E | 506 | 5/5 | 0.89 | 0.33 | - | 80,86,91,93 | 0 |
| 4 | SO4 | G | 509 | 5/5 | 0.81 | 0.27 | - | 75,83,99,102 | 0 |
| 4 | SO4 | B | 505 | 5/5 | 0.92 | 0.32 | - | 67,83,85,87 | 0 |
| 4 | SO4 | C | 516 | 5/5 | 0.83 | 0.29 | - | 111,116,121,126 | 0 |
| 4 | SO4 | C | 507 | 5/5 | 0.89 | 0.30 | - | 58,59,70,75 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 4 | SO4 | E | 511 | 5/5 | 0.83 | 0.28 | - | 63,86,95,95 | 0 |
| 4 | SO4 | B | 510 | 5/5 | 0.82 | 0.31 | - | 75,91,105,106 | 0 |
| 4 | SO4 | C | 513 | 5/5 | 0.92 | 0.35 | - | 55,62,71,72 | 0 |
| 4 | SO4 | E | 509 | 5/5 | 0.93 | 0.23 | - | 59,61,73,74 | 0 |
| 4 | SO4 | B | 513 | 5/5 | 0.90 | 0.20 | - | 68,71,82,83 | 0 |
| 4 | SO4 | D | 514 | 5/5 | 0.84 | 0.26 | - | 73,86,96,103 | 0 |
| 2 | GOL | D | 502 | 6/6 | 0.92 | 0.10 | - | 42,57,59,59 | 0 |
| 4 | SO4 | B | 515 | 5/5 | 0.84 | 0.43 | - | 89,95,97,102 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.