



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:14 AM UTC

PDB ID : 4NX0 / pdb\_00004nx0  
Title : Crystal structure of Abp-WT, a GH27-b-L-arabinopyranosidase from *Geobacillus stearothermophilus*  
Authors : Lansky, S.; Solomon, H.V.; Salama, R.; Belrhali, H.; Shoham, Y.; Shoham, G.  
Deposited on : 2013-12-08  
Resolution : 2.28 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

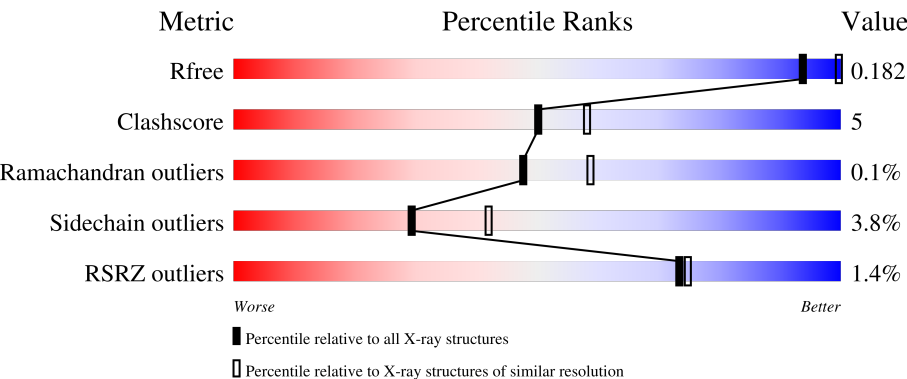
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 9078 (2.30-2.26)                                      |
| Clashscore            | 190562                      | 9802 (2.30-2.26)                                      |
| Ramachandran outliers | 187476                      | 9690 (2.30-2.26)                                      |
| Sidechain outliers    | 187428                      | 9691 (2.30-2.26)                                      |
| RSRZ outliers         | 180081                      | 9085 (2.30-2.26)                                      |

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

| Mol | Chain | Length | Quality of chain                          |
|-----|-------|--------|-------------------------------------------|
| 1   | A     | 448    | <div><div></div><div>87%8%</div></div>    |
| 1   | B     | 448    | <div><div>%</div><div>83%12%</div></div>  |
| 1   | C     | 448    | <div><div>2%</div><div>85%10%</div></div> |
| 1   | D     | 448    | <div><div></div><div>88%8%</div></div>    |
| 1   | E     | 448    | <div><div>%</div><div>87%8%</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  | C     | 503 | -         | X        | -       | -                |
| 2   | GOL  | C     | 505 | -         | -        | X       | -                |
| 2   | GOL  | D     | 502 | -         | -        | X       | -                |
| 2   | GOL  | D     | 503 | -         | X        | -       | -                |
| 2   | GOL  | D     | 505 | -         | -        | X       | -                |
| 2   | GOL  | E     | 505 | -         | X        | X       | -                |
| 2   | GOL  | F     | 502 | -         | -        | X       | -                |
| 4   | CIT  | A     | 515 | -         | X        | X       | -                |
| 4   | CIT  | B     | 520 | -         | -        | X       | -                |
| 4   | CIT  | C     | 519 | -         | X        | -       | -                |
| 4   | CIT  | G     | 513 | -         | X        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32820 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     | 430      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 3492  | 2233 | 598 | 636 | 25 |         |         |       |
| 1   | B     | 430      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 3496  | 2235 | 598 | 638 | 25 |         |         |       |
| 1   | C     | 431      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 3487  | 2230 | 598 | 634 | 25 |         |         |       |
| 1   | D     | 435      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 3506  | 2243 | 603 | 635 | 25 |         |         |       |
| 1   | E     | 430      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 3484  | 2228 | 597 | 634 | 25 |         |         |       |
| 1   | F     | 430      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3470  | 2219 | 596 | 630 | 25 |         |         |       |
| 1   | G     | 430      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 3481  | 2226 | 596 | 634 | 25 |         |         |       |
| 1   | H     | 430      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3470  | 2219 | 596 | 630 | 25 |         |         |       |

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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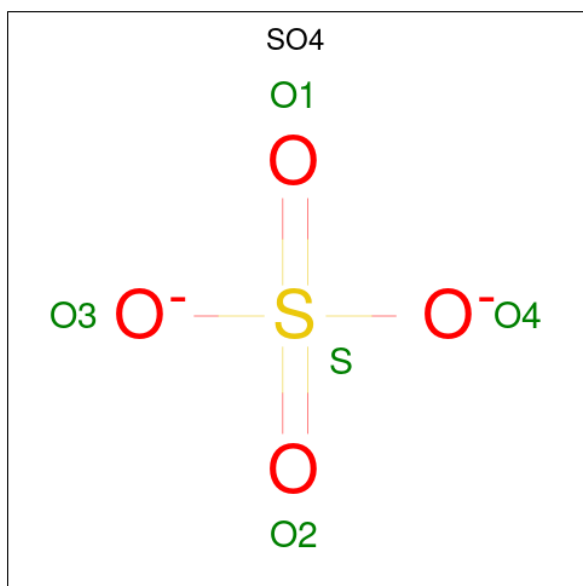
| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 2   | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | C     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | D     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | D     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | D     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | D     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | D     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | E     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | E     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | E     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | E     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | E     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | E     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | E     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | F     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | F     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | F     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | F     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | G     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |
| 2   | G     | 1        | Total<br>6 | C<br>3 | O<br>3 | 0       | 0       |

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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

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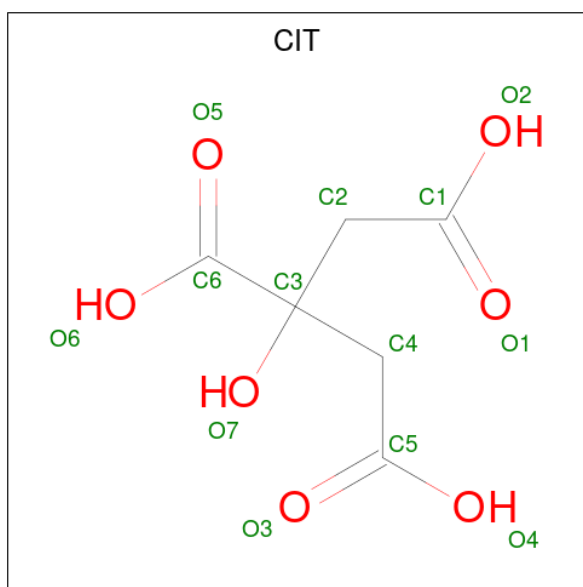
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula:  $C_6H_8O_7$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |
| 4   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 6 | 7 |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 5   | A     | 662      | Total | O   | 0       | 0       |
|     |       |          | 662   | 662 |         |         |
| 5   | B     | 625      | Total | O   | 0       | 0       |
|     |       |          | 625   | 625 |         |         |
| 5   | C     | 579      | Total | O   | 0       | 0       |
|     |       |          | 579   | 579 |         |         |
| 5   | D     | 536      | Total | O   | 0       | 0       |
|     |       |          | 536   | 536 |         |         |
| 5   | E     | 500      | Total | O   | 0       | 0       |
|     |       |          | 500   | 500 |         |         |
| 5   | F     | 495      | Total | O   | 0       | 0       |
|     |       |          | 495   | 495 |         |         |
| 5   | G     | 439      | Total | O   | 0       | 0       |
|     |       |          | 439   | 439 |         |         |

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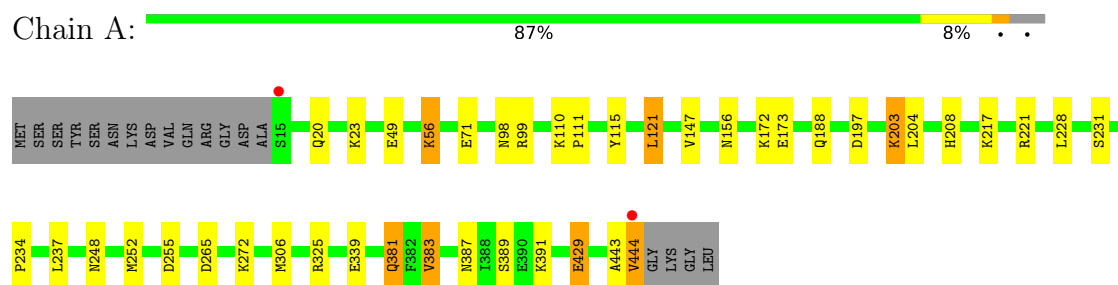
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | H     | 368      | Total<br>368 | O<br>368 | 0       | 0       |

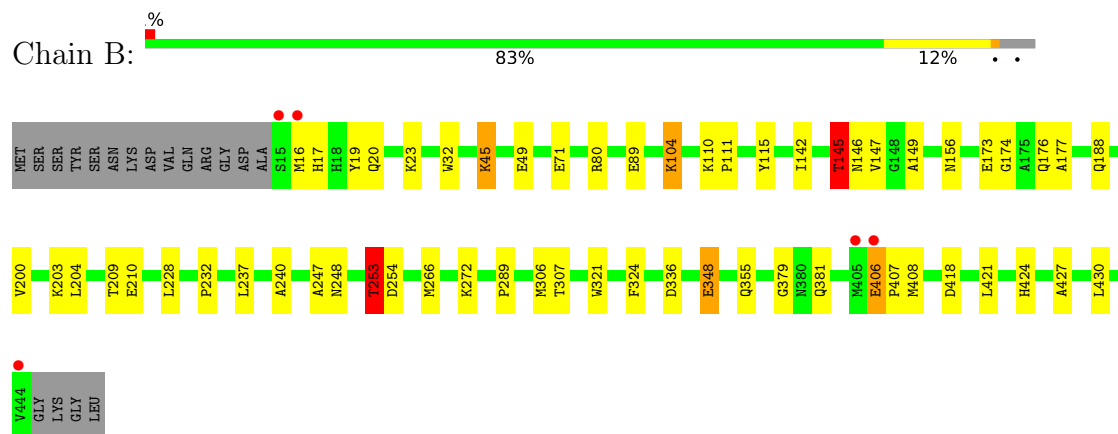
### 3 Residue-property plots [i](#)

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

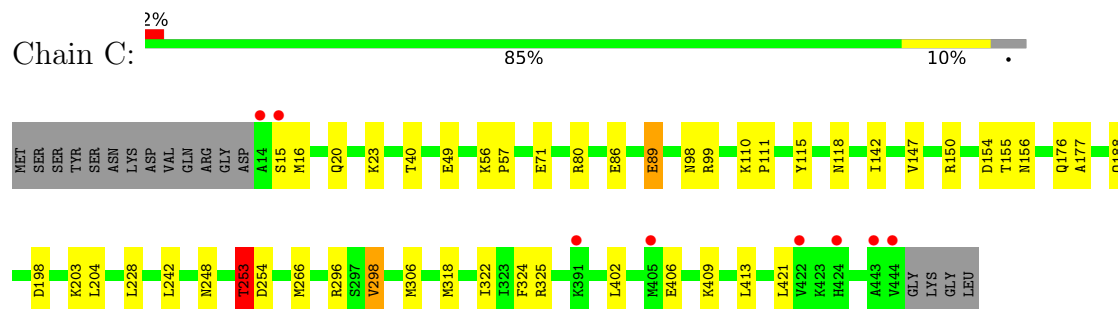
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



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

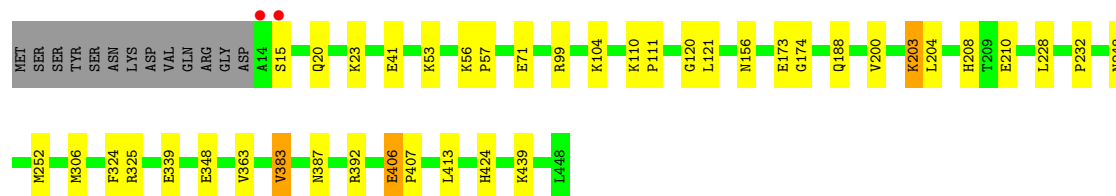


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



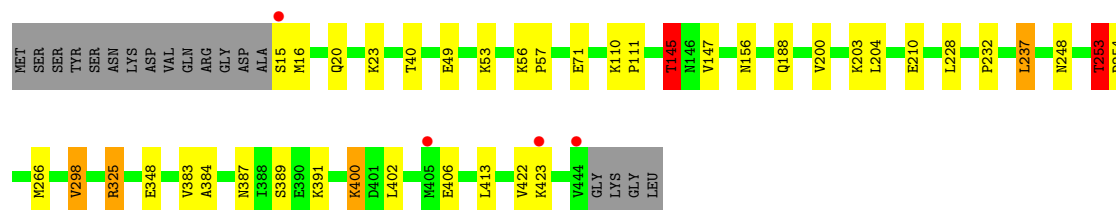
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

Chain D:  88% 8% ..



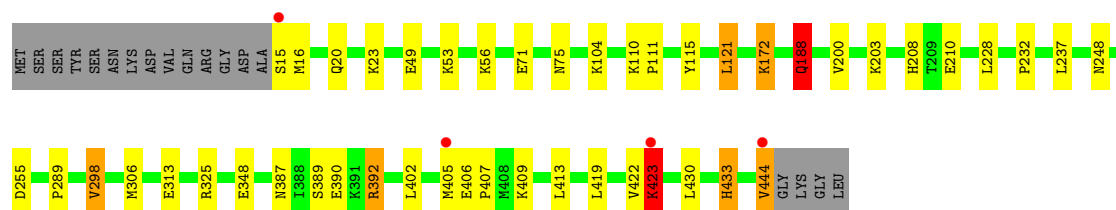
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

Chain E:  87% 8% ..



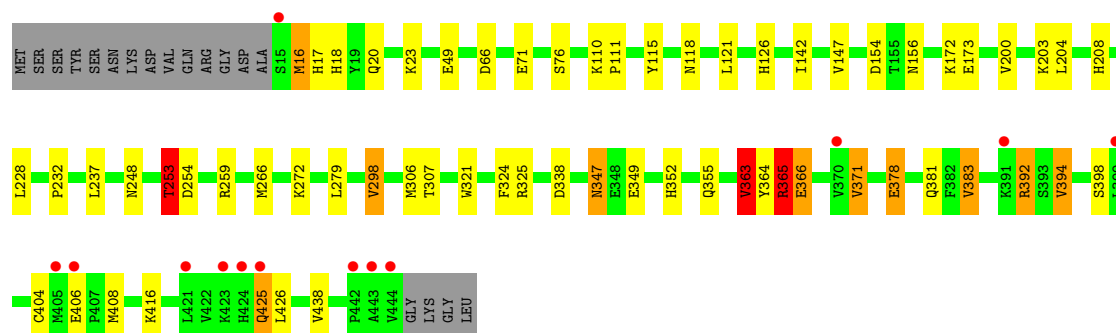
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

Chain F:  85% 9% ..



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

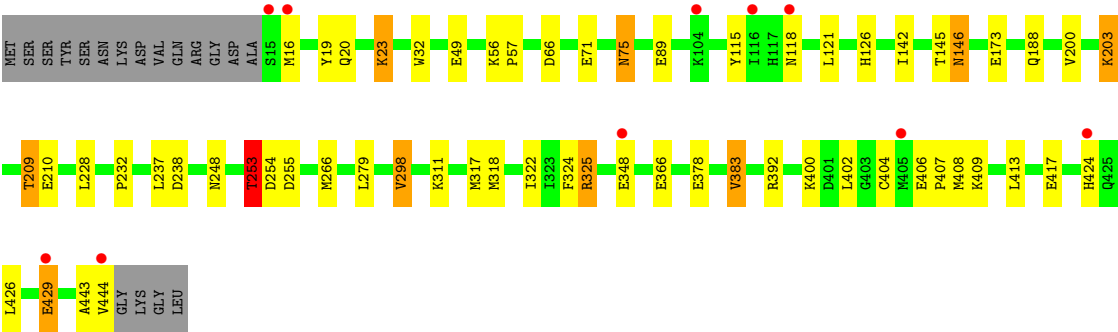
Chain G:  82% 11% ..



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

Chain H:  82% 11% ..





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 107.71Å 202.16Å 287.29Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 29.90 – 2.28<br>29.90 – 2.28                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.8 (29.90-2.28)<br>96.8 (29.90-2.28)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 5.45 (at 2.29Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.7.0029                                             | Depositor        |
| R, $R_{free}$                                                           | 0.146 , 0.177<br>0.155 , 0.182                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 13899 reflections (4.89%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 23.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.206                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 52.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 32820                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 28.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT, GOL, SO4

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

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 1.27         | 5/3606 (0.1%)   | 1.02        | 4/4895 (0.1%)   |
| 1   | B     | 1.26         | 10/3607 (0.3%)  | 0.99        | 5/4896 (0.1%)   |
| 1   | C     | 1.24         | 8/3595 (0.2%)   | 0.99        | 7/4880 (0.1%)   |
| 1   | D     | 1.22         | 6/3611 (0.2%)   | 0.98        | 5/4899 (0.1%)   |
| 1   | E     | 1.12         | 3/3595 (0.1%)   | 0.97        | 5/4881 (0.1%)   |
| 1   | F     | 1.12         | 3/3572 (0.1%)   | 0.97        | 3/4849 (0.1%)   |
| 1   | G     | 1.10         | 3/3589 (0.1%)   | 1.01        | 7/4872 (0.1%)   |
| 1   | H     | 1.13         | 4/3572 (0.1%)   | 1.00        | 6/4849 (0.1%)   |
| All | All   | 1.18         | 42/28747 (0.1%) | 0.99        | 42/39021 (0.1%) |

All (42) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 98  | ASN  | C-O    | -7.23 | 1.15        | 1.24     |
| 1   | C     | 98  | ASN  | C-O    | -7.04 | 1.15        | 1.24     |
| 1   | C     | 150 | ARG  | N-CA   | -6.98 | 1.37        | 1.46     |
| 1   | G     | 76  | SER  | C-O    | -6.56 | 1.17        | 1.24     |
| 1   | C     | 155 | THR  | C-O    | -6.46 | 1.15        | 1.24     |
| 1   | C     | 154 | ASP  | C-O    | -6.38 | 1.16        | 1.23     |
| 1   | C     | 242 | LEU  | C-O    | -6.34 | 1.16        | 1.24     |
| 1   | H     | 443 | ALA  | CA-C   | 6.31  | 1.60        | 1.52     |
| 1   | B     | 240 | ALA  | C-O    | -6.17 | 1.17        | 1.24     |
| 1   | D     | 325 | ARG  | C-O    | -6.06 | 1.16        | 1.24     |
| 1   | D     | 99  | ARG  | C-O    | -6.06 | 1.16        | 1.24     |
| 1   | C     | 80  | ARG  | C-O    | -5.96 | 1.16        | 1.24     |
| 1   | G     | 17  | HIS  | CG-ND1 | -5.91 | 1.31        | 1.38     |
| 1   | A     | 231 | SER  | CA-C   | 5.87  | 1.58        | 1.52     |
| 1   | B     | 80  | ARG  | C-O    | -5.87 | 1.17        | 1.24     |
| 1   | B     | 324 | PHE  | C-O    | -5.84 | 1.16        | 1.24     |
| 1   | B     | 237 | LEU  | C-O    | -5.79 | 1.16        | 1.24     |
| 1   | F     | 423 | LYS  | CA-CB  | 5.78  | 1.62        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 289 | PRO  | CA-C  | -5.66 | 1.47        | 1.53     |
| 1   | H     | 426 | LEU  | C-O   | -5.59 | 1.17        | 1.24     |
| 1   | H     | 23  | LYS  | C-O   | -5.52 | 1.17        | 1.24     |
| 1   | E     | 237 | LEU  | C-O   | -5.48 | 1.17        | 1.24     |
| 1   | E     | 325 | ARG  | C-O   | -5.45 | 1.17        | 1.24     |
| 1   | G     | 142 | ILE  | C-O   | -5.43 | 1.18        | 1.24     |
| 1   | B     | 418 | ASP  | C-O   | -5.39 | 1.17        | 1.23     |
| 1   | E     | 384 | ALA  | CA-C  | -5.39 | 1.46        | 1.52     |
| 1   | D     | 120 | GLY  | CA-C  | 5.37  | 1.58        | 1.51     |
| 1   | A     | 56  | LYS  | C-O   | -5.35 | 1.19        | 1.24     |
| 1   | C     | 99  | ARG  | C-O   | -5.32 | 1.17        | 1.24     |
| 1   | B     | 355 | GLN  | C-O   | -5.31 | 1.17        | 1.24     |
| 1   | B     | 427 | ALA  | C-O   | -5.25 | 1.17        | 1.23     |
| 1   | C     | 324 | PHE  | C-O   | -5.23 | 1.17        | 1.24     |
| 1   | H     | 317 | MET  | N-CA  | 5.23  | 1.52        | 1.46     |
| 1   | A     | 99  | ARG  | C-O   | -5.18 | 1.17        | 1.24     |
| 1   | A     | 325 | ARG  | C-O   | -5.18 | 1.16        | 1.23     |
| 1   | D     | 53  | LYS  | N-CA  | -5.16 | 1.39        | 1.46     |
| 1   | F     | 53  | LYS  | CA-C  | -5.15 | 1.46        | 1.52     |
| 1   | D     | 324 | PHE  | C-O   | -5.12 | 1.17        | 1.24     |
| 1   | B     | 149 | ALA  | N-CA  | -5.11 | 1.40        | 1.46     |
| 1   | B     | 247 | ALA  | N-CA  | -5.03 | 1.39        | 1.45     |
| 1   | D     | 252 | MET  | C-O   | -5.00 | 1.17        | 1.24     |
| 1   | F     | 289 | PRO  | CA-C  | -5.00 | 1.47        | 1.53     |

All (42) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 15  | SER  | N-CA-C  | 8.55  | 123.01      | 112.23   |
| 1   | F     | 298 | VAL  | N-CA-CB | -7.43 | 98.97       | 111.23   |
| 1   | E     | 298 | VAL  | N-CA-CB | -7.39 | 99.03       | 111.23   |
| 1   | G     | 394 | VAL  | N-CA-CB | 7.37  | 118.75      | 110.72   |
| 1   | H     | 253 | THR  | N-CA-CB | -7.32 | 98.95       | 111.69   |
| 1   | E     | 253 | THR  | N-CA-CB | -7.30 | 98.98       | 111.69   |
| 1   | B     | 253 | THR  | N-CA-CB | -7.20 | 99.17       | 111.69   |
| 1   | C     | 253 | THR  | N-CA-CB | -7.19 | 99.17       | 111.69   |
| 1   | H     | 383 | VAL  | CB-CA-C | 7.19  | 120.13      | 110.42   |
| 1   | G     | 253 | THR  | N-CA-CB | -7.19 | 99.18       | 111.69   |
| 1   | G     | 383 | VAL  | CB-CA-C | 7.13  | 120.05      | 110.42   |
| 1   | H     | 443 | ALA  | O-C-N   | -6.95 | 114.81      | 123.01   |
| 1   | G     | 298 | VAL  | N-CA-CB | -6.77 | 100.06      | 111.23   |
| 1   | H     | 209 | THR  | N-CA-CB | -6.68 | 100.30      | 110.12   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 188 | GLN  | N-CA-CB   | 6.68  | 119.93      | 110.12   |
| 1   | D     | 363 | VAL  | N-CA-C    | -6.54 | 104.48      | 110.82   |
| 1   | B     | 145 | THR  | CB-CA-C   | -6.44 | 96.47       | 111.09   |
| 1   | C     | 298 | VAL  | N-CA-CB   | -6.42 | 100.63      | 111.23   |
| 1   | A     | 443 | ALA  | CA-C-N    | 6.41  | 133.23      | 121.70   |
| 1   | A     | 443 | ALA  | C-N-CA    | 6.41  | 133.23      | 121.70   |
| 1   | D     | 439 | LYS  | CG-CD-CE  | 6.36  | 125.92      | 111.30   |
| 1   | E     | 145 | THR  | CB-CA-C   | -6.34 | 96.69       | 111.09   |
| 1   | G     | 366 | GLU  | CB-CA-C   | 6.32  | 120.55      | 109.80   |
| 1   | A     | 383 | VAL  | CB-CA-C   | 6.17  | 118.75      | 110.42   |
| 1   | H     | 298 | VAL  | N-CA-CB   | -6.08 | 101.19      | 111.23   |
| 1   | B     | 348 | GLU  | CB-CG-CD  | 5.85  | 122.55      | 112.60   |
| 1   | C     | 89  | GLU  | CB-CA-C   | -5.75 | 99.18       | 110.11   |
| 1   | G     | 363 | VAL  | CB-CA-C   | 5.61  | 119.75      | 112.24   |
| 1   | D     | 203 | LYS  | CG-CD-CE  | 5.60  | 124.18      | 111.30   |
| 1   | C     | 142 | ILE  | CB-CA-C   | -5.57 | 102.52      | 110.83   |
| 1   | D     | 383 | VAL  | CB-CA-C   | 5.51  | 117.61      | 110.12   |
| 1   | G     | 365 | ARG  | CB-CG-CD  | 5.45  | 123.83      | 111.30   |
| 1   | A     | 429 | GLU  | CB-CA-C   | -5.45 | 101.17      | 109.89   |
| 1   | C     | 142 | ILE  | CA-CB-CG1 | 5.39  | 119.57      | 110.40   |
| 1   | D     | 15  | SER  | N-CA-C    | 5.37  | 118.99      | 112.23   |
| 1   | E     | 348 | GLU  | CB-CG-CD  | 5.27  | 121.55      | 112.60   |
| 1   | C     | 325 | ARG  | NE-CZ-NH1 | -5.17 | 116.33      | 121.50   |
| 1   | B     | 32  | TRP  | N-CA-C    | 5.10  | 116.53      | 111.07   |
| 1   | F     | 348 | GLU  | CB-CG-CD  | 5.09  | 121.25      | 112.60   |
| 1   | E     | 423 | LYS  | CG-CD-CE  | 5.06  | 122.93      | 111.30   |
| 1   | B     | 104 | LYS  | CB-CA-C   | -5.04 | 101.64      | 109.61   |
| 1   | H     | 142 | ILE  | CA-CB-CG1 | -5.02 | 101.87      | 110.40   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3492  | 0        | 3370     | 35      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 3496  | 0        | 3369     | 41      | 0            |
| 1   | C     | 3487  | 0        | 3365     | 30      | 0            |
| 1   | D     | 3506  | 0        | 3394     | 28      | 0            |
| 1   | E     | 3484  | 0        | 3363     | 28      | 0            |
| 1   | F     | 3470  | 0        | 3346     | 31      | 0            |
| 1   | G     | 3481  | 0        | 3356     | 43      | 0            |
| 1   | H     | 3470  | 0        | 3346     | 35      | 0            |
| 2   | A     | 24    | 0        | 32       | 6       | 0            |
| 2   | B     | 54    | 0        | 72       | 8       | 0            |
| 2   | C     | 30    | 0        | 40       | 9       | 0            |
| 2   | D     | 30    | 0        | 40       | 11      | 0            |
| 2   | E     | 36    | 0        | 48       | 6       | 0            |
| 2   | F     | 24    | 0        | 32       | 7       | 0            |
| 2   | G     | 24    | 0        | 32       | 1       | 0            |
| 2   | H     | 18    | 0        | 24       | 4       | 0            |
| 3   | A     | 50    | 0        | 0        | 1       | 0            |
| 3   | B     | 50    | 0        | 0        | 3       | 0            |
| 3   | C     | 65    | 0        | 0        | 1       | 0            |
| 3   | D     | 60    | 0        | 0        | 1       | 0            |
| 3   | E     | 50    | 0        | 0        | 0       | 0            |
| 3   | F     | 55    | 0        | 0        | 1       | 0            |
| 3   | G     | 40    | 0        | 0        | 1       | 0            |
| 3   | H     | 55    | 0        | 0        | 3       | 0            |
| 4   | A     | 13    | 0        | 6        | 6       | 0            |
| 4   | B     | 13    | 0        | 5        | 8       | 0            |
| 4   | C     | 13    | 0        | 5        | 4       | 0            |
| 4   | E     | 13    | 0        | 5        | 2       | 0            |
| 4   | G     | 13    | 0        | 5        | 7       | 0            |
| 5   | A     | 662   | 0        | 0        | 17      | 0            |
| 5   | B     | 625   | 0        | 0        | 17      | 0            |
| 5   | C     | 579   | 0        | 0        | 14      | 0            |
| 5   | D     | 536   | 0        | 0        | 8       | 0            |
| 5   | E     | 500   | 0        | 0        | 4       | 0            |
| 5   | F     | 495   | 0        | 0        | 11      | 0            |
| 5   | G     | 439   | 0        | 0        | 17      | 0            |
| 5   | H     | 368   | 0        | 0        | 10      | 0            |
| All | All   | 32820 | 0        | 27255    | 298     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (298) 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) |
|--------------------|------------------|--------------------------|-------------------|
| 2:C:505:GOL:O3     | 2:C:505:GOL:C3   | 1.67                     | 1.40              |
| 4:A:515:CIT:O5     | 4:A:515:CIT:C5   | 1.75                     | 1.20              |
| 1:H:146:ASN:HB3    | 5:H:917:HOH:O    | 1.40                     | 1.18              |
| 4:C:519:CIT:O4     | 4:C:519:CIT:H21  | 1.47                     | 1.11              |
| 1:C:49:GLU:HG2     | 5:C:1111:HOH:O   | 1.53                     | 1.09              |
| 4:C:519:CIT:O6     | 4:C:519:CIT:O2   | 1.69                     | 1.08              |
| 4:G:513:CIT:O5     | 4:G:513:CIT:C5   | 1.94                     | 1.06              |
| 1:C:118:ASN:HB3    | 5:C:1124:HOH:O   | 1.55                     | 1.04              |
| 4:C:519:CIT:O2     | 4:C:519:CIT:C6   | 2.06                     | 1.02              |
| 4:A:515:CIT:H42    | 5:A:975:HOH:O    | 1.66                     | 0.95              |
| 1:B:348:GLU:HB2    | 5:B:1067:HOH:O   | 1.66                     | 0.93              |
| 1:D:174:GLY:H      | 2:D:502:GOL:H31  | 1.36                     | 0.91              |
| 1:G:352:HIS:HB2    | 5:G:942:HOH:O    | 1.71                     | 0.90              |
| 1:D:210:GLU:HB2    | 2:D:505:GOL:H11  | 1.55                     | 0.88              |
| 1:E:210:GLU:HB2    | 4:E:517:CIT:H21  | 1.56                     | 0.86              |
| 1:A:188[B]:GLN:HG2 | 5:A:875:HOH:O    | 1.77                     | 0.83              |
| 4:C:519:CIT:O4     | 4:C:519:CIT:C2   | 2.26                     | 0.83              |
| 1:E:40:THR:HG21    | 2:E:505:GOL:H11  | 1.61                     | 0.82              |
| 1:B:210:GLU:H      | 4:B:520:CIT:H22  | 1.44                     | 0.81              |
| 1:C:176:GLN:HB3    | 2:C:505:GOL:H2   | 1.61                     | 0.81              |
| 1:C:177:ALA:H      | 2:C:505:GOL:H31  | 1.44                     | 0.80              |
| 1:G:398:SER:HA     | 1:G:425:GLN:HB2  | 1.60                     | 0.80              |
| 1:F:228:LEU:H      | 1:F:248:ASN:HD22 | 1.29                     | 0.80              |
| 1:F:210:GLU:HB2    | 2:F:502:GOL:H11  | 1.67                     | 0.76              |
| 1:B:228:LEU:H      | 1:B:248:ASN:HD22 | 1.32                     | 0.76              |
| 1:E:228:LEU:H      | 1:E:248:ASN:HD22 | 1.32                     | 0.76              |
| 4:G:513:CIT:H41    | 5:G:834:HOH:O    | 1.85                     | 0.76              |
| 1:A:306:MET:HE2    | 5:A:993:HOH:O    | 1.87                     | 0.75              |
| 1:A:228:LEU:H      | 1:A:248:ASN:HD22 | 1.32                     | 0.75              |
| 1:H:228:LEU:H      | 1:H:248:ASN:HD22 | 1.34                     | 0.75              |
| 1:A:381:GLN:CD     | 5:A:1230:HOH:O   | 2.30                     | 0.75              |
| 1:E:188[A]:GLN:HG2 | 5:E:783:HOH:O    | 1.87                     | 0.74              |
| 4:G:513:CIT:C4     | 5:G:834:HOH:O    | 2.35                     | 0.74              |
| 1:B:210:GLU:HB2    | 4:B:520:CIT:H41  | 1.69                     | 0.74              |
| 1:G:228:LEU:H      | 1:G:248:ASN:HD22 | 1.36                     | 0.73              |
| 1:C:118:ASN:CB     | 5:C:1124:HOH:O   | 2.25                     | 0.73              |
| 1:H:238:ASP:OD2    | 5:H:850:HOH:O    | 2.07                     | 0.73              |
| 1:B:89:GLU:HG2     | 5:B:1197:HOH:O   | 1.88                     | 0.72              |
| 1:D:228:LEU:H      | 1:D:248:ASN:HD22 | 1.37                     | 0.72              |
| 1:C:228:LEU:H      | 1:C:248:ASN:HD22 | 1.37                     | 0.71              |
| 1:E:40:THR:CG2     | 2:E:505:GOL:H11  | 2.19                     | 0.71              |
| 4:A:515:CIT:O5     | 4:A:515:CIT:O4   | 2.07                     | 0.71              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:C:188[B]:GLN:HG2 | 5:C:834:HOH:O    | 1.89                     | 0.71              |
| 1:H:311:LYS:N      | 3:H:508:SO4:O3   | 2.19                     | 0.71              |
| 1:A:381:GLN:NE2    | 5:A:1230:HOH:O   | 2.22                     | 0.71              |
| 1:C:253:THR:HG23   | 1:C:254:ASP:O    | 1.92                     | 0.70              |
| 1:G:154[B]:ASP:OD2 | 5:G:691:HOH:O    | 2.09                     | 0.70              |
| 1:H:145:THR:OG1    | 5:H:846:HOH:O    | 2.10                     | 0.70              |
| 1:G:365:ARG:HD2    | 5:G:798:HOH:O    | 1.91                     | 0.70              |
| 1:G:416:LYS:HD3    | 5:G:969:HOH:O    | 1.92                     | 0.70              |
| 1:B:253:THR:HG23   | 1:B:254:ASP:O    | 1.92                     | 0.69              |
| 1:C:118:ASN:HB3    | 5:C:1114:HOH:O   | 1.91                     | 0.68              |
| 1:E:49:GLU:HG3     | 5:E:974:HOH:O    | 1.93                     | 0.68              |
| 4:A:515:CIT:C4     | 5:A:975:HOH:O    | 2.33                     | 0.68              |
| 1:G:253:THR:HG23   | 1:G:254:ASP:O    | 1.95                     | 0.67              |
| 1:G:364:TYR:CE2    | 1:G:371:VAL:HG13 | 2.30                     | 0.67              |
| 1:E:253:THR:HG23   | 1:E:254:ASP:O    | 1.95                     | 0.66              |
| 1:F:423:LYS:NZ     | 1:F:423:LYS:HB3  | 2.10                     | 0.66              |
| 3:B:513:SO4:O1     | 5:B:1225:HOH:O   | 2.13                     | 0.65              |
| 1:G:416:LYS:CD     | 5:G:969:HOH:O    | 2.45                     | 0.65              |
| 1:G:208:HIS:HD2    | 4:G:513:CIT:O7   | 1.79                     | 0.65              |
| 1:F:313:GLU:OE2    | 1:F:433:HIS:HD2  | 1.78                     | 0.65              |
| 1:E:145:THR:CG2    | 5:E:971:HOH:O    | 2.45                     | 0.65              |
| 1:A:172:LYS:NZ     | 5:A:1164:HOH:O   | 2.24                     | 0.63              |
| 1:C:40:THR:CG2     | 2:C:503:GOL:H2   | 2.29                     | 0.62              |
| 1:E:40:THR:OG1     | 2:E:505:GOL:H31  | 1.99                     | 0.62              |
| 1:H:253:THR:HG23   | 1:H:254:ASP:O    | 2.00                     | 0.62              |
| 1:D:306:MET:HE1    | 5:D:726:HOH:O    | 2.00                     | 0.62              |
| 5:F:1055:HOH:O     | 1:H:203:LYS:HE3  | 1.99                     | 0.61              |
| 2:C:505:GOL:C3     | 2:C:505:GOL:HO3  | 2.11                     | 0.61              |
| 1:B:306:MET:HE1    | 5:B:733:HOH:O    | 2.00                     | 0.61              |
| 1:D:41:GLU:CD      | 5:D:1046:HOH:O   | 2.42                     | 0.61              |
| 1:H:424:HIS:ND1    | 5:H:957:HOH:O    | 2.27                     | 0.61              |
| 4:G:513:CIT:C1     | 5:G:784:HOH:O    | 2.48                     | 0.60              |
| 1:F:306:MET:HE2    | 5:F:848:HOH:O    | 2.00                     | 0.60              |
| 1:G:347:ASN:HD22   | 1:G:347:ASN:C    | 2.09                     | 0.60              |
| 1:H:255:ASP:OD2    | 2:H:502:GOL:H12  | 2.01                     | 0.60              |
| 1:G:18:HIS:HE1     | 5:G:952:HOH:O    | 1.83                     | 0.59              |
| 1:B:177:ALA:H      | 2:B:503:GOL:H31  | 1.67                     | 0.59              |
| 1:H:188:GLN:HG3    | 5:H:752:HOH:O    | 2.00                     | 0.59              |
| 1:F:409:LYS:CD     | 5:F:1092:HOH:O   | 2.49                     | 0.59              |
| 1:E:325:ARG:HH22   | 2:E:504:GOL:H2   | 1.68                     | 0.59              |
| 1:G:364:TYR:CE2    | 1:G:371:VAL:CG1  | 2.86                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:145:THR:CG2   | 5:B:969:HOH:O    | 2.51                     | 0.59              |
| 1:B:210:GLU:H     | 4:B:520:CIT:C2   | 2.14                     | 0.59              |
| 3:H:505:SO4:O4    | 5:H:799:HOH:O    | 2.17                     | 0.58              |
| 1:A:265:ASP:HB3   | 5:A:768:HOH:O    | 2.02                     | 0.58              |
| 1:F:409:LYS:HD3   | 5:F:1092:HOH:O   | 2.04                     | 0.58              |
| 1:D:174:GLY:N     | 2:D:502:GOL:H31  | 2.12                     | 0.57              |
| 1:A:173:GLU:OE2   | 3:A:510:SO4:O3   | 2.23                     | 0.57              |
| 1:F:56:LYS:NZ     | 5:F:906:HOH:O    | 2.37                     | 0.57              |
| 1:A:255:ASP:OD2   | 2:A:501:GOL:C3   | 2.53                     | 0.57              |
| 4:E:517:CIT:O6    | 4:E:517:CIT:O2   | 2.23                     | 0.56              |
| 1:E:40:THR:CG2    | 2:E:505:GOL:C1   | 2.83                     | 0.56              |
| 1:D:208:HIS:HA    | 2:D:505:GOL:H2   | 1.88                     | 0.55              |
| 1:C:306:MET:HE1   | 5:C:731:HOH:O    | 2.04                     | 0.55              |
| 1:G:378:GLU:N     | 1:G:378:GLU:CD   | 2.64                     | 0.55              |
| 4:G:513:CIT:O5    | 4:G:513:CIT:O3   | 2.23                     | 0.55              |
| 1:H:392:ARG:CZ    | 1:H:429:GLU:HG2  | 2.36                     | 0.55              |
| 4:A:515:CIT:O1    | 4:A:515:CIT:C6   | 2.54                     | 0.55              |
| 2:F:502:GOL:H32   | 5:F:861:HOH:O    | 2.07                     | 0.55              |
| 1:G:392:ARG:NH1   | 3:G:510:SO4:O3   | 2.40                     | 0.55              |
| 1:B:17:HIS:HE1    | 3:B:511:SO4:O2   | 1.90                     | 0.55              |
| 1:A:221:ARG:HH21  | 2:A:502:GOL:H2   | 1.72                     | 0.54              |
| 4:B:520:CIT:O6    | 4:B:520:CIT:O2   | 2.25                     | 0.54              |
| 1:G:363:VAL:HG13  | 1:G:371:VAL:HG22 | 1.89                     | 0.54              |
| 1:B:174:GLY:H     | 2:B:503:GOL:H32  | 1.73                     | 0.54              |
| 1:A:208:HIS:HD2   | 4:A:515:CIT:O7   | 1.91                     | 0.53              |
| 1:H:210:GLU:HB2   | 2:H:503:GOL:H2   | 1.90                     | 0.53              |
| 4:B:520:CIT:O6    | 4:B:520:CIT:C1   | 2.56                     | 0.53              |
| 1:D:424:HIS:H     | 2:D:503:GOL:H32  | 1.74                     | 0.53              |
| 4:G:513:CIT:H42   | 5:G:834:HOH:O    | 2.05                     | 0.53              |
| 1:C:253:THR:CG2   | 1:C:254:ASP:O    | 2.57                     | 0.53              |
| 1:E:145:THR:HG22  | 5:E:971:HOH:O    | 2.07                     | 0.53              |
| 1:A:49[B]:GLU:OE2 | 1:A:115:TYR:OH   | 2.27                     | 0.53              |
| 1:B:406:GLU:HB2   | 1:B:407:PRO:CD   | 2.39                     | 0.52              |
| 1:B:176:GLN:HB3   | 2:B:503:GOL:H2   | 1.90                     | 0.52              |
| 1:B:253:THR:CG2   | 1:B:254:ASP:O    | 2.58                     | 0.52              |
| 1:F:390:GLU:OE2   | 1:F:433:HIS:HE1  | 1.91                     | 0.52              |
| 1:A:49[A]:GLU:OE2 | 1:A:115:TYR:OH   | 2.26                     | 0.52              |
| 1:F:208:HIS:HA    | 2:F:502:GOL:H2   | 1.91                     | 0.52              |
| 1:F:392:ARG:NH1   | 3:F:506:SO4:O1   | 2.43                     | 0.52              |
| 1:A:255:ASP:CG    | 2:A:501:GOL:H31  | 2.35                     | 0.52              |
| 1:E:40:THR:HG21   | 2:E:505:GOL:C1   | 2.33                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:G:147:VAL:O     | 5:G:790:HOH:O    | 2.18                     | 0.52              |
| 1:C:40:THR:HG21   | 2:C:503:GOL:H2   | 1.91                     | 0.52              |
| 1:D:104:LYS:HD3   | 5:D:1097:HOH:O   | 2.10                     | 0.52              |
| 1:H:32:TRP:CD1    | 2:H:501:GOL:H32  | 2.46                     | 0.51              |
| 1:H:16:MET:HG2    | 1:H:19:TYR:CZ    | 2.45                     | 0.51              |
| 2:B:504:GOL:C1    | 5:B:1104:HOH:O   | 2.58                     | 0.51              |
| 1:H:75:ASN:HD22   | 1:H:75:ASN:H     | 1.59                     | 0.51              |
| 1:B:204:LEU:HD11  | 1:D:156:ASN:HD21 | 1.76                     | 0.51              |
| 1:B:156:ASN:HD21  | 1:D:204:LEU:HD11 | 1.75                     | 0.51              |
| 3:C:508:SO4:O3    | 5:C:792:HOH:O    | 2.19                     | 0.51              |
| 1:G:259:ARG:NH1   | 2:G:502:GOL:O2   | 2.37                     | 0.51              |
| 1:B:336:ASP:OD1   | 3:B:514:SO4:O3   | 2.27                     | 0.50              |
| 1:B:173:GLU:HG3   | 5:B:1204:HOH:O   | 2.10                     | 0.50              |
| 1:B:142:ILE:HD12  | 1:B:147:VAL:HG23 | 1.92                     | 0.50              |
| 2:B:504:GOL:H11   | 5:B:1104:HOH:O   | 2.11                     | 0.50              |
| 1:C:253:THR:HG21  | 1:C:266:MET:HE1  | 1.94                     | 0.50              |
| 1:H:253:THR:CG2   | 1:H:254:ASP:O    | 2.60                     | 0.50              |
| 1:F:49:GLU:OE2    | 1:F:115:TYR:OH   | 2.27                     | 0.50              |
| 1:B:210:GLU:HG2   | 4:B:520:CIT:H21  | 1.95                     | 0.49              |
| 1:D:188:GLN:NE2   | 5:D:683:HOH:O    | 2.44                     | 0.49              |
| 1:E:253:THR:CG2   | 1:E:254:ASP:O    | 2.59                     | 0.49              |
| 1:B:253:THR:HG21  | 1:B:266:MET:HE1  | 1.95                     | 0.49              |
| 1:F:188:GLN:HG3   | 5:F:950:HOH:O    | 2.11                     | 0.49              |
| 1:B:20:GLN:NE2    | 1:B:23:LYS:HE3   | 2.28                     | 0.49              |
| 1:E:253:THR:HG21  | 1:E:266:MET:HE1  | 1.94                     | 0.49              |
| 1:G:253:THR:CG2   | 1:G:254:ASP:O    | 2.59                     | 0.49              |
| 1:C:49:GLU:OE2    | 1:C:115:TYR:OH   | 2.26                     | 0.49              |
| 1:G:404:CYS:SG    | 1:G:408:MET:HE3  | 2.53                     | 0.49              |
| 1:D:20:GLN:NE2    | 1:D:23:LYS:HE3   | 2.27                     | 0.49              |
| 1:A:272:LYS:CD    | 5:B:1041:HOH:O   | 2.60                     | 0.49              |
| 1:H:146:ASN:OD1   | 1:H:146:ASN:N    | 2.38                     | 0.49              |
| 1:G:49[A]:GLU:OE2 | 1:G:115:TYR:OH   | 2.27                     | 0.48              |
| 1:H:75:ASN:HD22   | 1:H:75:ASN:N     | 2.09                     | 0.48              |
| 1:E:15:SER:C      | 1:E:16:MET:HE2   | 2.39                     | 0.48              |
| 1:H:406:GLU:HB2   | 1:H:407:PRO:CD   | 2.44                     | 0.48              |
| 1:A:265:ASP:HB3   | 5:A:837:HOH:O    | 2.11                     | 0.48              |
| 1:B:20:GLN:HE21   | 1:B:23:LYS:HE3   | 1.78                     | 0.48              |
| 1:F:208:HIS:HB3   | 2:F:502:GOL:O1   | 2.14                     | 0.48              |
| 1:H:404:CYS:SG    | 1:H:408:MET:HE3  | 2.53                     | 0.48              |
| 1:D:174:GLY:H     | 2:D:502:GOL:C3   | 2.17                     | 0.48              |
| 1:G:20:GLN:OE1    | 1:G:23:LYS:HE3   | 2.13                     | 0.48              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:H:49:GLU:OE2     | 1:H:115:TYR:OH   | 2.28                     | 0.48              |
| 1:D:424:HIS:HB3    | 2:D:503:GOL:H11  | 1.95                     | 0.48              |
| 1:B:406:GLU:HB2    | 1:B:407:PRO:HD2  | 1.96                     | 0.48              |
| 1:B:45:LYS:NZ      | 5:B:1167:HOH:O   | 2.46                     | 0.47              |
| 1:B:146:ASN:OD1    | 1:B:146:ASN:N    | 2.38                     | 0.47              |
| 2:B:504:GOL:O3     | 5:B:1187:HOH:O   | 2.20                     | 0.47              |
| 1:D:20:GLN:HE21    | 1:D:23:LYS:HE3   | 1.79                     | 0.47              |
| 1:H:23:LYS:HG3     | 1:H:279:LEU:HD21 | 1.96                     | 0.47              |
| 1:A:110:LYS:HB3    | 1:A:111:PRO:HD3  | 1.97                     | 0.47              |
| 1:H:173:GLU:HA     | 3:H:509:SO4:O3   | 2.15                     | 0.47              |
| 1:A:203:LYS:HD3    | 5:A:1249:HOH:O   | 2.13                     | 0.47              |
| 1:B:16:MET:HG2     | 1:B:19:TYR:CZ    | 2.49                     | 0.47              |
| 1:G:253:THR:HG21   | 1:G:266:MET:HE1  | 1.96                     | 0.47              |
| 1:B:145:THR:HB     | 1:B:147:VAL:H    | 1.80                     | 0.47              |
| 1:F:255:ASP:OD2    | 2:F:504:GOL:H31  | 2.13                     | 0.47              |
| 2:F:502:GOL:C3     | 5:F:861:HOH:O    | 2.60                     | 0.47              |
| 1:E:20:GLN:NE2     | 1:E:23:LYS:HE3   | 2.29                     | 0.47              |
| 1:A:387:ASN:C      | 1:A:387:ASN:HD22 | 2.22                     | 0.47              |
| 1:C:296:ARG:NH1    | 2:C:503:GOL:H31  | 2.30                     | 0.47              |
| 1:G:355:GLN:HB3    | 5:G:799:HOH:O    | 2.14                     | 0.47              |
| 1:D:406:GLU:HB2    | 1:D:407:PRO:CD   | 2.46                     | 0.46              |
| 1:G:16:MET:HE3     | 1:G:16:MET:HA    | 1.97                     | 0.46              |
| 1:F:406:GLU:HB2    | 1:F:407:PRO:CD   | 2.45                     | 0.46              |
| 1:A:49[A]:GLU:OE1  | 5:A:1111:HOH:O   | 2.21                     | 0.46              |
| 1:A:387:ASN:ND2    | 1:A:389:SER:H    | 2.14                     | 0.46              |
| 1:A:387:ASN:HD22   | 1:A:389:SER:H    | 1.64                     | 0.46              |
| 1:A:444:VAL:HG12   | 5:A:1183:HOH:O   | 2.15                     | 0.46              |
| 2:D:502:GOL:O2     | 3:D:512:SO4:O3   | 2.33                     | 0.46              |
| 1:G:172:LYS:NZ     | 5:G:874:HOH:O    | 2.48                     | 0.46              |
| 1:D:188:GLN:HB3    | 5:D:1066:HOH:O   | 2.15                     | 0.45              |
| 1:D:424:HIS:HB2    | 5:D:1128:HOH:O   | 2.15                     | 0.45              |
| 1:D:210:GLU:HG2    | 2:D:505:GOL:H31  | 1.98                     | 0.45              |
| 1:B:200:VAL:HB     | 1:B:232:PRO:O    | 2.17                     | 0.45              |
| 1:F:20:GLN:NE2     | 1:F:23:LYS:HE3   | 2.31                     | 0.45              |
| 1:E:145:THR:HB     | 1:E:147:VAL:H    | 1.80                     | 0.45              |
| 1:A:172:LYS:HE3    | 5:A:1092:HOH:O   | 2.16                     | 0.45              |
| 1:G:154[A]:ASP:OD1 | 5:G:715:HOH:O    | 2.21                     | 0.45              |
| 1:B:379:GLY:HA3    | 5:B:965:HOH:O    | 2.16                     | 0.45              |
| 1:F:423:LYS:HB3    | 1:F:423:LYS:HZ2  | 1.78                     | 0.45              |
| 2:B:505:GOL:H31    | 1:E:53:LYS:NZ    | 2.32                     | 0.45              |
| 1:G:416:LYS:HB2    | 1:G:416:LYS:HE2  | 1.54                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:306:MET:HE1   | 5:A:717:HOH:O    | 2.17                     | 0.44              |
| 1:E:110:LYS:HB3   | 1:E:111:PRO:HD3  | 1.99                     | 0.44              |
| 1:E:400:LYS:HE3   | 1:E:400:LYS:HB2  | 1.71                     | 0.44              |
| 1:G:338:ASP:HA    | 5:G:1035:HOH:O   | 2.17                     | 0.44              |
| 1:H:200:VAL:HB    | 1:H:232:PRO:O    | 2.17                     | 0.44              |
| 1:A:217:LYS:HE3   | 2:A:502:GOL:O3   | 2.18                     | 0.44              |
| 1:H:417:GLU:HG3   | 5:H:816:HOH:O    | 2.15                     | 0.44              |
| 1:F:444:VAL:HA    | 5:F:863:HOH:O    | 2.18                     | 0.44              |
| 1:F:444:VAL:HG13  | 1:F:444:VAL:O    | 2.17                     | 0.44              |
| 1:C:16:MET:CE     | 5:C:926:HOH:O    | 2.66                     | 0.44              |
| 1:C:118:ASN:CG    | 5:C:1124:HOH:O   | 2.56                     | 0.44              |
| 1:D:339:GLU:HG3   | 5:D:930:HOH:O    | 2.17                     | 0.44              |
| 1:B:145:THR:HG22  | 5:B:969:HOH:O    | 2.15                     | 0.44              |
| 1:F:75:ASN:N      | 1:F:75:ASN:HD22  | 2.16                     | 0.44              |
| 1:B:49:GLU:OE2    | 1:B:115:TYR:OH   | 2.31                     | 0.44              |
| 1:B:424:HIS:HB2   | 5:B:1219:HOH:O   | 2.18                     | 0.44              |
| 1:C:110:LYS:HB3   | 1:C:111:PRO:HD3  | 2.00                     | 0.44              |
| 1:H:378:GLU:OE2   | 5:H:875:HOH:O    | 2.21                     | 0.44              |
| 1:H:279:LEU:HD23  | 1:H:279:LEU:C    | 2.42                     | 0.43              |
| 2:F:504:GOL:H32   | 5:F:755:HOH:O    | 2.17                     | 0.43              |
| 1:B:110:LYS:HB3   | 1:B:111:PRO:HD3  | 2.00                     | 0.43              |
| 1:C:20:GLN:NE2    | 1:C:23:LYS:HE3   | 2.33                     | 0.43              |
| 1:A:56:LYS:HD3    | 1:A:121:LEU:HD13 | 2.00                     | 0.43              |
| 1:H:253:THR:HG21  | 1:H:266:MET:HE1  | 1.99                     | 0.43              |
| 1:H:66:ASP:HA     | 1:H:126:HIS:HB2  | 2.01                     | 0.43              |
| 1:D:110:LYS:HB3   | 1:D:111:PRO:HD3  | 2.01                     | 0.43              |
| 1:D:173:GLU:HA    | 2:D:502:GOL:H11  | 1.99                     | 0.43              |
| 1:E:204:LEU:HD11  | 1:G:156:ASN:HD21 | 1.84                     | 0.43              |
| 2:C:504:GOL:H31   | 5:G:685:HOH:O    | 2.18                     | 0.43              |
| 1:D:56:LYS:N      | 1:D:57:PRO:CD    | 2.81                     | 0.43              |
| 1:G:66:ASP:HA     | 1:G:126:HIS:HB2  | 2.01                     | 0.43              |
| 1:F:423:LYS:HB3   | 1:F:423:LYS:HZ3  | 1.84                     | 0.43              |
| 1:A:204:LEU:HD11  | 1:C:156:ASN:HD21 | 1.83                     | 0.42              |
| 2:B:502:GOL:H11   | 5:B:1071:HOH:O   | 2.19                     | 0.42              |
| 2:H:502:GOL:H11   | 5:H:677:HOH:O    | 2.19                     | 0.42              |
| 1:A:255:ASP:OD2   | 2:A:501:GOL:H31  | 2.18                     | 0.42              |
| 1:E:387:ASN:HD22  | 1:E:389:SER:H    | 1.67                     | 0.42              |
| 1:G:110:LYS:HB3   | 1:G:111:PRO:HD3  | 2.00                     | 0.42              |
| 1:C:188[B]:GLN:CD | 5:C:834:HOH:O    | 2.62                     | 0.42              |
| 1:C:89:GLU:CG     | 5:C:1025:HOH:O   | 2.66                     | 0.42              |
| 5:A:1104:HOH:O    | 1:B:272:LYS:CD   | 2.67                     | 0.42              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:C:86:GLU:OE1     | 2:C:504:GOL:C1   | 2.68                     | 0.42              |
| 1:C:56:LYS:N       | 1:C:57:PRO:CD    | 2.83                     | 0.42              |
| 1:C:318:MET:O      | 1:C:322:ILE:HG12 | 2.20                     | 0.42              |
| 1:E:156:ASN:HD21   | 1:G:204:LEU:HD11 | 1.84                     | 0.42              |
| 1:H:56:LYS:N       | 1:H:57:PRO:CD    | 2.83                     | 0.42              |
| 1:H:75:ASN:N       | 1:H:75:ASN:ND2   | 2.64                     | 0.42              |
| 1:G:378:GLU:N      | 1:G:378:GLU:OE1  | 2.52                     | 0.42              |
| 1:F:56:LYS:HD3     | 1:F:121:LEU:HD13 | 2.02                     | 0.42              |
| 1:A:339:GLU:HG3    | 5:A:904:HOH:O    | 2.19                     | 0.42              |
| 1:E:56:LYS:N       | 1:E:57:PRO:CD    | 2.82                     | 0.42              |
| 1:H:406:GLU:HB2    | 1:H:407:PRO:HD2  | 2.01                     | 0.42              |
| 1:B:188[B]:GLN:NE2 | 5:B:1195:HOH:O   | 2.54                     | 0.41              |
| 1:G:272:LYS:CD     | 5:H:850:HOH:O    | 2.68                     | 0.41              |
| 1:B:209:THR:N      | 4:B:520:CIT:H22  | 2.36                     | 0.41              |
| 1:B:408:MET:HE1    | 5:B:1025:HOH:O   | 2.20                     | 0.41              |
| 1:E:200:VAL:HB     | 1:E:232:PRO:O    | 2.19                     | 0.41              |
| 1:F:110:LYS:HB3    | 1:F:111:PRO:HD3  | 2.03                     | 0.41              |
| 1:H:318:MET:O      | 1:H:322:ILE:HG12 | 2.20                     | 0.41              |
| 1:A:20:GLN:NE2     | 1:A:23:LYS:HE3   | 2.33                     | 0.41              |
| 1:E:387:ASN:ND2    | 1:E:389:SER:H    | 2.18                     | 0.41              |
| 1:G:324:PHE:O      | 1:G:325:ARG:HB2  | 2.20                     | 0.41              |
| 1:B:210:GLU:CG     | 4:B:520:CIT:H21  | 2.50                     | 0.41              |
| 1:C:16:MET:HE2     | 5:C:926:HOH:O    | 2.20                     | 0.41              |
| 1:D:200:VAL:HB     | 1:D:232:PRO:O    | 2.19                     | 0.41              |
| 1:E:20:GLN:HE21    | 1:E:23:LYS:HE3   | 1.84                     | 0.41              |
| 1:D:348:GLU:HG2    | 5:D:1123:HOH:O   | 2.20                     | 0.41              |
| 1:F:387:ASN:C      | 1:F:387:ASN:HD22 | 2.28                     | 0.41              |
| 1:G:347:ASN:HD22   | 1:G:349:GLU:H    | 1.68                     | 0.41              |
| 1:A:197:ASP:OD2    | 2:A:503:GOL:H11  | 2.21                     | 0.41              |
| 1:C:198:ASP:O      | 1:C:198:ASP:CG   | 2.64                     | 0.41              |
| 1:A:156:ASN:HD21   | 1:C:204:LEU:HD11 | 1.85                     | 0.41              |
| 1:F:406:GLU:HB2    | 1:F:407:PRO:HD2  | 2.03                     | 0.41              |
| 1:G:16:MET:HE2     | 1:G:16:MET:HB3   | 1.88                     | 0.41              |
| 5:C:1158:HOH:O     | 1:G:173:GLU:HB2  | 2.20                     | 0.41              |
| 1:D:387:ASN:C      | 1:D:387:ASN:HD22 | 2.29                     | 0.41              |
| 1:A:306:MET:CE     | 5:A:993:HOH:O    | 2.58                     | 0.41              |
| 1:D:210:GLU:CB     | 2:D:505:GOL:H11  | 2.38                     | 0.41              |
| 1:F:200:VAL:HB     | 1:F:232:PRO:O    | 2.20                     | 0.41              |
| 1:G:200:VAL:HB     | 1:G:232:PRO:O    | 2.20                     | 0.41              |
| 1:G:306:MET:O      | 1:G:307:THR:C    | 2.64                     | 0.41              |
| 1:A:234:PRO:HA     | 1:A:252:MET:O    | 2.20                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:387:ASN:ND2 | 1:F:389:SER:H    | 2.20                     | 0.40              |
| 1:B:306:MET:O   | 1:B:307:THR:C    | 2.64                     | 0.40              |
| 1:C:89:GLU:HG2  | 5:C:1025:HOH:O   | 2.21                     | 0.40              |
| 1:F:15:SER:HB2  | 1:F:16:MET:HE2   | 2.02                     | 0.40              |
| 1:H:203:LYS:HB2 | 1:H:203:LYS:HE2  | 1.78                     | 0.40              |
| 1:F:20:GLN:HE21 | 1:F:23:LYS:HE3   | 1.86                     | 0.40              |
| 1:F:172:LYS:HD3 | 5:F:692:HOH:O    | 2.21                     | 0.40              |
| 1:G:172:LYS:HE3 | 5:G:704:HOH:O    | 2.20                     | 0.40              |
| 1:G:279:LEU:C   | 1:G:279:LEU:HD23 | 2.46                     | 0.40              |
| 1:H:324:PHE:O   | 1:H:325:ARG:HB2  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 432/448 (96%)   | 418 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 1   | B     | 432/448 (96%)   | 413 (96%)  | 19 (4%)  | 0        | 100         | 100 |
| 1   | C     | 431/448 (96%)   | 416 (96%)  | 15 (4%)  | 0        | 100         | 100 |
| 1   | D     | 434/448 (97%)   | 419 (96%)  | 15 (4%)  | 0        | 100         | 100 |
| 1   | E     | 431/448 (96%)   | 416 (96%)  | 15 (4%)  | 0        | 100         | 100 |
| 1   | F     | 428/448 (96%)   | 413 (96%)  | 14 (3%)  | 1 (0%)   | 43          | 53  |
| 1   | G     | 430/448 (96%)   | 415 (96%)  | 15 (4%)  | 0        | 100         | 100 |
| 1   | H     | 428/448 (96%)   | 410 (96%)  | 17 (4%)  | 1 (0%)   | 43          | 53  |
| All | All   | 3446/3584 (96%) | 3320 (96%) | 124 (4%) | 2 (0%)   | 48          | 59  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 325 | ARG  |
| 1   | F     | 325 | ARG  |

### 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     | 373/383 (97%)   | 363 (97%)  | 10 (3%)  | 39          | 55 |
| 1   | B     | 373/383 (97%)   | 362 (97%)  | 11 (3%)  | 37          | 52 |
| 1   | C     | 371/383 (97%)   | 361 (97%)  | 10 (3%)  | 39          | 55 |
| 1   | D     | 372/383 (97%)   | 365 (98%)  | 7 (2%)   | 50          | 66 |
| 1   | E     | 372/383 (97%)   | 359 (96%)  | 13 (4%)  | 32          | 45 |
| 1   | F     | 369/383 (96%)   | 351 (95%)  | 18 (5%)  | 22          | 31 |
| 1   | G     | 371/383 (97%)   | 348 (94%)  | 23 (6%)  | 16          | 21 |
| 1   | H     | 369/383 (96%)   | 348 (94%)  | 21 (6%)  | 18          | 25 |
| All | All   | 2970/3064 (97%) | 2857 (96%) | 113 (4%) | 29          | 42 |

All (113) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 71  | GLU  |
| 1   | A     | 121 | LEU  |
| 1   | A     | 147 | VAL  |
| 1   | A     | 203 | LYS  |
| 1   | A     | 237 | LEU  |
| 1   | A     | 381 | GLN  |
| 1   | A     | 383 | VAL  |
| 1   | A     | 391 | LYS  |
| 1   | A     | 429 | GLU  |
| 1   | A     | 444 | VAL  |
| 1   | B     | 45  | LYS  |
| 1   | B     | 71  | GLU  |
| 1   | B     | 104 | LYS  |
| 1   | B     | 145 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 203 | LYS  |
| 1   | B     | 253 | THR  |
| 1   | B     | 321 | TRP  |
| 1   | B     | 381 | GLN  |
| 1   | B     | 406 | GLU  |
| 1   | B     | 421 | LEU  |
| 1   | B     | 430 | LEU  |
| 1   | C     | 71  | GLU  |
| 1   | C     | 147 | VAL  |
| 1   | C     | 203 | LYS  |
| 1   | C     | 253 | THR  |
| 1   | C     | 298 | VAL  |
| 1   | C     | 402 | LEU  |
| 1   | C     | 406 | GLU  |
| 1   | C     | 409 | LYS  |
| 1   | C     | 413 | LEU  |
| 1   | C     | 421 | LEU  |
| 1   | D     | 71  | GLU  |
| 1   | D     | 121 | LEU  |
| 1   | D     | 203 | LYS  |
| 1   | D     | 383 | VAL  |
| 1   | D     | 392 | ARG  |
| 1   | D     | 406 | GLU  |
| 1   | D     | 413 | LEU  |
| 1   | E     | 71  | GLU  |
| 1   | E     | 145 | THR  |
| 1   | E     | 203 | LYS  |
| 1   | E     | 237 | LEU  |
| 1   | E     | 253 | THR  |
| 1   | E     | 298 | VAL  |
| 1   | E     | 383 | VAL  |
| 1   | E     | 391 | LYS  |
| 1   | E     | 400 | LYS  |
| 1   | E     | 402 | LEU  |
| 1   | E     | 406 | GLU  |
| 1   | E     | 413 | LEU  |
| 1   | E     | 422 | VAL  |
| 1   | F     | 71  | GLU  |
| 1   | F     | 104 | LYS  |
| 1   | F     | 121 | LEU  |
| 1   | F     | 172 | LYS  |
| 1   | F     | 188 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 203 | LYS  |
| 1   | F     | 237 | LEU  |
| 1   | F     | 298 | VAL  |
| 1   | F     | 392 | ARG  |
| 1   | F     | 402 | LEU  |
| 1   | F     | 405 | MET  |
| 1   | F     | 413 | LEU  |
| 1   | F     | 419 | LEU  |
| 1   | F     | 422 | VAL  |
| 1   | F     | 423 | LYS  |
| 1   | F     | 430 | LEU  |
| 1   | F     | 433 | HIS  |
| 1   | F     | 444 | VAL  |
| 1   | G     | 16  | MET  |
| 1   | G     | 71  | GLU  |
| 1   | G     | 118 | ASN  |
| 1   | G     | 121 | LEU  |
| 1   | G     | 203 | LYS  |
| 1   | G     | 237 | LEU  |
| 1   | G     | 253 | THR  |
| 1   | G     | 298 | VAL  |
| 1   | G     | 321 | TRP  |
| 1   | G     | 347 | ASN  |
| 1   | G     | 363 | VAL  |
| 1   | G     | 365 | ARG  |
| 1   | G     | 366 | GLU  |
| 1   | G     | 371 | VAL  |
| 1   | G     | 378 | GLU  |
| 1   | G     | 381 | GLN  |
| 1   | G     | 383 | VAL  |
| 1   | G     | 392 | ARG  |
| 1   | G     | 394 | VAL  |
| 1   | G     | 406 | GLU  |
| 1   | G     | 425 | GLN  |
| 1   | G     | 426 | LEU  |
| 1   | G     | 438 | VAL  |
| 1   | H     | 20  | GLN  |
| 1   | H     | 71  | GLU  |
| 1   | H     | 75  | ASN  |
| 1   | H     | 89  | GLU  |
| 1   | H     | 118 | ASN  |
| 1   | H     | 121 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 146 | ASN  |
| 1   | H     | 203 | LYS  |
| 1   | H     | 209 | THR  |
| 1   | H     | 237 | LEU  |
| 1   | H     | 253 | THR  |
| 1   | H     | 298 | VAL  |
| 1   | H     | 348 | GLU  |
| 1   | H     | 366 | GLU  |
| 1   | H     | 383 | VAL  |
| 1   | H     | 400 | LYS  |
| 1   | H     | 402 | LEU  |
| 1   | H     | 409 | LYS  |
| 1   | H     | 413 | LEU  |
| 1   | H     | 429 | GLU  |
| 1   | H     | 444 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | GLN  |
| 1   | A     | 156 | ASN  |
| 1   | A     | 208 | HIS  |
| 1   | A     | 246 | ASN  |
| 1   | A     | 248 | ASN  |
| 1   | A     | 355 | GLN  |
| 1   | A     | 356 | ASN  |
| 1   | A     | 381 | GLN  |
| 1   | A     | 387 | ASN  |
| 1   | B     | 17  | HIS  |
| 1   | B     | 20  | GLN  |
| 1   | B     | 156 | ASN  |
| 1   | B     | 246 | ASN  |
| 1   | B     | 248 | ASN  |
| 1   | B     | 337 | ASN  |
| 1   | B     | 387 | ASN  |
| 1   | C     | 18  | HIS  |
| 1   | C     | 20  | GLN  |
| 1   | C     | 68  | GLN  |
| 1   | C     | 156 | ASN  |
| 1   | C     | 248 | ASN  |
| 1   | C     | 355 | GLN  |
| 1   | C     | 387 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 18  | HIS  |
| 1   | D     | 20  | GLN  |
| 1   | D     | 156 | ASN  |
| 1   | D     | 188 | GLN  |
| 1   | D     | 246 | ASN  |
| 1   | D     | 248 | ASN  |
| 1   | D     | 387 | ASN  |
| 1   | D     | 424 | HIS  |
| 1   | E     | 18  | HIS  |
| 1   | E     | 20  | GLN  |
| 1   | E     | 68  | GLN  |
| 1   | E     | 118 | ASN  |
| 1   | E     | 138 | GLN  |
| 1   | E     | 146 | ASN  |
| 1   | E     | 156 | ASN  |
| 1   | E     | 184 | GLN  |
| 1   | E     | 248 | ASN  |
| 1   | E     | 387 | ASN  |
| 1   | F     | 18  | HIS  |
| 1   | F     | 20  | GLN  |
| 1   | F     | 75  | ASN  |
| 1   | F     | 137 | HIS  |
| 1   | F     | 248 | ASN  |
| 1   | F     | 355 | GLN  |
| 1   | F     | 387 | ASN  |
| 1   | F     | 433 | HIS  |
| 1   | G     | 156 | ASN  |
| 1   | G     | 208 | HIS  |
| 1   | G     | 248 | ASN  |
| 1   | G     | 347 | ASN  |
| 1   | G     | 381 | GLN  |
| 1   | G     | 387 | ASN  |
| 1   | H     | 20  | GLN  |
| 1   | H     | 68  | GLN  |
| 1   | H     | 75  | ASN  |
| 1   | H     | 118 | ASN  |
| 1   | H     | 248 | ASN  |
| 1   | H     | 355 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

130 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | SO4  | C     | 511 | -    | 4,4,4        | 0.55 | 0           | 6,6,6       | 0.64 | 0           |
| 2   | GOL  | E     | 502 | -    | 5,5,5        | 0.62 | 0           | 5,5,5       | 0.46 | 0           |
| 2   | GOL  | D     | 505 | -    | 5,5,5        | 0.98 | 0           | 5,5,5       | 1.54 | 1 (20%)     |
| 3   | SO4  | B     | 511 | -    | 4,4,4        | 0.79 | 0           | 6,6,6       | 0.60 | 0           |
| 2   | GOL  | A     | 502 | -    | 5,5,5        | 0.62 | 0           | 5,5,5       | 0.36 | 0           |
| 3   | SO4  | A     | 513 | -    | 4,4,4        | 0.52 | 0           | 6,6,6       | 0.63 | 0           |
| 3   | SO4  | C     | 509 | -    | 4,4,4        | 0.51 | 0           | 6,6,6       | 0.15 | 0           |
| 2   | GOL  | A     | 504 | -    | 5,5,5        | 0.48 | 0           | 5,5,5       | 0.68 | 0           |
| 3   | SO4  | G     | 505 | -    | 4,4,4        | 0.45 | 0           | 6,6,6       | 0.65 | 0           |
| 3   | SO4  | D     | 506 | -    | 4,4,4        | 0.52 | 0           | 6,6,6       | 0.64 | 0           |
| 2   | GOL  | F     | 502 | -    | 5,5,5        | 0.51 | 0           | 5,5,5       | 0.66 | 0           |
| 4   | CIT  | C     | 519 | -    | 12,12,12     | 3.07 | 7 (58%)     | 17,17,17    | 3.61 | 9 (52%)     |
| 2   | GOL  | G     | 504 | -    | 5,5,5        | 0.51 | 0           | 5,5,5       | 0.95 | 0           |
| 2   | GOL  | E     | 506 | -    | 5,5,5        | 0.39 | 0           | 5,5,5       | 0.31 | 0           |
| 3   | SO4  | E     | 509 | -    | 4,4,4        | 0.75 | 0           | 6,6,6       | 1.34 | 1 (16%)     |
| 3   | SO4  | F     | 512 | -    | 4,4,4        | 0.69 | 0           | 6,6,6       | 0.81 | 0           |
| 3   | SO4  | H     | 504 | -    | 4,4,4        | 0.61 | 0           | 6,6,6       | 0.56 | 0           |
| 3   | SO4  | C     | 510 | -    | 4,4,4        | 0.87 | 0           | 6,6,6       | 0.42 | 0           |
| 3   | SO4  | F     | 509 | -    | 4,4,4        | 0.61 | 0           | 6,6,6       | 0.78 | 0           |
| 3   | SO4  | C     | 508 | -    | 4,4,4        | 0.59 | 0           | 6,6,6       | 0.53 | 0           |
| 3   | SO4  | C     | 518 | -    | 4,4,4        | 0.57 | 0           | 6,6,6       | 0.37 | 0           |
| 3   | SO4  | E     | 507 | -    | 4,4,4        | 0.58 | 0           | 6,6,6       | 0.63 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | SO4  | D     | 513 | -    | 4,4,4        | 0.69 | 0        | 6,6,6       | 0.80 | 0        |
| 2   | GOL  | B     | 505 | -    | 5,5,5        | 1.15 | 0        | 5,5,5       | 0.77 | 0        |
| 3   | SO4  | F     | 507 | -    | 4,4,4        | 0.63 | 0        | 6,6,6       | 0.35 | 0        |
| 3   | SO4  | F     | 514 | -    | 4,4,4        | 0.81 | 0        | 6,6,6       | 0.46 | 0        |
| 3   | SO4  | C     | 512 | -    | 4,4,4        | 0.63 | 0        | 6,6,6       | 0.72 | 0        |
| 3   | SO4  | F     | 506 | -    | 4,4,4        | 0.62 | 0        | 6,6,6       | 0.25 | 0        |
| 3   | SO4  | C     | 515 | -    | 4,4,4        | 0.79 | 0        | 6,6,6       | 1.30 | 1 (16%)  |
| 3   | SO4  | E     | 515 | -    | 4,4,4        | 0.85 | 0        | 6,6,6       | 0.69 | 0        |
| 3   | SO4  | F     | 510 | -    | 4,4,4        | 0.70 | 0        | 6,6,6       | 0.58 | 0        |
| 3   | SO4  | F     | 508 | -    | 4,4,4        | 1.00 | 0        | 6,6,6       | 0.91 | 0        |
| 3   | SO4  | H     | 513 | -    | 4,4,4        | 0.50 | 0        | 6,6,6       | 0.62 | 0        |
| 3   | SO4  | A     | 511 | -    | 4,4,4        | 0.74 | 0        | 6,6,6       | 0.79 | 0        |
| 2   | GOL  | B     | 501 | -    | 5,5,5        | 0.63 | 0        | 5,5,5       | 1.21 | 1 (20%)  |
| 3   | SO4  | B     | 518 | -    | 4,4,4        | 0.58 | 0        | 6,6,6       | 0.22 | 0        |
| 2   | GOL  | E     | 501 | -    | 5,5,5        | 0.55 | 0        | 5,5,5       | 0.25 | 0        |
| 2   | GOL  | B     | 506 | -    | 5,5,5        | 0.74 | 0        | 5,5,5       | 0.54 | 0        |
| 2   | GOL  | H     | 502 | -    | 5,5,5        | 0.43 | 0        | 5,5,5       | 0.99 | 0        |
| 3   | SO4  | A     | 505 | -    | 4,4,4        | 1.27 | 0        | 6,6,6       | 1.08 | 0        |
| 3   | SO4  | D     | 514 | -    | 4,4,4        | 0.62 | 0        | 6,6,6       | 0.38 | 0        |
| 3   | SO4  | D     | 510 | -    | 4,4,4        | 0.66 | 0        | 6,6,6       | 0.54 | 0        |
| 2   | GOL  | A     | 503 | -    | 5,5,5        | 0.84 | 0        | 5,5,5       | 2.28 | 2 (40%)  |
| 2   | GOL  | F     | 503 | -    | 5,5,5        | 0.71 | 0        | 5,5,5       | 0.35 | 0        |
| 3   | SO4  | C     | 507 | -    | 4,4,4        | 0.79 | 0        | 6,6,6       | 0.67 | 0        |
| 2   | GOL  | H     | 501 | -    | 5,5,5        | 0.65 | 0        | 5,5,5       | 0.55 | 0        |
| 3   | SO4  | A     | 509 | -    | 4,4,4        | 0.57 | 0        | 6,6,6       | 1.13 | 1 (16%)  |
| 3   | SO4  | H     | 511 | -    | 4,4,4        | 0.50 | 0        | 6,6,6       | 0.43 | 0        |
| 3   | SO4  | D     | 515 | -    | 4,4,4        | 0.62 | 0        | 6,6,6       | 0.47 | 0        |
| 2   | GOL  | D     | 503 | -    | 5,5,5        | 0.57 | 0        | 5,5,5       | 1.89 | 3 (60%)  |
| 3   | SO4  | H     | 514 | -    | 4,4,4        | 0.27 | 0        | 6,6,6       | 0.42 | 0        |
| 3   | SO4  | H     | 510 | -    | 4,4,4        | 0.61 | 0        | 6,6,6       | 0.46 | 0        |
| 3   | SO4  | G     | 512 | -    | 4,4,4        | 0.60 | 0        | 6,6,6       | 0.38 | 0        |
| 3   | SO4  | E     | 508 | -    | 4,4,4        | 0.82 | 0        | 6,6,6       | 1.05 | 0        |
| 3   | SO4  | F     | 513 | -    | 4,4,4        | 0.75 | 0        | 6,6,6       | 1.14 | 1 (16%)  |
| 3   | SO4  | A     | 506 | -    | 4,4,4        | 0.56 | 0        | 6,6,6       | 0.48 | 0        |
| 3   | SO4  | D     | 516 | -    | 4,4,4        | 0.64 | 0        | 6,6,6       | 0.82 | 0        |
| 2   | GOL  | B     | 508 | -    | 5,5,5        | 0.76 | 0        | 5,5,5       | 0.93 | 0        |
| 2   | GOL  | B     | 509 | -    | 5,5,5        | 0.68 | 0        | 5,5,5       | 0.85 | 0        |
| 3   | SO4  | C     | 514 | -    | 4,4,4        | 0.55 | 0        | 6,6,6       | 0.37 | 0        |
| 3   | SO4  | G     | 507 | -    | 4,4,4        | 0.76 | 0        | 6,6,6       | 0.51 | 0        |
| 3   | SO4  | H     | 507 | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 0.37 | 0        |
| 2   | GOL  | C     | 503 | -    | 5,5,5        | 2.32 | 3 (60%)  | 5,5,5       | 2.29 | 3 (60%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | SO4  | G     | 506 | -    | 4,4,4        | 0.79 | 0        | 6,6,6       | 0.90 | 0        |
| 3   | SO4  | H     | 508 | -    | 4,4,4        | 0.60 | 0        | 6,6,6       | 0.45 | 0        |
| 3   | SO4  | B     | 514 | -    | 4,4,4        | 0.59 | 0        | 6,6,6       | 0.60 | 0        |
| 3   | SO4  | E     | 514 | -    | 4,4,4        | 1.15 | 0        | 6,6,6       | 1.09 | 0        |
| 2   | GOL  | B     | 503 | -    | 5,5,5        | 0.93 | 0        | 5,5,5       | 1.53 | 1 (20%)  |
| 4   | CIT  | A     | 515 | -    | 12,12,12     | 1.79 | 4 (33%)  | 17,17,17    | 4.53 | 13 (76%) |
| 3   | SO4  | G     | 508 | -    | 4,4,4        | 0.26 | 0        | 6,6,6       | 0.31 | 0        |
| 3   | SO4  | B     | 510 | -    | 4,4,4        | 0.55 | 0        | 6,6,6       | 0.67 | 0        |
| 2   | GOL  | C     | 502 | -    | 5,5,5        | 0.60 | 0        | 5,5,5       | 0.60 | 0        |
| 2   | GOL  | H     | 503 | -    | 5,5,5        | 0.86 | 0        | 5,5,5       | 0.93 | 0        |
| 2   | GOL  | D     | 501 | -    | 5,5,5        | 0.84 | 0        | 5,5,5       | 0.57 | 0        |
| 3   | SO4  | D     | 517 | -    | 4,4,4        | 0.56 | 0        | 6,6,6       | 0.72 | 0        |
| 3   | SO4  | F     | 515 | -    | 4,4,4        | 0.58 | 0        | 6,6,6       | 0.47 | 0        |
| 2   | GOL  | G     | 503 | -    | 5,5,5        | 0.54 | 0        | 5,5,5       | 1.21 | 1 (20%)  |
| 3   | SO4  | B     | 515 | -    | 4,4,4        | 0.81 | 0        | 6,6,6       | 0.82 | 0        |
| 3   | SO4  | H     | 512 | -    | 4,4,4        | 0.51 | 0        | 6,6,6       | 0.70 | 0        |
| 2   | GOL  | E     | 503 | -    | 5,5,5        | 0.69 | 0        | 5,5,5       | 1.86 | 2 (40%)  |
| 3   | SO4  | C     | 506 | -    | 4,4,4        | 0.54 | 0        | 6,6,6       | 0.48 | 0        |
| 2   | GOL  | G     | 502 | -    | 5,5,5        | 0.37 | 0        | 5,5,5       | 0.49 | 0        |
| 2   | GOL  | F     | 501 | -    | 5,5,5        | 0.86 | 0        | 5,5,5       | 0.34 | 0        |
| 3   | SO4  | D     | 509 | -    | 4,4,4        | 0.90 | 0        | 6,6,6       | 1.59 | 1 (16%)  |
| 2   | GOL  | B     | 502 | -    | 5,5,5        | 0.54 | 0        | 5,5,5       | 0.70 | 0        |
| 2   | GOL  | C     | 504 | -    | 5,5,5        | 0.66 | 0        | 5,5,5       | 0.99 | 1 (20%)  |
| 3   | SO4  | B     | 519 | -    | 4,4,4        | 0.64 | 0        | 6,6,6       | 0.63 | 0        |
| 4   | CIT  | E     | 517 | -    | 12,12,12     | 1.47 | 2 (16%)  | 17,17,17    | 1.86 | 5 (29%)  |
| 3   | SO4  | A     | 514 | -    | 4,4,4        | 0.87 | 0        | 6,6,6       | 0.73 | 0        |
| 4   | CIT  | G     | 513 | -    | 12,12,12     | 2.07 | 5 (41%)  | 17,17,17    | 3.89 | 10 (58%) |
| 2   | GOL  | B     | 504 | -    | 5,5,5        | 0.69 | 0        | 5,5,5       | 1.27 | 1 (20%)  |
| 3   | SO4  | F     | 505 | -    | 4,4,4        | 0.64 | 0        | 6,6,6       | 0.52 | 0        |
| 3   | SO4  | B     | 517 | -    | 4,4,4        | 0.94 | 0        | 6,6,6       | 1.06 | 0        |
| 4   | CIT  | B     | 520 | -    | 12,12,12     | 2.28 | 3 (25%)  | 17,17,17    | 1.70 | 4 (23%)  |
| 2   | GOL  | B     | 507 | -    | 5,5,5        | 0.36 | 0        | 5,5,5       | 1.58 | 1 (20%)  |
| 3   | SO4  | C     | 516 | -    | 4,4,4        | 0.67 | 0        | 6,6,6       | 0.76 | 0        |
| 3   | SO4  | A     | 512 | -    | 4,4,4        | 1.11 | 0        | 6,6,6       | 1.36 | 1 (16%)  |
| 3   | SO4  | E     | 510 | -    | 4,4,4        | 0.67 | 0        | 6,6,6       | 0.35 | 0        |
| 3   | SO4  | B     | 516 | -    | 4,4,4        | 0.81 | 0        | 6,6,6       | 1.21 | 0        |
| 3   | SO4  | G     | 510 | -    | 4,4,4        | 0.59 | 0        | 6,6,6       | 0.23 | 0        |
| 3   | SO4  | A     | 510 | -    | 4,4,4        | 0.73 | 0        | 6,6,6       | 0.86 | 0        |
| 3   | SO4  | E     | 511 | -    | 4,4,4        | 0.62 | 0        | 6,6,6       | 1.28 | 1 (16%)  |
| 3   | SO4  | H     | 506 | -    | 4,4,4        | 0.78 | 0        | 6,6,6       | 0.74 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | SO4  | D     | 512 | -    | 4,4,4        | 0.62 | 0        | 6,6,6       | 1.18 | 0        |
| 2   | GOL  | C     | 505 | -    | 5,5,5        | 2.78 | 1 (20%)  | 5,5,5       | 1.77 | 2 (40%)  |
| 3   | SO4  | A     | 507 | -    | 4,4,4        | 0.73 | 0        | 6,6,6       | 0.71 | 0        |
| 3   | SO4  | G     | 511 | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.58 | 0        |
| 2   | GOL  | C     | 501 | -    | 5,5,5        | 0.26 | 0        | 5,5,5       | 0.73 | 0        |
| 2   | GOL  | E     | 505 | -    | 5,5,5        | 1.52 | 1 (20%)  | 5,5,5       | 2.67 | 4 (80%)  |
| 3   | SO4  | H     | 509 | -    | 4,4,4        | 0.76 | 0        | 6,6,6       | 0.85 | 0        |
| 3   | SO4  | A     | 508 | -    | 4,4,4        | 0.62 | 0        | 6,6,6       | 0.43 | 0        |
| 3   | SO4  | D     | 507 | -    | 4,4,4        | 0.63 | 0        | 6,6,6       | 0.30 | 0        |
| 2   | GOL  | D     | 502 | -    | 5,5,5        | 0.93 | 0        | 5,5,5       | 1.68 | 2 (40%)  |
| 2   | GOL  | F     | 504 | -    | 5,5,5        | 0.26 | 0        | 5,5,5       | 0.54 | 0        |
| 2   | GOL  | D     | 504 | -    | 5,5,5        | 0.68 | 0        | 5,5,5       | 1.41 | 1 (20%)  |
| 3   | SO4  | B     | 512 | -    | 4,4,4        | 0.77 | 0        | 6,6,6       | 1.09 | 0        |
| 3   | SO4  | E     | 512 | -    | 4,4,4        | 0.66 | 0        | 6,6,6       | 0.74 | 0        |
| 3   | SO4  | E     | 516 | -    | 4,4,4        | 0.62 | 0        | 6,6,6       | 0.36 | 0        |
| 3   | SO4  | C     | 513 | -    | 4,4,4        | 0.80 | 0        | 6,6,6       | 1.32 | 1 (16%)  |
| 3   | SO4  | G     | 509 | -    | 4,4,4        | 0.45 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | GOL  | E     | 504 | -    | 5,5,5        | 0.76 | 0        | 5,5,5       | 0.87 | 0        |
| 2   | GOL  | G     | 501 | -    | 5,5,5        | 0.64 | 0        | 5,5,5       | 0.91 | 0        |
| 3   | SO4  | B     | 513 | -    | 4,4,4        | 0.48 | 0        | 6,6,6       | 0.53 | 0        |
| 2   | GOL  | A     | 501 | -    | 5,5,5        | 0.64 | 0        | 5,5,5       | 0.53 | 0        |
| 3   | SO4  | D     | 508 | -    | 4,4,4        | 1.18 | 0        | 6,6,6       | 0.55 | 0        |
| 3   | SO4  | E     | 513 | -    | 4,4,4        | 0.67 | 0        | 6,6,6       | 0.83 | 0        |
| 3   | SO4  | C     | 517 | -    | 4,4,4        | 0.75 | 0        | 6,6,6       | 0.39 | 0        |
| 3   | SO4  | D     | 511 | -    | 4,4,4        | 0.75 | 0        | 6,6,6       | 1.85 | 1 (16%)  |
| 3   | SO4  | H     | 505 | -    | 4,4,4        | 0.51 | 0        | 6,6,6       | 0.42 | 0        |
| 3   | SO4  | F     | 511 | -    | 4,4,4        | 0.76 | 0        | 6,6,6       | 0.80 | 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  | B     | 504 | -    | -       | 2/4/4/4  | -     |
| 2   | GOL  | B     | 501 | -    | -       | 0/4/4/4  | -     |
| 2   | GOL  | C     | 502 | -    | -       | 2/4/4/4  | -     |
| 2   | GOL  | E     | 502 | -    | -       | 2/4/4/4  | -     |
| 2   | GOL  | E     | 501 | -    | -       | 2/4/4/4  | -     |
| 2   | GOL  | B     | 506 | -    | -       | 4/4/4/4  | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings |
|-----|------|-------|-----|------|---------|-------------|-------|
| 2   | GOL  | H     | 502 | -    | -       | 4/4/4/4     | -     |
| 2   | GOL  | B     | 507 | -    | -       | 1/4/4/4     | -     |
| 4   | CIT  | B     | 520 | -    | -       | 10/16/16/16 | -     |
| 2   | GOL  | D     | 505 | -    | -       | 4/4/4/4     | -     |
| 2   | GOL  | A     | 502 | -    | -       | 2/4/4/4     | -     |
| 2   | GOL  | H     | 503 | -    | -       | 4/4/4/4     | -     |
| 2   | GOL  | A     | 504 | -    | -       | 0/4/4/4     | -     |
| 2   | GOL  | D     | 501 | -    | -       | 0/4/4/4     | -     |
| 2   | GOL  | A     | 503 | -    | -       | 1/4/4/4     | -     |
| 2   | GOL  | F     | 502 | -    | -       | 4/4/4/4     | -     |
| 2   | GOL  | F     | 503 | -    | -       | 0/4/4/4     | -     |
| 2   | GOL  | E     | 506 | -    | -       | 2/4/4/4     | -     |
| 2   | GOL  | G     | 504 | -    | -       | 2/4/4/4     | -     |
| 4   | CIT  | C     | 519 | -    | -       | 8/16/16/16  | -     |
| 2   | GOL  | H     | 501 | -    | -       | 2/4/4/4     | -     |
| 2   | GOL  | G     | 503 | -    | -       | 2/4/4/4     | -     |
| 2   | GOL  | C     | 505 | -    | -       | 2/4/4/4     | -     |
| 2   | GOL  | C     | 501 | -    | -       | 1/4/4/4     | -     |
| 2   | GOL  | E     | 503 | -    | -       | 2/4/4/4     | -     |
| 2   | GOL  | E     | 505 | -    | -       | 2/4/4/4     | -     |
| 2   | GOL  | D     | 503 | -    | -       | 3/4/4/4     | -     |
| 2   | GOL  | B     | 505 | -    | -       | 0/4/4/4     | -     |
| 2   | GOL  | G     | 502 | -    | -       | 4/4/4/4     | -     |
| 2   | GOL  | D     | 502 | -    | -       | 0/4/4/4     | -     |
| 2   | GOL  | F     | 504 | -    | -       | 3/4/4/4     | -     |
| 2   | GOL  | D     | 504 | -    | -       | 0/4/4/4     | -     |
| 2   | GOL  | B     | 508 | -    | -       | 0/4/4/4     | -     |
| 2   | GOL  | B     | 509 | -    | -       | 2/4/4/4     | -     |
| 2   | GOL  | F     | 501 | -    | -       | 0/4/4/4     | -     |
| 2   | GOL  | C     | 503 | -    | -       | 4/4/4/4     | -     |
| 2   | GOL  | E     | 504 | -    | -       | 2/4/4/4     | -     |
| 2   | GOL  | G     | 501 | -    | -       | 0/4/4/4     | -     |
| 2   | GOL  | A     | 501 | -    | -       | 4/4/4/4     | -     |
| 2   | GOL  | B     | 502 | -    | -       | 2/4/4/4     | -     |
| 2   | GOL  | B     | 503 | -    | -       | 1/4/4/4     | -     |
| 2   | GOL  | C     | 504 | -    | -       | 0/4/4/4     | -     |
| 4   | CIT  | A     | 515 | -    | -       | 6/16/16/16  | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 4   | CIT  | E     | 517 | -    | -       | 7/16/16/16 | -     |
| 4   | CIT  | G     | 513 | -    | -       | 7/16/16/16 | -     |

All (26) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 4   | C     | 519 | CIT  | C3-C6 | 6.28  | 1.60        | 1.53     |
| 2   | C     | 505 | GOL  | O3-C3 | 6.01  | 1.67        | 1.42     |
| 4   | B     | 520 | CIT  | O7-C3 | 5.50  | 1.53        | 1.43     |
| 4   | C     | 519 | CIT  | O7-C3 | 4.96  | 1.52        | 1.43     |
| 4   | C     | 519 | CIT  | C4-C3 | 3.57  | 1.58        | 1.54     |
| 4   | B     | 520 | CIT  | C4-C3 | 3.43  | 1.58        | 1.54     |
| 4   | A     | 515 | CIT  | C2-C3 | 3.40  | 1.58        | 1.54     |
| 2   | C     | 503 | GOL  | O2-C2 | 3.35  | 1.53        | 1.43     |
| 4   | G     | 513 | CIT  | C2-C3 | 3.26  | 1.58        | 1.54     |
| 4   | G     | 513 | CIT  | C4-C3 | 3.04  | 1.57        | 1.54     |
| 4   | C     | 519 | CIT  | O1-C1 | 2.94  | 1.31        | 1.22     |
| 4   | B     | 520 | CIT  | O5-C6 | 2.82  | 1.30        | 1.22     |
| 4   | A     | 515 | CIT  | O5-C6 | 2.74  | 1.30        | 1.22     |
| 4   | C     | 519 | CIT  | C2-C1 | -2.71 | 1.42        | 1.50     |
| 2   | C     | 503 | GOL  | O1-C1 | 2.71  | 1.53        | 1.42     |
| 4   | C     | 519 | CIT  | O5-C6 | 2.67  | 1.30        | 1.22     |
| 4   | G     | 513 | CIT  | O5-C6 | 2.65  | 1.30        | 1.22     |
| 4   | A     | 515 | CIT  | O6-C6 | 2.41  | 1.39        | 1.30     |
| 2   | C     | 503 | GOL  | O3-C3 | 2.32  | 1.52        | 1.42     |
| 4   | A     | 515 | CIT  | O4-C5 | -2.32 | 1.23        | 1.30     |
| 4   | E     | 517 | CIT  | C3-C6 | 2.27  | 1.55        | 1.53     |
| 4   | C     | 519 | CIT  | C2-C3 | -2.23 | 1.51        | 1.54     |
| 4   | G     | 513 | CIT  | O7-C3 | 2.22  | 1.47        | 1.43     |
| 4   | E     | 517 | CIT  | O1-C1 | 2.12  | 1.29        | 1.22     |
| 4   | G     | 513 | CIT  | O4-C5 | -2.09 | 1.23        | 1.30     |
| 2   | E     | 505 | GOL  | C3-C2 | 2.05  | 1.59        | 1.51     |

All (76) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 4   | A     | 515 | CIT  | O5-C6-C3 | -11.49 | 99.83       | 122.09   |
| 4   | G     | 513 | CIT  | O5-C6-C3 | -10.25 | 102.24      | 122.09   |
| 4   | A     | 515 | CIT  | O6-C6-C3 | 8.09   | 128.67      | 113.14   |
| 4   | G     | 513 | CIT  | O6-C6-C3 | 8.00   | 128.50      | 113.14   |
| 4   | C     | 519 | CIT  | O2-C1-O1 | 7.39   | 142.34      | 123.33   |
| 4   | C     | 519 | CIT  | O7-C3-C6 | 6.54   | 118.23      | 108.96   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | A     | 515 | CIT  | C4-C3-C6 | -5.84 | 97.11       | 110.03   |
| 4   | A     | 515 | CIT  | C2-C3-C6 | 5.16  | 121.45      | 110.03   |
| 4   | G     | 513 | CIT  | C4-C3-C6 | -5.16 | 98.63       | 110.03   |
| 4   | C     | 519 | CIT  | O7-C3-C4 | 5.03  | 120.85      | 109.38   |
| 4   | C     | 519 | CIT  | O7-C3-C2 | -4.81 | 98.41       | 109.38   |
| 4   | C     | 519 | CIT  | O2-C1-C2 | -4.59 | 99.79       | 114.35   |
| 4   | E     | 517 | CIT  | O7-C3-C6 | -4.27 | 102.90      | 108.96   |
| 4   | A     | 515 | CIT  | O1-C1-C2 | -4.26 | 110.88      | 122.95   |
| 4   | B     | 520 | CIT  | C3-C2-C1 | 4.20  | 125.42      | 113.92   |
| 4   | A     | 515 | CIT  | O7-C3-C6 | 4.08  | 114.74      | 108.96   |
| 2   | C     | 503 | GOL  | O1-C1-C2 | 3.98  | 128.28      | 110.38   |
| 4   | C     | 519 | CIT  | C4-C3-C2 | -3.89 | 99.32       | 109.31   |
| 4   | G     | 513 | CIT  | C2-C3-C6 | 3.82  | 118.48      | 110.03   |
| 4   | A     | 515 | CIT  | O7-C3-C4 | 3.62  | 117.62      | 109.38   |
| 2   | E     | 505 | GOL  | C3-C2-C1 | 3.60  | 125.01      | 111.80   |
| 2   | A     | 503 | GOL  | C3-C2-C1 | -3.60 | 98.60       | 111.80   |
| 3   | D     | 511 | SO4  | O3-S-O2  | 3.53  | 128.03      | 109.56   |
| 4   | C     | 519 | CIT  | C3-C2-C1 | -3.40 | 104.63      | 113.92   |
| 4   | E     | 517 | CIT  | O6-C6-C3 | 3.39  | 119.65      | 113.14   |
| 4   | G     | 513 | CIT  | O7-C3-C4 | 3.31  | 116.93      | 109.38   |
| 2   | E     | 503 | GOL  | O2-C2-C1 | -3.20 | 95.95       | 109.18   |
| 4   | C     | 519 | CIT  | O6-C6-C3 | 3.16  | 119.20      | 113.14   |
| 2   | A     | 503 | GOL  | O3-C3-C2 | 3.08  | 124.25      | 110.38   |
| 3   | D     | 509 | SO4  | O4-S-O1  | -3.07 | 93.52       | 109.56   |
| 2   | E     | 505 | GOL  | O1-C1-C2 | 2.97  | 123.73      | 110.38   |
| 3   | E     | 509 | SO4  | O3-S-O1  | -2.93 | 94.22       | 109.56   |
| 2   | B     | 507 | GOL  | O1-C1-C2 | -2.89 | 97.36       | 110.38   |
| 4   | E     | 517 | CIT  | C3-C4-C5 | 2.88  | 121.79      | 113.92   |
| 2   | C     | 505 | GOL  | C3-C2-C1 | 2.83  | 122.18      | 111.80   |
| 4   | B     | 520 | CIT  | C4-C3-C6 | -2.79 | 103.87      | 110.03   |
| 4   | G     | 513 | CIT  | O4-C5-O3 | -2.77 | 116.22      | 123.33   |
| 4   | A     | 515 | CIT  | C4-C3-C2 | -2.70 | 102.38      | 109.31   |
| 2   | D     | 505 | GOL  | O2-C2-C3 | 2.69  | 120.34      | 109.18   |
| 2   | D     | 502 | GOL  | O2-C2-C3 | -2.65 | 98.22       | 109.18   |
| 4   | A     | 515 | CIT  | O4-C5-C4 | 2.64  | 122.72      | 114.35   |
| 2   | B     | 503 | GOL  | O3-C3-C2 | -2.62 | 98.56       | 110.38   |
| 4   | A     | 515 | CIT  | O2-C1-C2 | 2.62  | 122.64      | 114.35   |
| 2   | D     | 504 | GOL  | O1-C1-C2 | -2.57 | 98.80       | 110.38   |
| 4   | G     | 513 | CIT  | O4-C5-C4 | 2.56  | 122.46      | 114.35   |
| 4   | G     | 513 | CIT  | O7-C3-C6 | 2.55  | 112.57      | 108.96   |
| 2   | D     | 503 | GOL  | O2-C2-C3 | 2.53  | 119.65      | 109.18   |
| 4   | A     | 515 | CIT  | O7-C3-C2 | -2.52 | 103.63      | 109.38   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | D     | 503 | GOL  | O1-C1-C2 | -2.47 | 99.28       | 110.38   |
| 2   | E     | 505 | GOL  | O3-C3-C2 | 2.46  | 121.45      | 110.38   |
| 2   | E     | 505 | GOL  | O2-C2-C1 | -2.43 | 99.11       | 109.18   |
| 3   | A     | 512 | SO4  | O4-S-O2  | -2.40 | 97.03       | 109.56   |
| 3   | E     | 511 | SO4  | O4-S-O3  | 2.39  | 121.69      | 108.54   |
| 2   | C     | 503 | GOL  | O3-C3-C2 | 2.38  | 121.09      | 110.38   |
| 4   | A     | 515 | CIT  | O6-C6-O5 | 2.34  | 131.34      | 123.86   |
| 4   | B     | 520 | CIT  | C3-C4-C5 | 2.32  | 120.28      | 113.92   |
| 2   | G     | 503 | GOL  | O1-C1-C2 | -2.29 | 100.08      | 110.38   |
| 4   | C     | 519 | CIT  | O4-C5-O3 | -2.22 | 117.63      | 123.33   |
| 3   | C     | 515 | SO4  | O3-S-O1  | -2.22 | 97.97       | 109.56   |
| 2   | D     | 502 | GOL  | C3-C2-C1 | 2.20  | 119.87      | 111.80   |
| 2   | C     | 505 | GOL  | O2-C2-C1 | -2.20 | 100.08      | 109.18   |
| 3   | A     | 509 | SO4  | O4-S-O1  | -2.19 | 98.11       | 109.56   |
| 4   | G     | 513 | CIT  | C4-C3-C2 | -2.18 | 103.71      | 109.31   |
| 2   | B     | 504 | GOL  | O2-C2-C1 | -2.14 | 100.31      | 109.18   |
| 2   | E     | 503 | GOL  | O1-C1-C2 | -2.14 | 100.75      | 110.38   |
| 4   | A     | 515 | CIT  | O4-C5-O3 | -2.13 | 117.85      | 123.33   |
| 4   | E     | 517 | CIT  | O7-C3-C2 | -2.12 | 104.54      | 109.38   |
| 4   | G     | 513 | CIT  | C3-C2-C1 | 2.12  | 119.71      | 113.92   |
| 2   | B     | 501 | GOL  | C3-C2-C1 | -2.11 | 104.07      | 111.80   |
| 2   | C     | 504 | GOL  | O3-C3-C2 | -2.08 | 101.01      | 110.38   |
| 4   | B     | 520 | CIT  | O6-C6-C3 | 2.07  | 117.11      | 113.14   |
| 2   | D     | 503 | GOL  | O2-C2-C1 | -2.07 | 100.63      | 109.18   |
| 3   | C     | 513 | SO4  | O3-S-O2  | 2.06  | 120.32      | 109.56   |
| 3   | F     | 513 | SO4  | O4-S-O3  | -2.06 | 97.20       | 108.54   |
| 2   | C     | 503 | GOL  | O2-C2-C1 | 2.02  | 117.53      | 109.18   |
| 4   | E     | 517 | CIT  | O4-C5-O3 | -2.00 | 118.18      | 123.33   |

There are no chirality outliers.

All (110) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | A     | 501 | GOL  | O1-C1-C2-C3 |
| 2   | A     | 501 | GOL  | C1-C2-C3-O3 |
| 2   | A     | 501 | GOL  | O2-C2-C3-O3 |
| 2   | B     | 502 | GOL  | O1-C1-C2-C3 |
| 2   | B     | 506 | GOL  | O1-C1-C2-O2 |
| 2   | B     | 506 | GOL  | O1-C1-C2-C3 |
| 2   | C     | 502 | GOL  | C1-C2-C3-O3 |
| 2   | C     | 503 | GOL  | O1-C1-C2-C3 |
| 2   | C     | 503 | GOL  | C1-C2-C3-O3 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | C     | 505 | GOL  | O1-C1-C2-O2 |
| 2   | C     | 505 | GOL  | O1-C1-C2-C3 |
| 2   | D     | 503 | GOL  | O1-C1-C2-C3 |
| 2   | D     | 505 | GOL  | O1-C1-C2-C3 |
| 2   | E     | 501 | GOL  | C1-C2-C3-O3 |
| 2   | E     | 503 | GOL  | C1-C2-C3-O3 |
| 2   | E     | 504 | GOL  | C1-C2-C3-O3 |
| 2   | F     | 502 | GOL  | O1-C1-C2-O2 |
| 2   | F     | 502 | GOL  | O1-C1-C2-C3 |
| 2   | F     | 502 | GOL  | C1-C2-C3-O3 |
| 2   | F     | 502 | GOL  | O2-C2-C3-O3 |
| 2   | F     | 504 | GOL  | C1-C2-C3-O3 |
| 2   | G     | 502 | GOL  | O1-C1-C2-C3 |
| 2   | G     | 502 | GOL  | C1-C2-C3-O3 |
| 2   | G     | 504 | GOL  | O1-C1-C2-C3 |
| 2   | H     | 501 | GOL  | C1-C2-C3-O3 |
| 2   | H     | 502 | GOL  | O1-C1-C2-C3 |
| 2   | H     | 502 | GOL  | C1-C2-C3-O3 |
| 2   | H     | 503 | GOL  | O1-C1-C2-C3 |
| 4   | A     | 515 | CIT  | C1-C2-C3-C4 |
| 4   | B     | 520 | CIT  | C1-C2-C3-O7 |
| 4   | B     | 520 | CIT  | C1-C2-C3-C4 |
| 4   | B     | 520 | CIT  | C2-C3-C6-O5 |
| 4   | B     | 520 | CIT  | C2-C3-C6-O6 |
| 4   | B     | 520 | CIT  | O7-C3-C6-O5 |
| 4   | B     | 520 | CIT  | O7-C3-C6-O6 |
| 4   | C     | 519 | CIT  | C2-C3-C4-C5 |
| 4   | C     | 519 | CIT  | O7-C3-C4-C5 |
| 4   | E     | 517 | CIT  | O7-C3-C6-O5 |
| 4   | E     | 517 | CIT  | O7-C3-C6-O6 |
| 4   | E     | 517 | CIT  | C4-C3-C6-O5 |
| 4   | E     | 517 | CIT  | C4-C3-C6-O6 |
| 4   | G     | 513 | CIT  | C1-C2-C3-O7 |
| 4   | G     | 513 | CIT  | C1-C2-C3-C4 |
| 4   | A     | 515 | CIT  | C1-C2-C3-O7 |
| 4   | A     | 515 | CIT  | C1-C2-C3-C6 |
| 4   | B     | 520 | CIT  | C1-C2-C3-C6 |
| 4   | G     | 513 | CIT  | C1-C2-C3-C6 |
| 2   | C     | 503 | GOL  | O1-C1-C2-O2 |
| 2   | E     | 503 | GOL  | O2-C2-C3-O3 |
| 4   | C     | 519 | CIT  | C6-C3-C4-C5 |
| 2   | A     | 502 | GOL  | C1-C2-C3-O3 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | B     | 503 | GOL  | O1-C1-C2-C3 |
| 2   | B     | 504 | GOL  | C1-C2-C3-O3 |
| 2   | B     | 506 | GOL  | C1-C2-C3-O3 |
| 2   | B     | 509 | GOL  | C1-C2-C3-O3 |
| 2   | C     | 501 | GOL  | O1-C1-C2-C3 |
| 2   | D     | 503 | GOL  | C1-C2-C3-O3 |
| 2   | D     | 505 | GOL  | C1-C2-C3-O3 |
| 2   | E     | 502 | GOL  | O1-C1-C2-C3 |
| 2   | E     | 505 | GOL  | C1-C2-C3-O3 |
| 2   | E     | 506 | GOL  | O1-C1-C2-C3 |
| 2   | G     | 503 | GOL  | O1-C1-C2-C3 |
| 2   | A     | 501 | GOL  | O1-C1-C2-O2 |
| 2   | A     | 502 | GOL  | O2-C2-C3-O3 |
| 2   | D     | 505 | GOL  | O1-C1-C2-O2 |
| 2   | E     | 504 | GOL  | O2-C2-C3-O3 |
| 2   | E     | 505 | GOL  | O2-C2-C3-O3 |
| 2   | G     | 502 | GOL  | O1-C1-C2-O2 |
| 2   | G     | 502 | GOL  | O2-C2-C3-O3 |
| 2   | G     | 503 | GOL  | O1-C1-C2-O2 |
| 2   | H     | 501 | GOL  | O2-C2-C3-O3 |
| 2   | H     | 502 | GOL  | O2-C2-C3-O3 |
| 2   | H     | 503 | GOL  | O1-C1-C2-O2 |
| 2   | B     | 502 | GOL  | O1-C1-C2-O2 |
| 2   | B     | 504 | GOL  | O2-C2-C3-O3 |
| 2   | C     | 502 | GOL  | O2-C2-C3-O3 |
| 2   | D     | 503 | GOL  | O2-C2-C3-O3 |
| 2   | E     | 501 | GOL  | O2-C2-C3-O3 |
| 2   | E     | 506 | GOL  | O1-C1-C2-O2 |
| 2   | G     | 504 | GOL  | O1-C1-C2-O2 |
| 2   | H     | 502 | GOL  | O1-C1-C2-O2 |
| 4   | C     | 519 | CIT  | C1-C2-C3-O7 |
| 2   | A     | 503 | GOL  | O1-C1-C2-O2 |
| 2   | B     | 507 | GOL  | O1-C1-C2-O2 |
| 2   | D     | 505 | GOL  | O2-C2-C3-O3 |
| 2   | F     | 504 | GOL  | O1-C1-C2-O2 |
| 2   | F     | 504 | GOL  | O2-C2-C3-O3 |
| 4   | B     | 520 | CIT  | O7-C3-C4-C5 |
| 4   | C     | 519 | CIT  | C1-C2-C3-C4 |
| 2   | B     | 506 | GOL  | O2-C2-C3-O3 |
| 4   | E     | 517 | CIT  | C2-C3-C4-C5 |
| 4   | E     | 517 | CIT  | O1-C1-C2-C3 |
| 4   | E     | 517 | CIT  | O2-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | A     | 515 | CIT  | C4-C3-C6-O5 |
| 4   | G     | 513 | CIT  | C4-C3-C6-O5 |
| 2   | H     | 503 | GOL  | C1-C2-C3-O3 |
| 4   | C     | 519 | CIT  | C1-C2-C3-C6 |
| 2   | E     | 502 | GOL  | O1-C1-C2-O2 |
| 2   | H     | 503 | GOL  | O2-C2-C3-O3 |
| 4   | A     | 515 | CIT  | C2-C3-C4-C5 |
| 4   | A     | 515 | CIT  | O7-C3-C4-C5 |
| 2   | B     | 509 | GOL  | O2-C2-C3-O3 |
| 2   | C     | 503 | GOL  | O2-C2-C3-O3 |
| 4   | G     | 513 | CIT  | O7-C3-C4-C5 |
| 4   | B     | 520 | CIT  | O1-C1-C2-C3 |
| 4   | B     | 520 | CIT  | O2-C1-C2-C3 |
| 4   | G     | 513 | CIT  | O1-C1-C2-C3 |
| 4   | C     | 519 | CIT  | C3-C4-C5-O3 |
| 4   | C     | 519 | CIT  | C3-C4-C5-O4 |
| 4   | G     | 513 | CIT  | O2-C1-C2-C3 |

There are no ring outliers.

37 monomers are involved in 89 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | D     | 505 | GOL  | 4       | 0            |
| 3   | B     | 511 | SO4  | 1       | 0            |
| 2   | A     | 502 | GOL  | 2       | 0            |
| 2   | F     | 502 | GOL  | 5       | 0            |
| 4   | C     | 519 | CIT  | 4       | 0            |
| 3   | C     | 508 | SO4  | 1       | 0            |
| 2   | B     | 505 | GOL  | 1       | 0            |
| 3   | F     | 506 | SO4  | 1       | 0            |
| 2   | H     | 502 | GOL  | 2       | 0            |
| 2   | A     | 503 | GOL  | 1       | 0            |
| 2   | H     | 501 | GOL  | 1       | 0            |
| 2   | D     | 503 | GOL  | 2       | 0            |
| 2   | C     | 503 | GOL  | 3       | 0            |
| 3   | H     | 508 | SO4  | 1       | 0            |
| 3   | B     | 514 | SO4  | 1       | 0            |
| 2   | B     | 503 | GOL  | 3       | 0            |
| 4   | A     | 515 | CIT  | 6       | 0            |
| 2   | H     | 503 | GOL  | 1       | 0            |
| 2   | G     | 502 | GOL  | 1       | 0            |
| 2   | B     | 502 | GOL  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | C     | 504 | GOL  | 2       | 0            |
| 4   | E     | 517 | CIT  | 2       | 0            |
| 4   | G     | 513 | CIT  | 7       | 0            |
| 2   | B     | 504 | GOL  | 3       | 0            |
| 4   | B     | 520 | CIT  | 8       | 0            |
| 3   | G     | 510 | SO4  | 1       | 0            |
| 3   | A     | 510 | SO4  | 1       | 0            |
| 3   | D     | 512 | SO4  | 1       | 0            |
| 2   | C     | 505 | GOL  | 4       | 0            |
| 2   | E     | 505 | GOL  | 5       | 0            |
| 3   | H     | 509 | SO4  | 1       | 0            |
| 2   | D     | 502 | GOL  | 5       | 0            |
| 2   | F     | 504 | GOL  | 2       | 0            |
| 2   | E     | 504 | GOL  | 1       | 0            |
| 3   | B     | 513 | SO4  | 1       | 0            |
| 2   | A     | 501 | GOL  | 3       | 0            |
| 3   | H     | 505 | SO4  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| 1   | A     | 430/448 (95%)   | -0.80  | 2 (0%) 87 88  | 8, 13, 35, 96         | 4 (0%)  |
| 1   | B     | 430/448 (95%)   | -0.68  | 5 (1%) 76 78  | 9, 17, 36, 91         | 4 (0%)  |
| 1   | C     | 431/448 (96%)   | -0.58  | 8 (1%) 66 68  | 9, 18, 50, 107        | 2 (0%)  |
| 1   | D     | 435/448 (97%)   | -0.51  | 2 (0%) 87 88  | 10, 22, 45, 88        | 1 (0%)  |
| 1   | E     | 430/448 (95%)   | -0.43  | 4 (0%) 81 82  | 11, 23, 56, 114       | 3 (0%)  |
| 1   | F     | 430/448 (95%)   | -0.29  | 4 (0%) 81 82  | 16, 27, 53, 116       | 0       |
| 1   | G     | 430/448 (95%)   | 0.12   | 13 (3%) 52 54 | 11, 32, 61, 111       | 3 (0%)  |
| 1   | H     | 430/448 (95%)   | 0.38   | 10 (2%) 61 63 | 22, 37, 61, 115       | 0       |
| All | All   | 3446/3584 (96%) | -0.35  | 48 (1%) 73 75 | 8, 23, 53, 116        | 17 (0%) |

All (48) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 444 | VAL  | 8.0  |
| 1   | G     | 444 | VAL  | 7.9  |
| 1   | A     | 444 | VAL  | 7.6  |
| 1   | E     | 444 | VAL  | 7.4  |
| 1   | C     | 14  | ALA  | 7.3  |
| 1   | C     | 444 | VAL  | 7.1  |
| 1   | F     | 444 | VAL  | 6.0  |
| 1   | E     | 15  | SER  | 5.6  |
| 1   | B     | 15  | SER  | 5.3  |
| 1   | F     | 405 | MET  | 4.9  |
| 1   | C     | 405 | MET  | 4.8  |
| 1   | D     | 14  | ALA  | 4.7  |
| 1   | G     | 443 | ALA  | 4.5  |
| 1   | G     | 405 | MET  | 4.1  |
| 1   | A     | 15  | SER  | 3.6  |
| 1   | F     | 15  | SER  | 3.5  |

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*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 15  | SER  | 3.4  |
| 1   | H     | 15  | SER  | 3.4  |
| 1   | H     | 405 | MET  | 3.2  |
| 1   | G     | 391 | LYS  | 3.2  |
| 1   | G     | 421 | LEU  | 3.1  |
| 1   | C     | 15  | SER  | 3.1  |
| 1   | B     | 405 | MET  | 3.1  |
| 1   | H     | 424 | HIS  | 3.0  |
| 1   | B     | 444 | VAL  | 3.0  |
| 1   | E     | 405 | MET  | 3.0  |
| 1   | D     | 15  | SER  | 2.8  |
| 1   | G     | 442 | PRO  | 2.8  |
| 1   | F     | 423 | LYS  | 2.7  |
| 1   | C     | 443 | ALA  | 2.7  |
| 1   | G     | 423 | LYS  | 2.7  |
| 1   | G     | 424 | HIS  | 2.6  |
| 1   | H     | 16  | MET  | 2.5  |
| 1   | H     | 118 | ASN  | 2.5  |
| 1   | E     | 423 | LYS  | 2.5  |
| 1   | C     | 424 | HIS  | 2.5  |
| 1   | H     | 104 | LYS  | 2.4  |
| 1   | H     | 116 | ILE  | 2.4  |
| 1   | G     | 406 | GLU  | 2.4  |
| 1   | B     | 406 | GLU  | 2.2  |
| 1   | H     | 348 | GLU  | 2.2  |
| 1   | G     | 399 | LEU  | 2.2  |
| 1   | G     | 425 | GLN  | 2.2  |
| 1   | C     | 422 | VAL  | 2.1  |
| 1   | B     | 16  | MET  | 2.1  |
| 1   | C     | 391 | LYS  | 2.1  |
| 1   | G     | 370 | VAL  | 2.1  |
| 1   | H     | 429 | GLU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | SO4  | E     | 516 | 5/5   | 0.55 | 0.14 | 91,102,118,122             | 0     |
| 3   | SO4  | G     | 508 | 5/5   | 0.61 | 0.16 | 96,103,128,136             | 0     |
| 3   | SO4  | H     | 514 | 5/5   | 0.61 | 0.13 | 101,112,123,125            | 0     |
| 3   | SO4  | H     | 507 | 5/5   | 0.64 | 0.13 | 104,110,115,123            | 0     |
| 3   | SO4  | G     | 510 | 5/5   | 0.71 | 0.14 | 90,99,107,116              | 0     |
| 3   | SO4  | H     | 505 | 5/5   | 0.71 | 0.13 | 75,97,102,103              | 0     |
| 3   | SO4  | D     | 516 | 5/5   | 0.72 | 0.15 | 75,76,93,95                | 0     |
| 3   | SO4  | F     | 515 | 5/5   | 0.73 | 0.12 | 90,102,112,113             | 0     |
| 3   | SO4  | E     | 507 | 5/5   | 0.73 | 0.17 | 78,97,117,120              | 0     |
| 3   | SO4  | C     | 518 | 5/5   | 0.73 | 0.14 | 83,92,120,127              | 0     |
| 3   | SO4  | A     | 513 | 5/5   | 0.74 | 0.14 | 74,76,86,93                | 0     |
| 3   | SO4  | D     | 513 | 5/5   | 0.76 | 0.14 | 71,82,108,108              | 0     |
| 3   | SO4  | D     | 515 | 5/5   | 0.77 | 0.13 | 76,91,101,105              | 0     |
| 3   | SO4  | F     | 508 | 5/5   | 0.78 | 0.20 | 54,67,89,95                | 0     |
| 3   | SO4  | F     | 511 | 5/5   | 0.78 | 0.19 | 54,74,86,91                | 0     |
| 3   | SO4  | E     | 510 | 5/5   | 0.78 | 0.15 | 84,91,94,107               | 0     |
| 3   | SO4  | H     | 512 | 5/5   | 0.78 | 0.12 | 81,83,96,96                | 0     |
| 3   | SO4  | C     | 507 | 5/5   | 0.78 | 0.17 | 72,81,101,102              | 0     |
| 3   | SO4  | D     | 511 | 5/5   | 0.79 | 0.17 | 49,62,78,78                | 0     |
| 3   | SO4  | H     | 509 | 5/5   | 0.80 | 0.18 | 43,46,66,74                | 5     |
| 3   | SO4  | H     | 510 | 5/5   | 0.80 | 0.17 | 78,82,95,96                | 0     |
| 2   | GOL  | G     | 502 | 6/6   | 0.80 | 0.18 | 56,68,77,82                | 0     |
| 3   | SO4  | H     | 508 | 5/5   | 0.80 | 0.13 | 69,71,88,94                | 0     |
| 3   | SO4  | F     | 506 | 5/5   | 0.81 | 0.13 | 86,87,108,111              | 0     |
| 3   | SO4  | C     | 506 | 5/5   | 0.81 | 0.10 | 76,77,94,94                | 0     |
| 3   | SO4  | G     | 512 | 5/5   | 0.81 | 0.14 | 80,91,99,104               | 0     |
| 3   | SO4  | D     | 507 | 5/5   | 0.81 | 0.13 | 78,96,97,105               | 0     |
| 3   | SO4  | B     | 518 | 5/5   | 0.81 | 0.13 | 102,103,116,122            | 0     |
| 3   | SO4  | E     | 509 | 5/5   | 0.82 | 0.22 | 46,60,77,91                | 5     |
| 2   | GOL  | C     | 505 | 6/6   | 0.82 | 0.20 | 21,27,34,43                | 0     |
| 3   | SO4  | E     | 513 | 5/5   | 0.82 | 0.14 | 75,76,88,92                | 0     |
| 2   | GOL  | B     | 505 | 6/6   | 0.82 | 0.20 | 43,54,65,67                | 0     |
| 3   | SO4  | D     | 514 | 5/5   | 0.82 | 0.14 | 62,91,99,102               | 0     |
| 3   | SO4  | G     | 511 | 5/5   | 0.82 | 0.12 | 82,101,104,113             | 0     |
| 3   | SO4  | F     | 507 | 5/5   | 0.82 | 0.15 | 71,88,91,99                | 5     |
| 2   | GOL  | D     | 503 | 6/6   | 0.83 | 0.16 | 43,49,54,62                | 0     |
| 3   | SO4  | B     | 519 | 5/5   | 0.83 | 0.14 | 56,73,88,106               | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | GOL  | G     | 504 | 6/6   | 0.83 | 0.20 | 52,58,67,71                 | 0     |
| 2   | GOL  | F     | 503 | 6/6   | 0.83 | 0.18 | 59,67,71,72                 | 0     |
| 3   | SO4  | H     | 504 | 5/5   | 0.84 | 0.11 | 73,79,92,107                | 0     |
| 3   | SO4  | B     | 513 | 5/5   | 0.84 | 0.14 | 79,94,112,117               | 0     |
| 3   | SO4  | D     | 510 | 5/5   | 0.84 | 0.14 | 66,78,95,97                 | 0     |
| 3   | SO4  | G     | 505 | 5/5   | 0.84 | 0.19 | 71,98,113,117               | 0     |
| 3   | SO4  | F     | 505 | 5/5   | 0.84 | 0.12 | 72,75,85,96                 | 0     |
| 2   | GOL  | B     | 508 | 6/6   | 0.84 | 0.17 | 63,65,68,70                 | 0     |
| 3   | SO4  | C     | 509 | 5/5   | 0.84 | 0.12 | 104,108,116,118             | 0     |
| 2   | GOL  | E     | 506 | 6/6   | 0.84 | 0.18 | 58,72,74,75                 | 0     |
| 3   | SO4  | A     | 514 | 5/5   | 0.85 | 0.15 | 48,62,67,83                 | 0     |
| 3   | SO4  | C     | 508 | 5/5   | 0.85 | 0.12 | 74,75,79,82                 | 0     |
| 3   | SO4  | F     | 510 | 5/5   | 0.85 | 0.19 | 62,74,79,88                 | 0     |
| 3   | SO4  | C     | 514 | 5/5   | 0.86 | 0.12 | 65,79,88,91                 | 0     |
| 3   | SO4  | E     | 515 | 5/5   | 0.86 | 0.18 | 52,70,82,84                 | 0     |
| 3   | SO4  | F     | 513 | 5/5   | 0.86 | 0.19 | 56,60,79,90                 | 0     |
| 3   | SO4  | H     | 506 | 5/5   | 0.86 | 0.16 | 59,63,68,77                 | 0     |
| 3   | SO4  | F     | 514 | 5/5   | 0.86 | 0.21 | 59,70,77,89                 | 0     |
| 2   | GOL  | B     | 503 | 6/6   | 0.86 | 0.15 | 29,31,43,48                 | 0     |
| 2   | GOL  | H     | 502 | 6/6   | 0.86 | 0.20 | 52,62,74,81                 | 0     |
| 3   | SO4  | B     | 516 | 5/5   | 0.86 | 0.19 | 51,67,68,72                 | 0     |
| 3   | SO4  | H     | 511 | 5/5   | 0.86 | 0.11 | 70,92,95,103                | 0     |
| 3   | SO4  | B     | 517 | 5/5   | 0.86 | 0.17 | 39,41,60,63                 | 0     |
| 2   | GOL  | B     | 507 | 6/6   | 0.86 | 0.17 | 54,64,72,76                 | 0     |
| 4   | CIT  | E     | 517 | 13/13 | 0.86 | 0.16 | 35,64,73,87                 | 0     |
| 2   | GOL  | D     | 505 | 6/6   | 0.87 | 0.16 | 32,36,39,50                 | 0     |
| 2   | GOL  | C     | 503 | 6/6   | 0.87 | 0.19 | 18,24,28,33                 | 6     |
| 2   | GOL  | H     | 503 | 6/6   | 0.87 | 0.15 | 38,42,49,53                 | 0     |
| 2   | GOL  | F     | 502 | 6/6   | 0.87 | 0.14 | 40,47,49,56                 | 0     |
| 3   | SO4  | G     | 506 | 5/5   | 0.87 | 0.15 | 45,80,86,98                 | 0     |
| 2   | GOL  | A     | 502 | 6/6   | 0.87 | 0.17 | 54,66,71,72                 | 0     |
| 3   | SO4  | B     | 511 | 5/5   | 0.87 | 0.17 | 45,58,66,67                 | 5     |
| 2   | GOL  | B     | 506 | 6/6   | 0.87 | 0.16 | 56,67,71,71                 | 0     |
| 3   | SO4  | E     | 514 | 5/5   | 0.87 | 0.19 | 41,52,66,79                 | 0     |
| 3   | SO4  | F     | 512 | 5/5   | 0.87 | 0.15 | 64,69,90,96                 | 0     |
| 2   | GOL  | C     | 504 | 6/6   | 0.88 | 0.13 | 36,38,44,56                 | 0     |
| 3   | SO4  | D     | 508 | 5/5   | 0.88 | 0.22 | 48,59,67,81                 | 0     |
| 2   | GOL  | F     | 504 | 6/6   | 0.88 | 0.16 | 50,57,62,66                 | 0     |
| 3   | SO4  | F     | 509 | 5/5   | 0.88 | 0.17 | 56,75,85,85                 | 0     |
| 2   | GOL  | B     | 509 | 6/6   | 0.88 | 0.15 | 50,58,65,66                 | 0     |
| 3   | SO4  | B     | 512 | 5/5   | 0.88 | 0.21 | 44,48,51,65                 | 5     |
| 3   | SO4  | C     | 515 | 5/5   | 0.88 | 0.15 | 49,58,72,74                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | SO4  | A     | 507 | 5/5   | 0.88 | 0.15 | 39,52,60,70                 | 5     |
| 4   | CIT  | C     | 519 | 13/13 | 0.88 | 0.13 | 26,45,62,62                 | 0     |
| 3   | SO4  | D     | 506 | 5/5   | 0.88 | 0.11 | 72,74,85,96                 | 0     |
| 3   | SO4  | D     | 509 | 5/5   | 0.89 | 0.17 | 45,56,68,71                 | 0     |
| 3   | SO4  | E     | 512 | 5/5   | 0.89 | 0.15 | 50,66,84,88                 | 0     |
| 3   | SO4  | B     | 514 | 5/5   | 0.89 | 0.20 | 61,66,79,82                 | 5     |
| 3   | SO4  | C     | 517 | 5/5   | 0.89 | 0.20 | 56,64,78,90                 | 0     |
| 3   | SO4  | D     | 512 | 5/5   | 0.89 | 0.17 | 60,73,82,87                 | 0     |
| 3   | SO4  | E     | 508 | 5/5   | 0.89 | 0.14 | 39,43,56,60                 | 5     |
| 3   | SO4  | A     | 512 | 5/5   | 0.89 | 0.19 | 41,41,58,59                 | 0     |
| 2   | GOL  | E     | 505 | 6/6   | 0.90 | 0.20 | 32,45,48,49                 | 0     |
| 3   | SO4  | A     | 506 | 5/5   | 0.90 | 0.17 | 66,66,86,88                 | 0     |
| 4   | CIT  | B     | 520 | 13/13 | 0.90 | 0.12 | 31,46,59,64                 | 0     |
| 2   | GOL  | E     | 503 | 6/6   | 0.90 | 0.14 | 50,57,62,65                 | 0     |
| 3   | SO4  | A     | 508 | 5/5   | 0.90 | 0.24 | 62,73,75,86                 | 0     |
| 3   | SO4  | C     | 511 | 5/5   | 0.91 | 0.13 | 67,67,82,88                 | 0     |
| 2   | GOL  | H     | 501 | 6/6   | 0.91 | 0.12 | 32,43,45,48                 | 0     |
| 3   | SO4  | G     | 507 | 5/5   | 0.91 | 0.12 | 40,46,60,61                 | 5     |
| 3   | SO4  | C     | 510 | 5/5   | 0.91 | 0.20 | 51,60,76,78                 | 0     |
| 3   | SO4  | A     | 509 | 5/5   | 0.92 | 0.15 | 55,62,69,75                 | 0     |
| 3   | SO4  | A     | 511 | 5/5   | 0.92 | 0.18 | 39,53,58,69                 | 0     |
| 2   | GOL  | E     | 504 | 6/6   | 0.92 | 0.17 | 37,56,61,63                 | 0     |
| 2   | GOL  | G     | 503 | 6/6   | 0.92 | 0.11 | 29,36,38,44                 | 0     |
| 3   | SO4  | C     | 513 | 5/5   | 0.92 | 0.16 | 43,45,49,62                 | 0     |
| 2   | GOL  | A     | 504 | 6/6   | 0.92 | 0.12 | 38,45,53,54                 | 0     |
| 4   | CIT  | G     | 513 | 13/13 | 0.92 | 0.11 | 35,44,66,66                 | 0     |
| 2   | GOL  | G     | 501 | 6/6   | 0.93 | 0.11 | 40,49,64,65                 | 0     |
| 4   | CIT  | A     | 515 | 13/13 | 0.93 | 0.12 | 15,29,39,49                 | 13    |
| 2   | GOL  | D     | 504 | 6/6   | 0.93 | 0.10 | 31,37,44,54                 | 0     |
| 2   | GOL  | D     | 502 | 6/6   | 0.93 | 0.10 | 31,35,39,41                 | 0     |
| 3   | SO4  | B     | 510 | 5/5   | 0.93 | 0.16 | 68,70,76,86                 | 0     |
| 2   | GOL  | C     | 502 | 6/6   | 0.93 | 0.11 | 31,38,49,63                 | 0     |
| 2   | GOL  | B     | 502 | 6/6   | 0.94 | 0.09 | 32,37,45,57                 | 0     |
| 2   | GOL  | E     | 501 | 6/6   | 0.94 | 0.10 | 35,49,58,64                 | 0     |
| 3   | SO4  | A     | 505 | 5/5   | 0.94 | 0.14 | 32,35,47,64                 | 0     |
| 2   | GOL  | A     | 501 | 6/6   | 0.94 | 0.10 | 28,38,48,60                 | 0     |
| 3   | SO4  | C     | 516 | 5/5   | 0.94 | 0.15 | 40,58,64,72                 | 0     |
| 2   | GOL  | F     | 501 | 6/6   | 0.94 | 0.09 | 25,32,35,37                 | 0     |
| 3   | SO4  | D     | 517 | 5/5   | 0.94 | 0.12 | 34,35,49,51                 | 5     |
| 2   | GOL  | B     | 504 | 6/6   | 0.95 | 0.10 | 30,35,38,40                 | 0     |
| 2   | GOL  | D     | 501 | 6/6   | 0.96 | 0.07 | 18,22,23,24                 | 0     |
| 3   | SO4  | E     | 511 | 5/5   | 0.96 | 0.13 | 39,41,44,55                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | GOL  | A     | 503 | 6/6   | 0.96 | 0.08 | 14,18,19,24                 | 0     |
| 2   | GOL  | C     | 501 | 6/6   | 0.96 | 0.05 | 18,20,21,22                 | 0     |
| 2   | GOL  | E     | 502 | 6/6   | 0.96 | 0.07 | 22,26,27,32                 | 0     |
| 3   | SO4  | C     | 512 | 5/5   | 0.97 | 0.12 | 40,46,54,54                 | 0     |
| 2   | GOL  | B     | 501 | 6/6   | 0.97 | 0.08 | 18,25,27,34                 | 0     |
| 3   | SO4  | H     | 513 | 5/5   | 0.97 | 0.11 | 53,53,57,60                 | 0     |
| 3   | SO4  | B     | 515 | 5/5   | 0.98 | 0.09 | 23,35,38,39                 | 0     |
| 3   | SO4  | G     | 509 | 5/5   | 0.99 | 0.04 | 24,25,28,29                 | 0     |
| 3   | SO4  | A     | 510 | 5/5   | 0.99 | 0.05 | 23,24,26,37                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.