



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:34 PM UTC

PDB ID : 4NZF / pdb\_00004nzf  
Title : Crystal structure of Abp-D197A (a GH27-b-L-arabinopyranosidase from *Geobacillus stearothermophilus*), in complex with arabinose  
Authors : Lansky, S.; Solomon, H.V.; Salama, R.; Belrhali, H.; Shoham, Y.; Shoham, G.  
Deposited on : 2013-12-12  
Resolution : 2.19 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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>.

---

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                                                             |

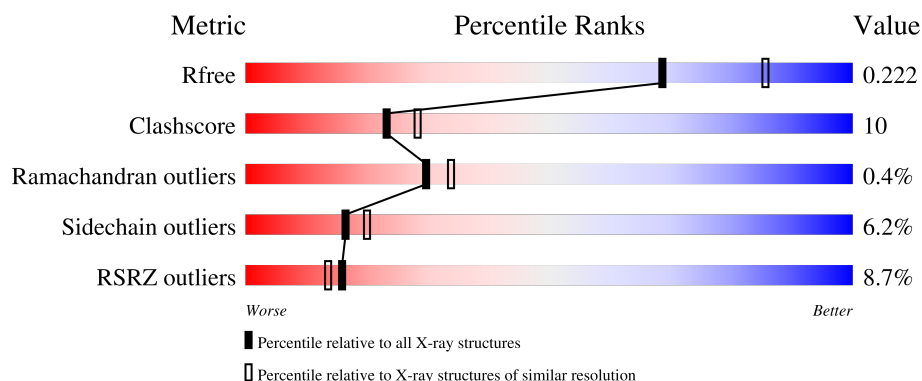
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 6164 (2.20-2.20)                                      |
| Clashscore            | 190562                      | 6851 (2.20-2.20)                                      |
| Ramachandran outliers | 187476                      | 6768 (2.20-2.20)                                      |
| Sidechain outliers    | 187428                      | 6769 (2.20-2.20)                                      |
| RSRZ outliers         | 180081                      | 6166 (2.20-2.20)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>0%</div> <div>82% 12% . .</div> </div> |
| 1   | B     | 448    | <div> <div>0%</div> <div>81% 12% . .</div> </div> |
| 1   | C     | 448    | <div> <div>2%</div> <div>81% 14% . .</div> </div> |
| 1   | D     | 448    | <div> <div>0%</div> <div>78% 17% . .</div> </div> |
| 1   | E     | 448    | <div> <div>3%</div> <div>83% 12% . .</div> </div> |

*Continued on next page...*

*Continued from previous page...*

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

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | GOL  | A     | 501 | -         | -        | X       | -                |
| 2   | GOL  | D     | 503 | -         | -        | X       | -                |
| 2   | GOL  | H     | 502 | -         | -        | X       | -                |
| 5   | CIT  | A     | 515 | -         | X        | X       | -                |
| 5   | CIT  | B     | 519 | -         | X        | X       | -                |
| 5   | CIT  | C     | 519 | -         | -        | X       | -                |
| 5   | CIT  | D     | 515 | -         | -        | X       | -                |
| 5   | CIT  | E     | 517 | -         | -        | X       | -                |

## 2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Abp, a GH27 beta-L-arabinopyranosidase.

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

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



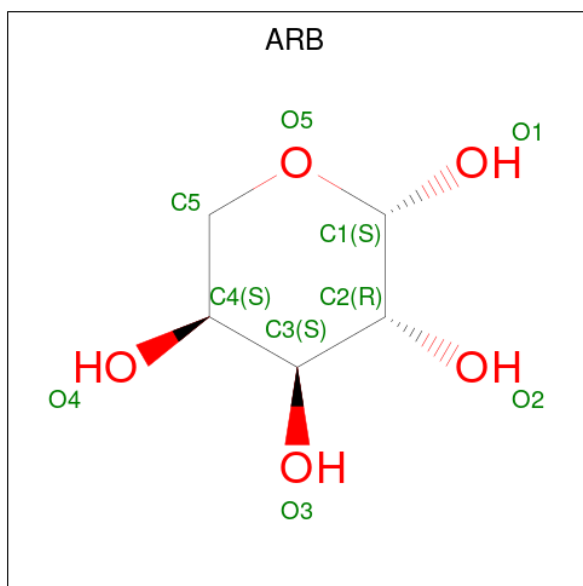
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 2   | B     | 1        | Total | C | O | 0    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

*Continued on next page...*

Continued from previous page...

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

- Molecule 3 is beta-L-arabinopyranose (CCD ID: ARB) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



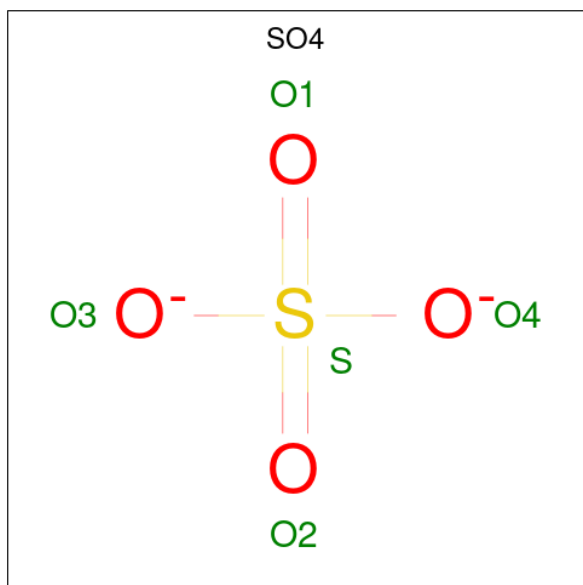
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 5 | 5 |         |         |
| 3   | B     | 1        | Total | C | O | 0    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

Continued on next page...

Continued from previous page...

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

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



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

Continued on next page...

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

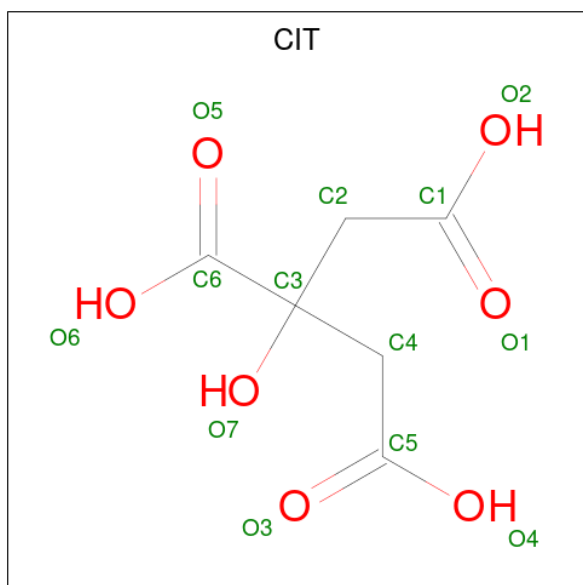
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | E     | 1        | Total | O | S | 0    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

*Continued on next page...*

Continued from previous page...

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

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula:  $C_6H_8O_7$ ).



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

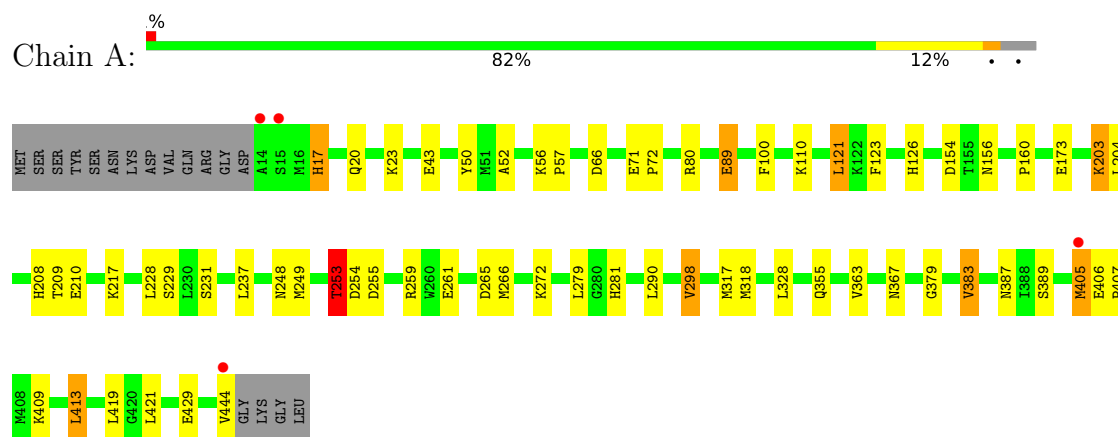
- Molecule 6 is water.

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

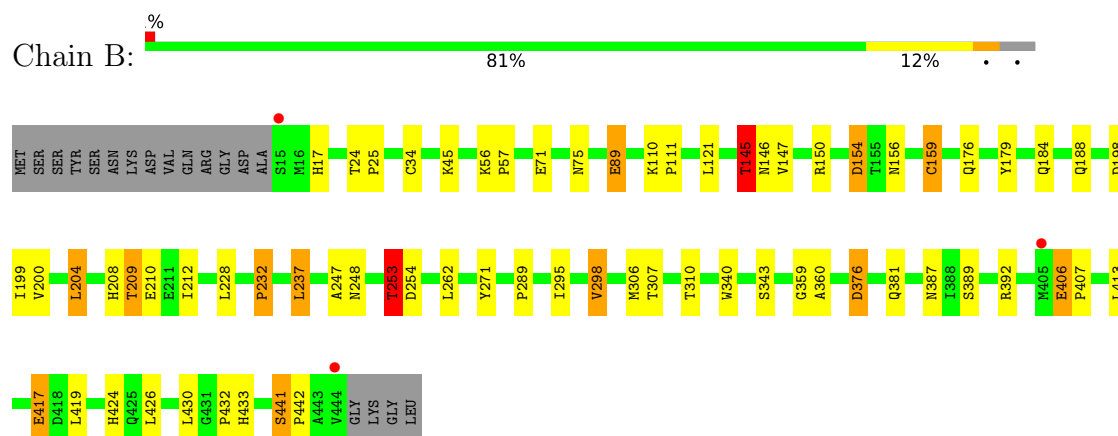
### 3 Residue-property plots [i](#)

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.

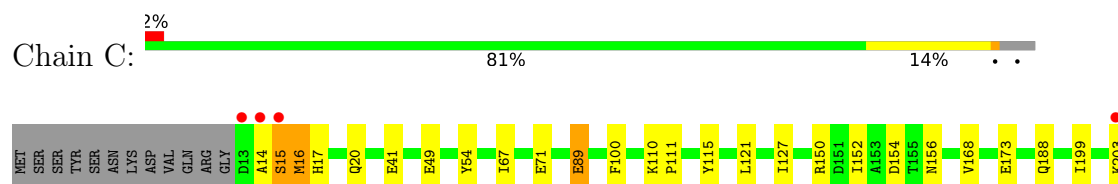
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

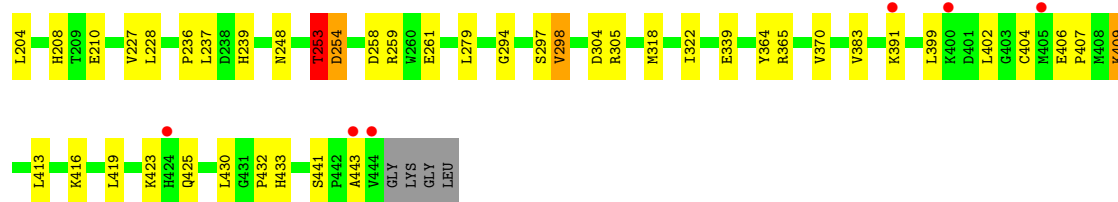


- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



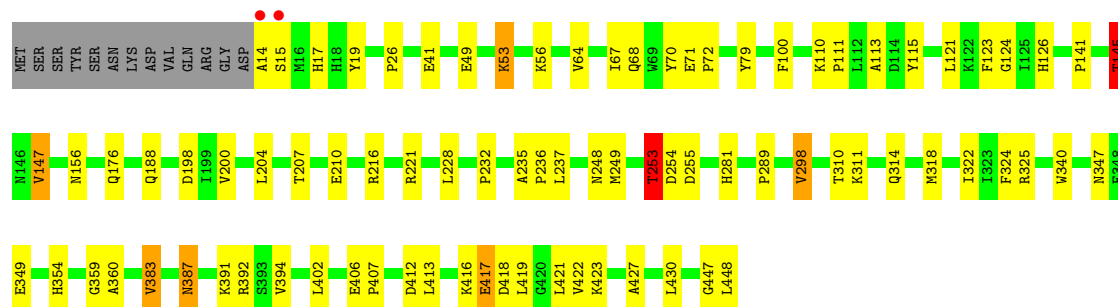
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase





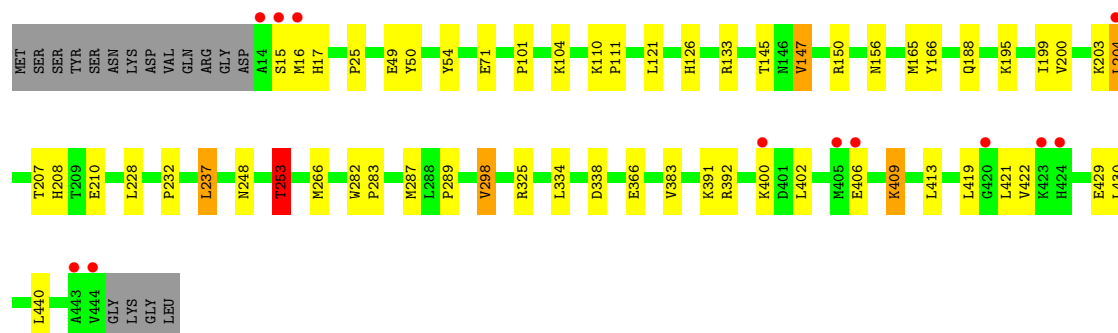
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

Chain D: 78% 17% ..



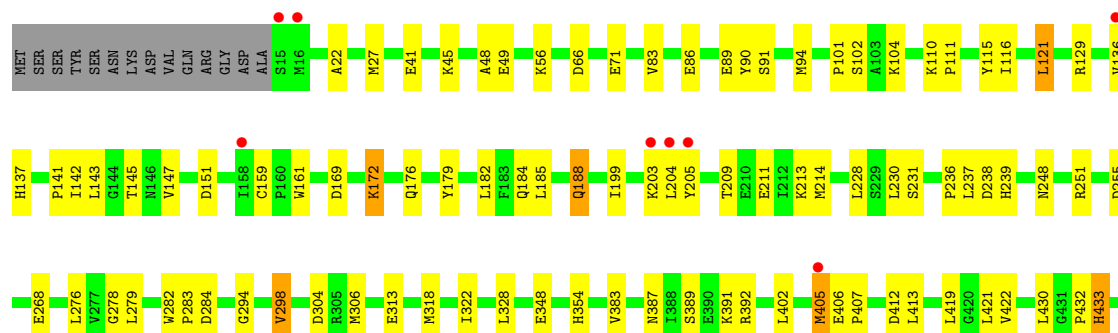
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

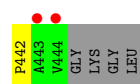
Chain E: 3% 83% 12% ..



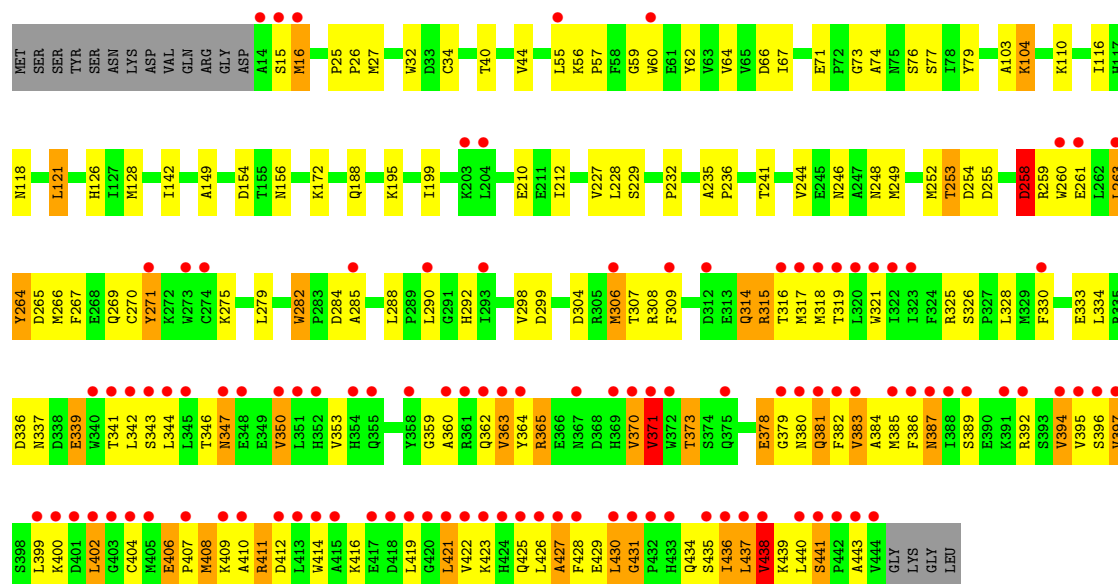
- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase

Chain F: 2% 75% 20% ..

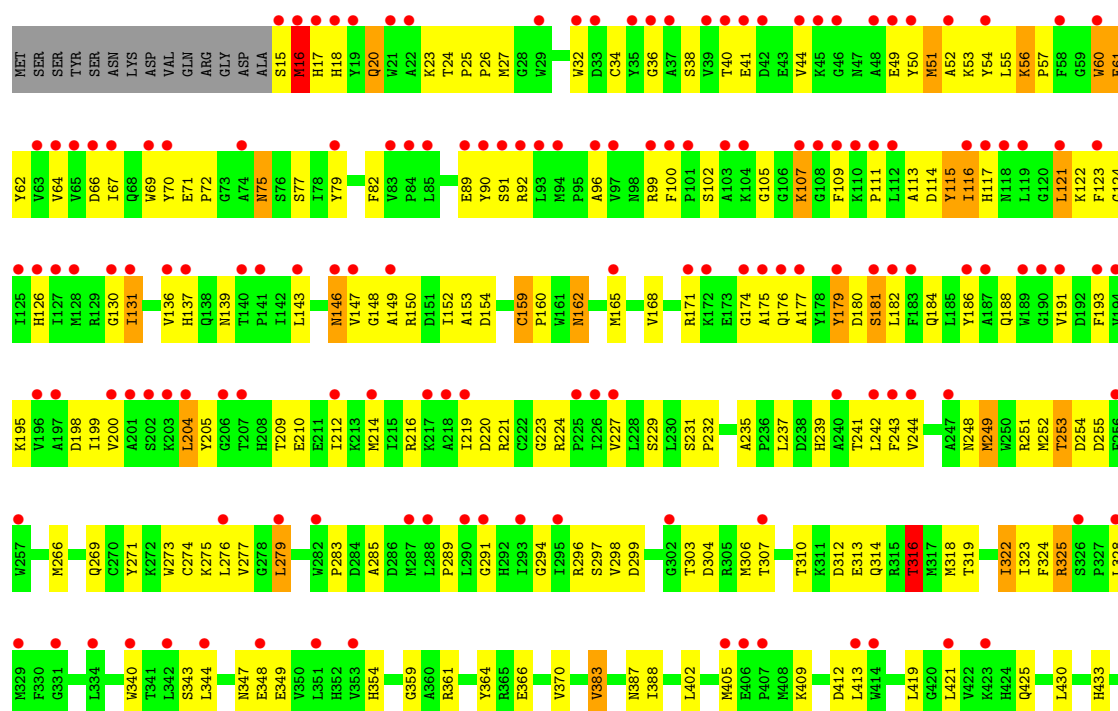




- Molecule 1: Abp, a GH27 beta-L-arabinopyranosidase



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



|      |     |     |     |
|------|-----|-----|-----|
| S441 |     |     |     |
| F442 |     |     |     |
| A443 |     |     |     |
| V444 |     |     |     |
| GLY  | LYS | GLY | LEU |



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 107.60Å 201.50Å 286.91Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 34.71 – 2.19<br>34.71 – 2.19                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 89.0 (34.71-2.19)<br>89.0 (34.71-2.19)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.22 (at 2.20Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.7.0029                                             | Depositor        |
| R, $R_{free}$                                                           | 0.168 , 0.219<br>0.176 , 0.222                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 14318 reflections (4.51%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 24.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.800                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 48.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 31507                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 35.0                                                        | wwPDB-VP         |

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

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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     | 1.45         | 11/3600 (0.3%)  | 1.20        | 11/4887 (0.2%)  |
| 1   | B     | 1.33         | 9/3587 (0.3%)   | 1.18        | 14/4869 (0.3%)  |
| 1   | C     | 1.22         | 6/3600 (0.2%)   | 1.12        | 10/4887 (0.2%)  |
| 1   | D     | 1.34         | 10/3608 (0.3%)  | 1.16        | 13/4895 (0.3%)  |
| 1   | E     | 1.15         | 2/3582 (0.1%)   | 1.11        | 5/4863 (0.1%)   |
| 1   | F     | 1.13         | 2/3569 (0.1%)   | 1.14        | 8/4845 (0.2%)   |
| 1   | G     | 1.31         | 13/3608 (0.4%)  | 1.30        | 17/4898 (0.3%)  |
| 1   | H     | 1.16         | 5/3594 (0.1%)   | 1.23        | 18/4877 (0.4%)  |
| All | All   | 1.27         | 58/28748 (0.2%) | 1.18        | 96/39021 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | E     | 0                   | 1                   |

All (58) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 253 | THR  | CB-CG2 | -7.08 | 1.29        | 1.52     |
| 1   | A     | 328 | LEU  | N-CA   | -6.88 | 1.38        | 1.46     |
| 1   | A     | 52  | ALA  | C-O    | -6.72 | 1.16        | 1.24     |
| 1   | A     | 231 | SER  | N-CA   | 6.05  | 1.51        | 1.46     |
| 1   | A     | 160 | PRO  | C-O    | -6.03 | 1.16        | 1.24     |
| 1   | D     | 383 | VAL  | N-CA   | -6.01 | 1.39        | 1.46     |
| 1   | G     | 370 | VAL  | C-O    | 5.96  | 1.30        | 1.24     |
| 1   | G     | 314 | GLN  | C-O    | 5.93  | 1.30        | 1.24     |
| 1   | A     | 123 | PHE  | CA-C   | -5.92 | 1.45        | 1.52     |
| 1   | B     | 237 | LEU  | C-O    | -5.92 | 1.16        | 1.24     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 53  | LYS  | N-CA  | -5.92 | 1.38        | 1.46     |
| 1   | B     | 376 | ASP  | C-O   | -5.84 | 1.15        | 1.23     |
| 1   | B     | 271 | TYR  | N-CA  | 5.74  | 1.53        | 1.46     |
| 1   | G     | 328 | LEU  | CA-C  | -5.71 | 1.46        | 1.53     |
| 1   | C     | 150 | ARG  | N-CA  | -5.69 | 1.38        | 1.46     |
| 1   | G     | 128 | MET  | C-O   | -5.63 | 1.17        | 1.23     |
| 1   | H     | 299 | ASP  | CA-C  | 5.60  | 1.61        | 1.53     |
| 1   | B     | 262 | LEU  | C-O   | -5.60 | 1.16        | 1.24     |
| 1   | G     | 438 | VAL  | CA-CB | 5.59  | 1.61        | 1.54     |
| 1   | A     | 43  | GLU  | C-O   | -5.56 | 1.17        | 1.24     |
| 1   | G     | 431 | GLY  | C-N   | 5.49  | 1.40        | 1.33     |
| 1   | E     | 150 | ARG  | C-O   | -5.48 | 1.17        | 1.24     |
| 1   | F     | 22  | ALA  | C-O   | 5.47  | 1.30        | 1.24     |
| 1   | G     | 437 | LEU  | C-O   | 5.46  | 1.30        | 1.24     |
| 1   | H     | 285 | ALA  | CA-C  | -5.45 | 1.44        | 1.52     |
| 1   | F     | 48  | ALA  | CA-C  | 5.44  | 1.59        | 1.52     |
| 1   | A     | 17  | HIS  | CA-C  | 5.43  | 1.60        | 1.52     |
| 1   | A     | 318 | MET  | C-O   | -5.41 | 1.17        | 1.24     |
| 1   | G     | 261 | GLU  | C-O   | 5.37  | 1.30        | 1.24     |
| 1   | H     | 383 | VAL  | CA-C  | -5.33 | 1.46        | 1.52     |
| 1   | C     | 168 | VAL  | N-CA  | -5.33 | 1.39        | 1.46     |
| 1   | B     | 179 | TYR  | C-O   | -5.32 | 1.18        | 1.24     |
| 1   | G     | 261 | GLU  | CA-C  | 5.28  | 1.59        | 1.52     |
| 1   | G     | 264 | TYR  | C-O   | 5.27  | 1.30        | 1.24     |
| 1   | A     | 80  | ARG  | C-O   | -5.27 | 1.17        | 1.24     |
| 1   | C     | 152 | ILE  | C-O   | -5.25 | 1.18        | 1.24     |
| 1   | C     | 127 | ILE  | C-O   | 5.23  | 1.29        | 1.24     |
| 1   | B     | 75  | ASN  | C-O   | -5.23 | 1.20        | 1.23     |
| 1   | G     | 271 | TYR  | CA-C  | 5.21  | 1.59        | 1.52     |
| 1   | B     | 426 | LEU  | CA-C  | -5.20 | 1.46        | 1.52     |
| 1   | A     | 355 | GLN  | CA-C  | 5.20  | 1.59        | 1.52     |
| 1   | H     | 61  | GLU  | CA-C  | 5.17  | 1.57        | 1.52     |
| 1   | B     | 289 | PRO  | CA-CB | -5.16 | 1.48        | 1.53     |
| 1   | G     | 427 | ALA  | C-O   | 5.16  | 1.29        | 1.23     |
| 1   | D     | 141 | PRO  | N-CA  | -5.15 | 1.41        | 1.47     |
| 1   | B     | 25  | PRO  | C-O   | -5.14 | 1.18        | 1.24     |
| 1   | D     | 418 | ASP  | CA-C  | -5.13 | 1.46        | 1.52     |
| 1   | C     | 227 | VAL  | CA-C  | 5.13  | 1.58        | 1.52     |
| 1   | D     | 427 | ALA  | C-O   | -5.11 | 1.17        | 1.23     |
| 1   | D     | 64  | VAL  | C-O   | 5.10  | 1.29        | 1.24     |
| 1   | E     | 25  | PRO  | CA-C  | 5.09  | 1.56        | 1.52     |
| 1   | G     | 110 | LYS  | N-CA  | -5.07 | 1.41        | 1.46     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 289 | PRO  | CA-C  | -5.06 | 1.48        | 1.52     |
| 1   | D     | 113 | ALA  | N-CA  | -5.04 | 1.40        | 1.46     |
| 1   | D     | 68  | GLN  | N-CA  | 5.04  | 1.52        | 1.46     |
| 1   | D     | 26  | PRO  | CA-C  | -5.03 | 1.46        | 1.52     |
| 1   | C     | 304 | ASP  | C-O   | -5.02 | 1.17        | 1.23     |
| 1   | H     | 387 | ASN  | N-CA  | -5.00 | 1.40        | 1.46     |

All (96) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 15  | SER  | N-CA-C  | 9.97  | 124.51      | 111.75   |
| 1   | G     | 315 | ARG  | N-CA-C  | -9.25 | 101.18      | 111.07   |
| 1   | G     | 32  | TRP  | N-CA-C  | 7.92  | 119.69      | 111.14   |
| 1   | B     | 24  | THR  | CA-C-N  | -7.51 | 112.64      | 120.38   |
| 1   | B     | 24  | THR  | C-N-CA  | -7.51 | 112.64      | 120.38   |
| 1   | A     | 100 | PHE  | CA-C-N  | -7.21 | 112.28      | 119.56   |
| 1   | A     | 100 | PHE  | C-N-CA  | -7.21 | 112.28      | 119.56   |
| 1   | H     | 131 | ILE  | CA-C-N  | -7.15 | 112.63      | 119.85   |
| 1   | H     | 131 | ILE  | C-N-CA  | -7.15 | 112.63      | 119.85   |
| 1   | C     | 298 | VAL  | N-CA-CB | -7.09 | 99.53       | 111.23   |
| 1   | A     | 363 | VAL  | N-CA-C  | -7.03 | 104.00      | 110.82   |
| 1   | E     | 49  | GLU  | N-CA-C  | -6.89 | 103.83      | 111.82   |
| 1   | B     | 298 | VAL  | N-CA-CB | -6.86 | 103.24      | 112.16   |
| 1   | D     | 147 | VAL  | N-CA-C  | -6.85 | 99.92       | 109.45   |
| 1   | B     | 204 | LEU  | N-CA-C  | 6.63  | 119.84      | 111.69   |
| 1   | H     | 322 | ILE  | CB-CA-C | -6.55 | 103.31      | 111.70   |
| 1   | E     | 298 | VAL  | N-CA-CB | -6.52 | 103.69      | 112.16   |
| 1   | C     | 89  | GLU  | CB-CA-C | -6.50 | 98.31       | 110.01   |
| 1   | H     | 162 | ASN  | N-CA-C  | 6.44  | 118.95      | 108.26   |
| 1   | E     | 253 | THR  | N-CA-CB | -6.42 | 100.94      | 111.66   |
| 1   | F     | 231 | SER  | CB-CA-C | -6.42 | 102.93      | 110.76   |
| 1   | G     | 212 | ILE  | N-CA-C  | -6.39 | 104.29      | 110.42   |
| 1   | E     | 204 | LEU  | N-CA-C  | 6.38  | 118.31      | 111.36   |
| 1   | C     | 425 | GLN  | N-CA-C  | 6.33  | 118.69      | 109.07   |
| 1   | A     | 298 | VAL  | N-CA-CB | -6.26 | 100.90      | 111.23   |
| 1   | F     | 136 | VAL  | N-CA-C  | -6.26 | 105.63      | 111.45   |
| 1   | A     | 367 | ASN  | CB-CA-C | -6.15 | 102.72      | 111.95   |
| 1   | C     | 253 | THR  | N-CA-CB | -6.15 | 101.39      | 111.66   |
| 1   | D     | 216 | ARG  | N-CA-C  | -6.09 | 104.72      | 111.36   |
| 1   | H     | 316 | THR  | N-CA-C  | -5.96 | 104.86      | 111.36   |
| 1   | F     | 298 | VAL  | N-CA-CB | -5.95 | 104.43      | 112.16   |
| 1   | A     | 253 | THR  | N-CA-CB | -5.92 | 100.53      | 111.53   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 383 | VAL  | CB-CA-C  | 5.86  | 118.33      | 110.42   |
| 1   | A     | 413 | LEU  | N-CA-C   | 5.83  | 117.72      | 111.36   |
| 1   | H     | 139 | ASN  | N-CA-C   | 5.81  | 119.57      | 111.90   |
| 1   | B     | 295 | ILE  | N-CA-C   | -5.78 | 104.99      | 110.42   |
| 1   | F     | 318 | MET  | N-CA-C   | -5.73 | 105.12      | 111.36   |
| 1   | G     | 282 | TRP  | N-CA-C   | 5.72  | 119.81      | 108.59   |
| 1   | H     | 316 | THR  | N-CA-CB  | 5.70  | 118.59      | 110.16   |
| 1   | D     | 123 | PHE  | CA-C-N   | -5.68 | 118.26      | 122.18   |
| 1   | D     | 123 | PHE  | C-N-CA   | -5.68 | 118.26      | 122.18   |
| 1   | G     | 306 | MET  | N-CA-C   | -5.66 | 100.66      | 109.72   |
| 1   | B     | 34  | CYS  | N-CA-C   | -5.65 | 106.06      | 113.12   |
| 1   | H     | 54  | TYR  | N-CA-C   | 5.62  | 119.40      | 112.54   |
| 1   | B     | 253 | THR  | N-CA-CB  | -5.62 | 102.28      | 111.66   |
| 1   | A     | 50  | TYR  | N-CA-C   | -5.59 | 105.27      | 111.36   |
| 1   | H     | 56  | LYS  | CA-C-N   | -5.57 | 112.98      | 119.32   |
| 1   | H     | 56  | LYS  | C-N-CA   | -5.57 | 112.98      | 119.32   |
| 1   | F     | 179 | TYR  | N-CA-C   | -5.52 | 105.34      | 111.36   |
| 1   | F     | 159 | CYS  | N-CA-C   | -5.48 | 102.74      | 110.31   |
| 1   | B     | 441 | SER  | CA-C-N   | 5.45  | 125.76      | 119.93   |
| 1   | B     | 441 | SER  | C-N-CA   | 5.45  | 125.76      | 119.93   |
| 1   | H     | 285 | ALA  | N-CA-C   | -5.45 | 106.22      | 112.92   |
| 1   | B     | 212 | ILE  | N-CA-C   | -5.45 | 105.22      | 110.72   |
| 1   | D     | 56  | LYS  | CA-C-N   | -5.43 | 114.22      | 119.87   |
| 1   | D     | 56  | LYS  | C-N-CA   | -5.43 | 114.22      | 119.87   |
| 1   | D     | 253 | THR  | N-CA-CB  | -5.41 | 101.46      | 111.53   |
| 1   | G     | 411 | ARG  | CB-CG-CD | -5.41 | 98.85       | 111.30   |
| 1   | H     | 159 | CYS  | CA-C-N   | 5.40  | 125.22      | 119.28   |
| 1   | H     | 159 | CYS  | C-N-CA   | 5.40  | 125.22      | 119.28   |
| 1   | C     | 254 | ASP  | N-CA-C   | -5.39 | 103.78      | 110.41   |
| 1   | C     | 67  | ILE  | N-CA-C   | 5.35  | 117.33      | 109.63   |
| 1   | D     | 124 | GLY  | N-CA-C   | 5.34  | 120.54      | 111.19   |
| 1   | B     | 159 | CYS  | N-CA-C   | -5.34 | 101.31      | 109.64   |
| 1   | G     | 246 | ASN  | N-CA-C   | 5.34  | 120.44      | 113.88   |
| 1   | D     | 298 | VAL  | N-CA-CB  | -5.33 | 105.23      | 112.16   |
| 1   | G     | 373 | THR  | N-CA-C   | 5.33  | 118.14      | 109.24   |
| 1   | E     | 298 | VAL  | CB-CA-C  | 5.33  | 118.15      | 111.65   |
| 1   | H     | 179 | TYR  | N-CA-C   | -5.27 | 105.44      | 111.14   |
| 1   | D     | 394 | VAL  | CB-CA-C  | -5.27 | 104.38      | 110.91   |
| 1   | D     | 354 | HIS  | N-CA-C   | 5.24  | 116.68      | 111.07   |
| 1   | G     | 306 | MET  | CA-C-N   | -5.24 | 113.12      | 120.82   |
| 1   | G     | 306 | MET  | C-N-CA   | -5.24 | 113.12      | 120.82   |
| 1   | B     | 145 | THR  | CB-CA-C  | -5.22 | 99.25       | 111.09   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 1   | G     | 439    | LYS  | N-CA-C  | 5.21  | 117.20      | 108.23   |
| 1   | D     | 145    | THR  | CB-CA-C | -5.21 | 99.26       | 111.09   |
| 1   | G     | 64     | VAL  | N-CA-C  | 5.21  | 114.79      | 106.88   |
| 1   | G     | 326    | SER  | N-CA-C  | -5.20 | 102.65      | 110.24   |
| 1   | A     | 110    | LYS  | CA-C-N  | -5.18 | 113.20      | 118.85   |
| 1   | A     | 110    | LYS  | C-N-CA  | -5.18 | 113.20      | 118.85   |
| 1   | C     | 305    | ARG  | N-CA-C  | 5.16  | 116.36      | 108.42   |
| 1   | H     | 51     | MET  | N-CA-C  | -5.12 | 105.39      | 110.97   |
| 1   | G     | 371    | VAL  | N-CA-C  | 5.11  | 115.26      | 108.11   |
| 1   | G     | 383    | VAL  | CB-CA-C | 5.06  | 119.56      | 110.65   |
| 1   | F     | 83     | VAL  | CA-C-N  | -5.06 | 115.51      | 120.52   |
| 1   | F     | 83     | VAL  | C-N-CA  | -5.06 | 115.51      | 120.52   |
| 1   | G     | 67     | ILE  | N-CA-C  | 5.06  | 119.86      | 109.34   |
| 1   | C     | 339[A] | GLU  | N-CA-C  | -5.05 | 105.96      | 111.82   |
| 1   | C     | 339[B] | GLU  | N-CA-C  | -5.05 | 105.96      | 111.82   |
| 1   | B     | 154    | ASP  | CB-CA-C | -5.04 | 101.82      | 109.89   |
| 1   | G     | 438    | VAL  | N-CA-C  | 5.03  | 115.15      | 108.11   |
| 1   | H     | 77     | SER  | N-CA-C  | -5.03 | 107.00      | 113.23   |
| 1   | D     | 298    | VAL  | N-CA-C  | -5.02 | 107.81      | 112.43   |
| 1   | H     | 16     | MET  | CB-CA-C | 5.01  | 118.31      | 110.19   |
| 1   | H     | 204    | LEU  | N-CA-C  | 5.01  | 116.43      | 111.07   |
| 1   | B     | 209    | THR  | N-CA-CB | -5.01 | 102.75      | 110.01   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | E     | 165 | MET  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3489  | 0        | 3372     | 48      | 0            |
| 1   | B     | 3482  | 0        | 3360     | 43      | 0            |
| 1   | C     | 3492  | 0        | 3370     | 37      | 0            |
| 1   | D     | 3503  | 0        | 3395     | 52      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | E     | 3477  | 0        | 3356     | 35      | 0            |
| 1   | F     | 3467  | 0        | 3347     | 49      | 0            |
| 1   | G     | 3494  | 0        | 3376     | 136     | 0            |
| 1   | H     | 3483  | 0        | 3373     | 158     | 0            |
| 2   | A     | 6     | 0        | 8        | 8       | 0            |
| 2   | B     | 18    | 0        | 24       | 2       | 0            |
| 2   | C     | 30    | 0        | 40       | 2       | 0            |
| 2   | D     | 18    | 0        | 24       | 7       | 0            |
| 2   | E     | 24    | 0        | 32       | 3       | 0            |
| 2   | F     | 6     | 0        | 8        | 0       | 0            |
| 2   | G     | 6     | 0        | 8        | 1       | 0            |
| 2   | H     | 12    | 0        | 16       | 4       | 0            |
| 3   | A     | 10    | 0        | 10       | 0       | 0            |
| 3   | B     | 10    | 0        | 10       | 0       | 0            |
| 3   | C     | 10    | 0        | 10       | 0       | 0            |
| 3   | D     | 10    | 0        | 10       | 0       | 0            |
| 3   | E     | 10    | 0        | 10       | 0       | 0            |
| 3   | F     | 10    | 0        | 10       | 1       | 0            |
| 3   | G     | 10    | 0        | 10       | 3       | 0            |
| 3   | H     | 10    | 0        | 10       | 0       | 0            |
| 4   | A     | 60    | 0        | 0        | 1       | 0            |
| 4   | B     | 70    | 0        | 0        | 4       | 0            |
| 4   | C     | 60    | 0        | 0        | 4       | 0            |
| 4   | D     | 50    | 0        | 0        | 5       | 0            |
| 4   | E     | 55    | 0        | 0        | 2       | 0            |
| 4   | F     | 55    | 0        | 0        | 0       | 0            |
| 4   | G     | 35    | 0        | 0        | 0       | 0            |
| 4   | H     | 25    | 0        | 0        | 0       | 0            |
| 5   | A     | 13    | 0        | 5        | 6       | 0            |
| 5   | B     | 13    | 0        | 5        | 6       | 0            |
| 5   | C     | 13    | 0        | 5        | 9       | 0            |
| 5   | D     | 13    | 0        | 5        | 7       | 0            |
| 5   | E     | 13    | 0        | 5        | 9       | 0            |
| 5   | G     | 13    | 0        | 5        | 3       | 0            |
| 6   | A     | 540   | 0        | 0        | 21      | 1            |
| 6   | B     | 465   | 0        | 0        | 13      | 1            |
| 6   | C     | 421   | 0        | 0        | 10      | 0            |
| 6   | D     | 380   | 0        | 0        | 11      | 0            |
| 6   | E     | 388   | 0        | 0        | 8       | 0            |
| 6   | F     | 298   | 0        | 0        | 11      | 0            |
| 6   | G     | 264   | 0        | 0        | 36      | 0            |
| 6   | H     | 176   | 0        | 0        | 37      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 31507 | 0        | 27219    | 572     | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (572) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:G:347:ASN:HA     | 6:G:785:HOH:O    | 1.48                     | 1.10              |
| 1:A:17:HIS:CE1     | 6:A:1094:HOH:O   | 2.18                     | 0.96              |
| 1:G:363:VAL:HG13   | 1:G:371:VAL:HG23 | 1.47                     | 0.93              |
| 1:A:406:GLU:HB2    | 1:A:407:PRO:HD2  | 1.49                     | 0.92              |
| 1:G:188[B]:GLN:HG3 | 6:G:731:HOH:O    | 1.70                     | 0.90              |
| 1:G:346:THR:HG21   | 6:G:846:HOH:O    | 1.73                     | 0.87              |
| 1:H:324:PHE:O      | 6:H:761:HOH:O    | 1.93                     | 0.85              |
| 1:H:82:PHE:HA      | 6:H:658:HOH:O    | 1.76                     | 0.85              |
| 1:G:431:GLY:HA3    | 6:G:666:HOH:O    | 1.77                     | 0.84              |
| 1:B:228:LEU:H      | 1:B:248:ASN:HD22 | 1.22                     | 0.83              |
| 1:F:228:LEU:H      | 1:F:248:ASN:HD22 | 1.22                     | 0.83              |
| 1:G:292:HIS:ND1    | 1:G:336:ASP:OD2  | 2.10                     | 0.83              |
| 1:H:425[B]:GLN:NE2 | 6:H:766:HOH:O    | 2.08                     | 0.82              |
| 1:D:210:GLU:H      | 5:D:515:CIT:H22  | 1.44                     | 0.82              |
| 1:E:145:THR:HG23   | 6:E:841:HOH:O    | 1.81                     | 0.81              |
| 1:G:318:MET:HB3    | 6:G:835:HOH:O    | 1.80                     | 0.80              |
| 1:H:56:LYS:HB2     | 6:H:742:HOH:O    | 1.82                     | 0.80              |
| 1:A:228:LEU:H      | 1:A:248:ASN:HD22 | 1.31                     | 0.79              |
| 1:B:210:GLU:H      | 5:B:519:CIT:H41  | 1.47                     | 0.78              |
| 1:G:77:SER:OG      | 1:G:299:ASP:OD1  | 2.01                     | 0.77              |
| 1:A:154:ASP:HB2    | 6:A:744:HOH:O    | 1.85                     | 0.77              |
| 1:C:228:LEU:H      | 1:C:248:ASN:HD22 | 1.32                     | 0.77              |
| 1:E:208:HIS:HA     | 5:E:517:CIT:O5   | 1.85                     | 0.76              |
| 1:C:14:ALA:HB3     | 6:C:958:HOH:O    | 1.85                     | 0.76              |
| 1:A:89:GLU:H       | 1:A:89:GLU:CD    | 1.94                     | 0.75              |
| 1:D:417:GLU:CB     | 6:D:810:HOH:O    | 2.34                     | 0.75              |
| 1:H:340:TRP:O      | 1:H:343:SER:OG   | 2.04                     | 0.75              |
| 1:C:188[B]:GLN:CD  | 6:C:830:HOH:O    | 2.30                     | 0.75              |
| 1:H:70:TYR:CE2     | 6:H:649:HOH:O    | 2.40                     | 0.75              |
| 1:G:266:MET:HE3    | 1:G:285:ALA:HB1  | 1.69                     | 0.74              |
| 1:H:92:ARG:HD3     | 1:H:181:SER:OG   | 1.87                     | 0.73              |
| 1:E:228:LEU:H      | 1:E:248:ASN:HD22 | 1.34                     | 0.73              |
| 1:H:56:LYS:CB      | 6:H:742:HOH:O    | 2.35                     | 0.73              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:H:159:CYS:SG     | 1:H:198:ASP:OD1  | 2.45                     | 0.73              |
| 1:H:184:GLN:HA     | 6:H:646:HOH:O    | 1.89                     | 0.73              |
| 1:G:408:MET:HE2    | 1:G:441:SER:O    | 1.89                     | 0.72              |
| 1:H:223:GLY:N      | 6:H:760:HOH:O    | 2.17                     | 0.72              |
| 1:G:304:ASP:OD1    | 1:G:304:ASP:C    | 2.31                     | 0.72              |
| 1:D:17:HIS:CE1     | 6:D:782:HOH:O    | 2.41                     | 0.72              |
| 1:B:406:GLU:HB2    | 1:B:407:PRO:CD   | 2.20                     | 0.71              |
| 1:G:27:MET:HE2     | 1:G:59:GLY:C     | 2.15                     | 0.71              |
| 1:G:363:VAL:CG1    | 1:G:371:VAL:HG23 | 2.20                     | 0.71              |
| 1:A:406:GLU:HB2    | 1:A:407:PRO:CD   | 2.21                     | 0.70              |
| 1:H:318:MET:O      | 1:H:322:ILE:HG12 | 1.91                     | 0.70              |
| 1:C:253:THR:HG23   | 1:C:254:ASP:O    | 1.91                     | 0.70              |
| 1:D:448:LEU:C      | 6:D:824:HOH:O    | 2.34                     | 0.70              |
| 1:F:41:GLU:OE2     | 1:F:102:SER:OG   | 2.07                     | 0.70              |
| 1:H:114:ASP:HA     | 6:H:746:HOH:O    | 1.92                     | 0.69              |
| 1:G:342:LEU:HD12   | 1:G:342:LEU:O    | 1.93                     | 0.69              |
| 1:D:417:GLU:HB2    | 6:D:810:HOH:O    | 1.93                     | 0.68              |
| 1:B:210:GLU:HG2    | 5:B:519:CIT:H42  | 1.76                     | 0.68              |
| 1:G:378:GLU:N      | 1:G:378:GLU:OE1  | 2.27                     | 0.67              |
| 2:A:501:GOL:C1     | 6:A:1086:HOH:O   | 2.42                     | 0.67              |
| 1:F:129:ARG:NH1    | 1:F:211:GLU:OE2  | 2.22                     | 0.67              |
| 1:G:342:LEU:HD12   | 1:G:342:LEU:C    | 2.20                     | 0.66              |
| 1:D:228:LEU:H      | 1:D:248:ASN:HD22 | 1.43                     | 0.66              |
| 1:G:362:GLN:NE2    | 6:G:837:HOH:O    | 2.28                     | 0.65              |
| 1:G:275:LYS:HE3    | 1:H:244:VAL:HG11 | 1.78                     | 0.65              |
| 1:G:412:ASP:OD2    | 1:G:436:ILE:HD11 | 1.95                     | 0.65              |
| 1:C:14:ALA:CB      | 6:C:958:HOH:O    | 2.41                     | 0.65              |
| 1:C:210:GLU:HB2    | 5:C:519:CIT:H41  | 1.76                     | 0.65              |
| 1:H:130:GLY:C      | 6:H:634:HOH:O    | 2.38                     | 0.65              |
| 1:H:252[B]:MET:HE2 | 1:H:273:TRP:CB   | 2.26                     | 0.65              |
| 1:A:208:HIS:C      | 5:A:515:CIT:O6   | 2.39                     | 0.65              |
| 1:B:145:THR:HG23   | 6:B:945:HOH:O    | 1.96                     | 0.65              |
| 4:D:510:SO4:O2     | 6:D:961:HOH:O    | 2.13                     | 0.65              |
| 1:H:75:ASN:N       | 1:H:75:ASN:HD22  | 1.94                     | 0.65              |
| 1:H:252[B]:MET:HE2 | 1:H:273:TRP:HB2  | 1.77                     | 0.65              |
| 1:H:182:LEU:O      | 1:H:186:TYR:CD2  | 2.50                     | 0.65              |
| 1:A:210:GLU:HB2    | 5:A:515:CIT:H22  | 1.79                     | 0.64              |
| 1:A:265:ASP:HB3    | 6:A:975:HOH:O    | 1.96                     | 0.64              |
| 1:H:20:GLN:HE21    | 1:H:20:GLN:N     | 1.95                     | 0.64              |
| 1:A:173:GLU:OE2    | 4:A:506:SO4:O4   | 2.14                     | 0.64              |
| 1:G:378:GLU:CD     | 1:G:378:GLU:H    | 2.05                     | 0.64              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:G:255:ASP:OD1    | 2:G:501:GOL:H11  | 1.98                     | 0.64              |
| 2:A:501:GOL:C2     | 6:A:1086:HOH:O   | 2.45                     | 0.64              |
| 1:G:334:LEU:O      | 1:G:337:ASN:ND2  | 2.30                     | 0.64              |
| 1:D:210:GLU:HB2    | 5:D:515:CIT:H41  | 1.80                     | 0.64              |
| 1:H:254:ASP:O      | 1:H:255:ASP:C    | 2.42                     | 0.63              |
| 5:B:519:CIT:O1     | 6:B:1049:HOH:O   | 2.16                     | 0.63              |
| 1:E:16:MET:HE3     | 1:E:16:MET:HA    | 1.79                     | 0.63              |
| 5:G:510:CIT:H22    | 5:G:510:CIT:O3   | 1.97                     | 0.63              |
| 1:H:210:GLU:OE1    | 1:H:210:GLU:HA   | 1.99                     | 0.63              |
| 1:B:253:THR:HG23   | 1:B:254:ASP:O    | 1.98                     | 0.62              |
| 1:H:66:ASP:HA      | 1:H:126:HIS:HB2  | 1.82                     | 0.62              |
| 1:D:255:ASP:OD2    | 2:D:501:GOL:H31  | 2.00                     | 0.62              |
| 1:G:394:VAL:HA     | 1:G:429:GLU:HA   | 1.82                     | 0.62              |
| 4:B:507:SO4:O3     | 6:B:1031:HOH:O   | 2.15                     | 0.62              |
| 1:G:347:ASN:HD22   | 1:G:350:VAL:H    | 1.47                     | 0.62              |
| 1:G:306:MET:O      | 1:G:307:THR:C    | 2.40                     | 0.62              |
| 1:D:255:ASP:CG     | 2:D:501:GOL:H31  | 2.25                     | 0.61              |
| 1:D:188:GLN:NE2    | 6:D:820:HOH:O    | 2.32                     | 0.61              |
| 1:F:110:LYS:HB3    | 1:F:111:PRO:HD3  | 1.82                     | 0.61              |
| 1:A:208:HIS:HA     | 5:A:515:CIT:O6   | 2.00                     | 0.61              |
| 1:G:428:PHE:O      | 1:G:430:LEU:HD22 | 2.00                     | 0.61              |
| 1:C:49:GLU:OE2     | 1:C:115:TYR:OH   | 2.17                     | 0.61              |
| 1:C:210:GLU:H      | 5:C:519:CIT:H22  | 1.65                     | 0.61              |
| 1:G:210:GLU:H      | 5:G:510:CIT:H42  | 1.65                     | 0.61              |
| 1:A:89:GLU:CG      | 6:A:856:HOH:O    | 2.49                     | 0.60              |
| 1:B:253:THR:CG2    | 1:B:254:ASP:O    | 2.49                     | 0.60              |
| 1:A:203:LYS:HE3    | 6:A:1127:HOH:O   | 2.02                     | 0.60              |
| 1:E:325:ARG:HD2    | 6:E:984:HOH:O    | 2.01                     | 0.60              |
| 1:F:45:LYS:NZ      | 6:F:838:HOH:O    | 2.23                     | 0.60              |
| 1:G:346:THR:CG2    | 6:G:846:HOH:O    | 2.38                     | 0.60              |
| 1:G:350:VAL:HG22   | 1:G:437:LEU:HD23 | 1.84                     | 0.60              |
| 1:H:175:ALA:N      | 2:H:502:GOL:H32  | 2.16                     | 0.60              |
| 1:G:66:ASP:OD2     | 1:G:195:LYS:NZ   | 2.35                     | 0.60              |
| 1:H:179:TYR:CD2    | 1:H:214:MET:HE3  | 2.37                     | 0.60              |
| 1:A:208:HIS:CA     | 5:A:515:CIT:O6   | 2.50                     | 0.60              |
| 1:G:350:VAL:HG22   | 1:G:437:LEU:CD2  | 2.32                     | 0.60              |
| 1:A:154:ASP:CB     | 6:A:744:HOH:O    | 2.43                     | 0.60              |
| 1:G:154[B]:ASP:OD2 | 6:G:653:HOH:O    | 2.16                     | 0.59              |
| 1:B:156:ASN:HD21   | 1:D:204:LEU:HD11 | 1.67                     | 0.59              |
| 1:A:255:ASP:OD2    | 2:A:501:GOL:C1   | 2.50                     | 0.59              |
| 1:D:253:THR:CG2    | 1:D:254:ASP:O    | 2.50                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:E:188:GLN:HG2    | 6:E:831:HOH:O    | 2.02                     | 0.59              |
| 1:G:365:ARG:HB2    | 1:G:370:VAL:HG22 | 1.85                     | 0.59              |
| 1:B:176:GLN:HB3    | 2:B:503:GOL:H31  | 1.84                     | 0.59              |
| 1:G:347:ASN:HB3    | 1:G:350:VAL:HB   | 1.83                     | 0.59              |
| 1:G:344:LEU:HD21   | 6:G:804:HOH:O    | 2.02                     | 0.59              |
| 1:H:252[A]:MET:HG2 | 1:H:273:TRP:CD1  | 2.37                     | 0.59              |
| 1:H:136:VAL:HG21   | 1:H:153:ALA:HB2  | 1.85                     | 0.59              |
| 1:G:228:LEU:H      | 1:G:248:ASN:HD22 | 1.51                     | 0.59              |
| 1:G:279:LEU:C      | 1:G:279:LEU:HD23 | 2.28                     | 0.58              |
| 1:F:161:TRP:O      | 6:F:674:HOH:O    | 2.17                     | 0.58              |
| 1:B:210:GLU:CG     | 5:B:519:CIT:H42  | 2.33                     | 0.58              |
| 1:G:252:MET:O      | 6:G:842:HOH:O    | 2.17                     | 0.58              |
| 1:H:102:SER:OG     | 1:H:111:PRO:HB2  | 2.04                     | 0.58              |
| 1:A:156:ASN:HD21   | 1:C:204:LEU:HD11 | 1.69                     | 0.58              |
| 1:G:330:PHE:CE2    | 1:G:334:LEU:HD23 | 2.39                     | 0.58              |
| 1:H:159:CYS:CB     | 1:H:198:ASP:OD1  | 2.52                     | 0.58              |
| 1:G:308:ARG:CB     | 6:G:830:HOH:O    | 2.52                     | 0.58              |
| 1:G:315:ARG:N      | 6:G:804:HOH:O    | 2.37                     | 0.58              |
| 1:A:253:THR:HG21   | 1:A:266:MET:HE1  | 1.86                     | 0.57              |
| 1:D:176:GLN:HB3    | 2:D:503:GOL:H32  | 1.86                     | 0.57              |
| 1:F:184:GLN:O      | 1:F:188:GLN:HG2  | 2.04                     | 0.57              |
| 1:G:314:GLN:HB3    | 6:G:804:HOH:O    | 2.03                     | 0.57              |
| 1:H:17:HIS:HB2     | 6:H:670:HOH:O    | 2.04                     | 0.57              |
| 2:C:505:GOL:H2     | 4:C:510:SO4:O3   | 2.05                     | 0.57              |
| 1:G:339:GLU:OE2    | 1:G:339:GLU:N    | 2.37                     | 0.57              |
| 1:G:421:LEU:HD12   | 1:G:422:VAL:N    | 2.18                     | 0.57              |
| 1:H:107:LYS:O      | 6:H:659:HOH:O    | 2.17                     | 0.57              |
| 1:H:107:LYS:HA     | 1:H:107:LYS:CE   | 2.34                     | 0.57              |
| 2:A:501:GOL:H11    | 6:A:1086:HOH:O   | 2.05                     | 0.57              |
| 1:H:70:TYR:HE2     | 6:H:649:HOH:O    | 1.81                     | 0.57              |
| 1:H:105:GLY:O      | 6:H:710:HOH:O    | 2.18                     | 0.57              |
| 1:D:49:GLU:OE1     | 1:D:115:TYR:OH   | 2.21                     | 0.57              |
| 6:A:845:HOH:O      | 2:E:504:GOL:H12  | 2.05                     | 0.57              |
| 1:B:204:LEU:HD11   | 1:D:156:ASN:HD21 | 1.69                     | 0.57              |
| 1:G:266:MET:O      | 1:G:269:GLN:N    | 2.37                     | 0.57              |
| 1:A:253:THR:HG23   | 1:A:254:ASP:O    | 2.04                     | 0.56              |
| 2:A:501:GOL:O2     | 6:A:1086:HOH:O   | 2.18                     | 0.56              |
| 1:E:366:GLU:HB2    | 6:E:953:HOH:O    | 2.04                     | 0.56              |
| 1:G:103:ALA:O      | 1:G:104:LYS:C    | 2.47                     | 0.56              |
| 1:G:172:LYS:NZ     | 6:G:677:HOH:O    | 2.34                     | 0.56              |
| 1:G:253:THR:HG23   | 1:G:254:ASP:O    | 2.06                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:G:380:ASN:ND2   | 6:G:730:HOH:O      | 2.19                     | 0.56              |
| 1:G:385:MET:HE3   | 1:G:397:VAL:HG12   | 1.88                     | 0.56              |
| 1:C:208:HIS:ND1   | 5:C:519:CIT:O5     | 2.31                     | 0.56              |
| 1:H:38:SER:O      | 1:H:296:ARG:NH2    | 2.33                     | 0.56              |
| 1:H:179:TYR:CE2   | 1:H:214:MET:HE3    | 2.41                     | 0.56              |
| 1:G:337:ASN:CG    | 6:G:843:HOH:O      | 2.48                     | 0.56              |
| 1:H:49:GLU:OE2    | 1:H:115:TYR:OH     | 2.24                     | 0.56              |
| 1:H:252[B]:MET:SD | 1:H:266[B]:MET:CE  | 2.93                     | 0.56              |
| 1:D:253:THR:HG22  | 1:D:254:ASP:O      | 2.06                     | 0.55              |
| 1:F:188:GLN:HG3   | 6:F:791:HOH:O      | 2.05                     | 0.55              |
| 1:H:313:GLU:OE2   | 6:H:667:HOH:O      | 2.18                     | 0.55              |
| 1:A:279:LEU:HD23  | 1:A:279:LEU:C      | 2.31                     | 0.55              |
| 1:D:67:ILE:HD13   | 1:D:79:TYR:CE1     | 2.41                     | 0.55              |
| 1:F:392:ARG:NH1   | 6:F:640:HOH:O      | 2.39                     | 0.55              |
| 1:H:248:ASN:ND2   | 6:H:739:HOH:O      | 2.39                     | 0.55              |
| 1:H:113:ALA:O     | 1:H:117:HIS:ND1    | 2.40                     | 0.55              |
| 1:H:239:HIS:HA    | 6:H:664:HOH:O      | 2.06                     | 0.55              |
| 1:C:253:THR:CG2   | 1:C:254:ASP:O      | 2.55                     | 0.55              |
| 1:H:67:ILE:CG1    | 1:H:126:HIS:CE1    | 2.89                     | 0.55              |
| 1:H:200:VAL:HB    | 1:H:232:PRO:O      | 2.07                     | 0.54              |
| 1:F:151:ASP:O     | 1:F:172:LYS:HG2    | 2.08                     | 0.54              |
| 1:H:130:GLY:O     | 1:H:165:MET:CE     | 2.56                     | 0.54              |
| 1:G:396:SER:CB    | 1:G:427:ALA:HB2    | 2.37                     | 0.54              |
| 1:G:395:VAL:HB    | 1:G:430:LEU:HD23   | 1.90                     | 0.54              |
| 1:H:67:ILE:HG13   | 1:H:126:HIS:CE1    | 2.42                     | 0.54              |
| 1:H:312:ASP:O     | 1:H:316:THR:HG23   | 2.08                     | 0.54              |
| 1:B:154:ASP:OD2   | 6:B:782:HOH:O      | 2.18                     | 0.54              |
| 1:D:412:ASP:C     | 1:D:412:ASP:OD1    | 2.49                     | 0.54              |
| 5:E:517:CIT:H22   | 6:E:670:HOH:O      | 2.08                     | 0.54              |
| 1:H:198:ASP:O     | 1:H:198:ASP:OD2    | 2.26                     | 0.54              |
| 1:F:405:MET:HE2   | 1:F:405:MET:HA     | 1.90                     | 0.54              |
| 1:G:421:LEU:HD11  | 1:G:423:LYS:HE3    | 1.90                     | 0.54              |
| 1:F:306:MET:HE2   | 6:F:682:HOH:O      | 2.07                     | 0.53              |
| 1:H:27:MET:HA     | 1:H:328:LEU:O      | 2.07                     | 0.53              |
| 1:G:16:MET:HE3    | 1:G:16:MET:HA      | 1.89                     | 0.53              |
| 1:H:56:LYS:N      | 1:H:57:PRO:CD      | 2.71                     | 0.53              |
| 1:H:150:ARG:HD2   | 6:H:627:HOH:O      | 2.08                     | 0.53              |
| 1:H:252[B]:MET:SD | 1:H:266[B]:MET:HE1 | 2.49                     | 0.53              |
| 1:H:253:THR:HB    | 6:H:606:HOH:O      | 2.08                     | 0.53              |
| 1:B:150:ARG:HD2   | 6:B:725:HOH:O      | 2.07                     | 0.53              |
| 5:C:519:CIT:O1    | 5:C:519:CIT:C6     | 2.57                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:F:49:GLU:OE2     | 1:F:115:TYR:OH   | 2.23                     | 0.53              |
| 1:F:387:ASN:ND2    | 1:F:389:SER:H    | 2.07                     | 0.53              |
| 1:B:340:TRP:O      | 1:B:343:SER:OG   | 2.26                     | 0.53              |
| 1:D:387:ASN:C      | 1:D:387:ASN:HD22 | 2.15                     | 0.53              |
| 1:H:131:ILE:CD1    | 1:H:152:ILE:HD11 | 2.39                     | 0.53              |
| 1:G:341:THR:O      | 1:G:344:LEU:HB2  | 2.09                     | 0.53              |
| 1:G:381:GLN:NE2    | 1:G:404:CYS:SG   | 2.82                     | 0.53              |
| 1:H:115:TYR:O      | 1:H:115:TYR:CG   | 2.62                     | 0.53              |
| 1:B:210:GLU:H      | 5:B:519:CIT:C4   | 2.20                     | 0.52              |
| 1:D:325:ARG:HD2    | 6:D:979:HOH:O    | 2.07                     | 0.52              |
| 1:H:412:ASP:C      | 1:H:412:ASP:OD1  | 2.49                     | 0.52              |
| 1:D:176:GLN:H      | 2:D:503:GOL:C3   | 2.22                     | 0.52              |
| 1:H:92:ARG:HD3     | 1:H:181:SER:HG   | 1.74                     | 0.52              |
| 1:B:406:GLU:HB2    | 1:B:407:PRO:HD2  | 1.90                     | 0.52              |
| 1:E:101:PRO:O      | 1:E:104:LYS:HB2  | 2.09                     | 0.52              |
| 1:G:346:THR:CB     | 6:G:846:HOH:O    | 2.57                     | 0.52              |
| 1:H:252[B]:MET:HE3 | 1:H:283:PRO:CB   | 2.40                     | 0.52              |
| 1:H:297:SER:CB     | 6:H:615:HOH:O    | 2.57                     | 0.52              |
| 1:H:123:PHE:CD2    | 1:H:191:VAL:HG22 | 2.45                     | 0.52              |
| 1:H:70:TYR:O       | 1:H:72:PRO:HD3   | 2.09                     | 0.52              |
| 1:C:17:HIS:CE1     | 6:C:779:HOH:O    | 2.62                     | 0.52              |
| 4:C:508:SO4:O3     | 6:C:1007:HOH:O   | 2.18                     | 0.52              |
| 1:H:273:TRP:CE3    | 1:H:276:LEU:HD23 | 2.45                     | 0.52              |
| 1:E:210:GLU:HB2    | 5:E:517:CIT:H22  | 1.91                     | 0.52              |
| 1:F:406:GLU:HB2    | 1:F:407:PRO:HD2  | 1.92                     | 0.52              |
| 1:H:324:PHE:O      | 1:H:325:ARG:HB2  | 2.10                     | 0.52              |
| 1:A:387:ASN:HD22   | 1:A:389:SER:H    | 1.58                     | 0.52              |
| 1:C:318:MET:O      | 1:C:322:ILE:HG12 | 2.10                     | 0.52              |
| 6:A:1140:HOH:O     | 2:E:504:GOL:H32  | 2.11                     | 0.51              |
| 1:F:204:LEU:HB2    | 1:F:205:TYR:CD2  | 2.44                     | 0.51              |
| 1:G:347:ASN:CG     | 6:G:785:HOH:O    | 2.52                     | 0.51              |
| 1:G:406:GLU:HG3    | 1:G:407:PRO:O    | 2.10                     | 0.51              |
| 1:G:363:VAL:HG13   | 1:G:371:VAL:O    | 2.10                     | 0.51              |
| 1:G:410:ALA:HB2    | 1:G:440:LEU:HD23 | 1.92                     | 0.51              |
| 1:H:306:MET:O      | 1:H:307:THR:C    | 2.53                     | 0.51              |
| 1:H:316:THR:HG21   | 1:H:433:HIS:O    | 2.10                     | 0.51              |
| 1:D:281:HIS:O      | 1:D:281:HIS:ND1  | 2.43                     | 0.51              |
| 1:G:318:MET:CB     | 6:G:835:HOH:O    | 2.48                     | 0.51              |
| 1:G:319:THR:OG1    | 1:G:414:TRP:NE1  | 2.34                     | 0.51              |
| 1:D:417:GLU:HB3    | 6:D:810:HOH:O    | 2.06                     | 0.51              |
| 1:D:392:ARG:NH1    | 4:D:512:SO4:O4   | 2.44                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:D:423:LYS:HE3    | 2:D:502:GOL:H2   | 1.93                     | 0.51              |
| 1:E:253:THR:HG21   | 1:E:266:MET:HE1  | 1.92                     | 0.51              |
| 1:H:23:LYS:HA      | 1:H:279:LEU:CD2  | 2.40                     | 0.51              |
| 1:B:306:MET:CE     | 6:B:674:HOH:O    | 2.58                     | 0.51              |
| 1:D:318:MET:O      | 1:D:322:ILE:HG12 | 2.11                     | 0.51              |
| 1:G:353:VAL:O      | 1:G:353:VAL:HG12 | 2.10                     | 0.51              |
| 1:H:252[B]:MET:HE3 | 1:H:283:PRO:HB3  | 1.91                     | 0.51              |
| 1:B:306:MET:HE1    | 6:B:674:HOH:O    | 2.11                     | 0.51              |
| 1:D:406:GLU:HB2    | 1:D:407:PRO:CD   | 2.41                     | 0.51              |
| 1:G:308:ARG:HB2    | 6:G:830:HOH:O    | 2.09                     | 0.51              |
| 1:H:107:LYS:HA     | 1:H:107:LYS:HE2  | 1.93                     | 0.51              |
| 1:A:259:ARG:NH2    | 1:A:261:GLU:OE2  | 2.44                     | 0.51              |
| 1:F:282:TRP:O      | 1:F:283:PRO:C    | 2.54                     | 0.51              |
| 1:H:52:ALA:HA      | 6:H:742:HOH:O    | 2.09                     | 0.51              |
| 1:H:64:VAL:HG22    | 1:H:124:GLY:HA3  | 1.93                     | 0.51              |
| 1:G:314:GLN:CB     | 6:G:804:HOH:O    | 2.59                     | 0.50              |
| 1:H:90:TYR:CE1     | 1:H:143:LEU:HD12 | 2.45                     | 0.50              |
| 1:A:89:GLU:CD      | 1:A:89:GLU:N     | 2.68                     | 0.50              |
| 1:H:24:THR:O       | 1:H:25:PRO:C     | 2.49                     | 0.50              |
| 1:A:154:ASP:OD1    | 6:A:1101:HOH:O   | 2.18                     | 0.50              |
| 1:D:210:GLU:CG     | 5:D:515:CIT:H21  | 2.41                     | 0.50              |
| 1:H:89:GLU:HB3     | 1:H:90:TYR:CE2   | 2.47                     | 0.50              |
| 1:B:145:THR:HG21   | 1:B:147:VAL:HG22 | 1.93                     | 0.50              |
| 1:F:176:GLN:OE1    | 1:F:214:MET:HG2  | 2.12                     | 0.50              |
| 1:A:89:GLU:HG3     | 6:A:856:HOH:O    | 2.11                     | 0.50              |
| 1:G:275:LYS:CE     | 1:H:244:VAL:HG11 | 2.41                     | 0.50              |
| 1:H:100:PHE:CD1    | 1:H:109:PHE:HE1  | 2.30                     | 0.50              |
| 1:H:297:SER:HB2    | 6:H:615:HOH:O    | 2.11                     | 0.50              |
| 1:E:204:LEU:HD11   | 1:G:156:ASN:HD21 | 1.75                     | 0.50              |
| 1:G:290:LEU:HD21   | 1:G:317:MET:CE   | 2.41                     | 0.50              |
| 1:D:200:VAL:HB     | 1:D:232:PRO:O    | 2.12                     | 0.50              |
| 1:A:255:ASP:CG     | 2:A:501:GOL:H12  | 2.36                     | 0.49              |
| 1:D:67:ILE:HG13    | 1:D:126:HIS:CE1  | 2.47                     | 0.49              |
| 1:H:252[B]:MET:HE1 | 1:H:324:PHE:CZ   | 2.47                     | 0.49              |
| 1:G:421:LEU:HD12   | 1:G:422:VAL:CA   | 2.42                     | 0.49              |
| 1:C:416:LYS:HD2    | 6:C:948:HOH:O    | 2.12                     | 0.49              |
| 1:F:56:LYS:HD3     | 1:F:121:LEU:HD13 | 1.93                     | 0.49              |
| 1:F:91:SER:OG      | 1:F:141:PRO:O    | 2.22                     | 0.49              |
| 1:H:310:THR:O      | 1:H:314:GLN:HG3  | 2.12                     | 0.49              |
| 1:D:207:THR:N      | 4:D:506:SO4:O1   | 2.45                     | 0.49              |
| 1:G:333:GLU:OE2    | 1:G:334:LEU:N    | 2.45                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:H:319:THR:O      | 1:H:323:ILE:HG22 | 2.13                     | 0.49              |
| 1:A:387:ASN:ND2    | 1:A:389:SER:H    | 2.11                     | 0.49              |
| 1:H:61:GLU:C       | 6:H:744:HOH:O    | 2.56                     | 0.49              |
| 1:G:25:PRO:HG3     | 1:G:282:TRP:CE3  | 2.48                     | 0.49              |
| 1:H:253:THR:HG22   | 1:H:254:ASP:O    | 2.12                     | 0.49              |
| 1:B:146:ASN:CB     | 6:B:801:HOH:O    | 2.60                     | 0.48              |
| 1:F:145:THR:O      | 6:F:881:HOH:O    | 2.19                     | 0.48              |
| 1:G:364:TYR:O      | 1:G:370:VAL:HA   | 2.12                     | 0.48              |
| 1:B:306:MET:O      | 1:B:307:THR:C    | 2.56                     | 0.48              |
| 1:H:62:TYR:N       | 6:H:744:HOH:O    | 2.46                     | 0.48              |
| 1:H:231:SER:HB2    | 1:H:232:PRO:HA   | 1.95                     | 0.48              |
| 1:D:210:GLU:H      | 5:D:515:CIT:C2   | 2.19                     | 0.48              |
| 1:E:145:THR:HG22   | 1:E:147:VAL:HG13 | 1.94                     | 0.48              |
| 1:F:348:GLU:HG2    | 6:F:647:HOH:O    | 2.13                     | 0.48              |
| 1:H:124:GLY:HA2    | 1:H:193:PHE:O    | 2.12                     | 0.48              |
| 1:H:252[B]:MET:CE  | 1:H:273:TRP:HB2  | 2.43                     | 0.48              |
| 5:D:515:CIT:H41    | 6:D:634:HOH:O    | 2.13                     | 0.48              |
| 1:F:387:ASN:HD22   | 1:F:389:SER:H    | 1.62                     | 0.48              |
| 1:G:56:LYS:HB3     | 1:G:57:PRO:HD3   | 1.94                     | 0.48              |
| 1:G:284:ASP:OD1    | 6:G:777:HOH:O    | 2.20                     | 0.48              |
| 1:B:432:PRO:O      | 1:B:433:HIS:HB2  | 2.14                     | 0.48              |
| 1:H:220:ASP:C      | 6:H:776:HOH:O    | 2.56                     | 0.48              |
| 1:H:266[B]:MET:HE3 | 1:H:269:GLN:HB2  | 1.94                     | 0.48              |
| 1:G:384:ALA:HA     | 1:G:436:ILE:O    | 2.13                     | 0.48              |
| 1:H:348:GLU:O      | 1:H:348:GLU:CD   | 2.56                     | 0.48              |
| 1:H:67:ILE:HB      | 1:H:126:HIS:CE1  | 2.48                     | 0.48              |
| 1:H:291:GLY:O      | 1:H:306:MET:HA   | 2.13                     | 0.48              |
| 1:E:208:HIS:HE1    | 6:E:610:HOH:O    | 1.96                     | 0.47              |
| 1:H:159:CYS:HB3    | 1:H:162:ASN:O    | 2.14                     | 0.47              |
| 1:H:229:SER:HA     | 1:H:249:MET:O    | 2.14                     | 0.47              |
| 1:C:423:LYS:N      | 4:C:516:SO4:O3   | 2.32                     | 0.47              |
| 1:D:176:GLN:CB     | 2:D:503:GOL:H32  | 2.44                     | 0.47              |
| 1:G:142:ILE:HD11   | 1:G:149:ALA:HA   | 1.95                     | 0.47              |
| 1:H:75:ASN:N       | 1:H:75:ASN:ND2   | 2.61                     | 0.47              |
| 1:G:76:SER:OG      | 1:G:77:SER:N     | 2.47                     | 0.47              |
| 1:G:266:MET:HE3    | 1:G:321:TRP:CH2  | 2.49                     | 0.47              |
| 1:G:288:LEU:HD22   | 1:G:317:MET:HE3  | 1.96                     | 0.47              |
| 1:H:55:LEU:C       | 1:H:57:PRO:HD2   | 2.39                     | 0.47              |
| 1:G:66:ASP:HA      | 1:G:126:HIS:HB2  | 1.96                     | 0.47              |
| 1:H:131:ILE:HD13   | 1:H:152:ILE:HD11 | 1.96                     | 0.47              |
| 1:D:310:THR:O      | 1:D:314:GLN:HG3  | 2.14                     | 0.47              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:E:210:GLU:HG2    | 5:E:517:CIT:H41  | 1.94                     | 0.47              |
| 1:F:86:GLU:HB3     | 1:F:94:MET:O     | 2.14                     | 0.47              |
| 1:F:209:THR:O      | 1:F:213:LYS:HG3  | 2.15                     | 0.47              |
| 1:G:241:THR:HG21   | 1:H:271:TYR:CE1  | 2.50                     | 0.47              |
| 1:G:434:GLN:NE2    | 6:G:784:HOH:O    | 2.48                     | 0.47              |
| 1:B:417[B]:GLU:CD  | 6:B:860:HOH:O    | 2.57                     | 0.47              |
| 1:F:89:GLU:C       | 6:F:690:HOH:O    | 2.57                     | 0.47              |
| 1:F:387:ASN:HD22   | 1:F:387:ASN:C    | 2.22                     | 0.47              |
| 1:G:387:ASN:ND2    | 1:G:389:SER:OG   | 2.46                     | 0.47              |
| 1:A:255:ASP:OD1    | 2:A:501:GOL:H12  | 2.14                     | 0.47              |
| 1:C:399:LEU:HB3    | 1:C:404:CYS:HB2  | 1.97                     | 0.47              |
| 1:D:110:LYS:HB3    | 1:D:111:PRO:HD3  | 1.97                     | 0.47              |
| 1:E:210:GLU:CG     | 5:E:517:CIT:H41  | 2.45                     | 0.47              |
| 1:G:399:LEU:HA     | 1:G:402:LEU:HB2  | 1.95                     | 0.47              |
| 1:H:67:ILE:HD12    | 1:H:126:HIS:CE1  | 2.50                     | 0.47              |
| 1:H:69:TRP:HA      | 1:H:99:ARG:HH22  | 1.79                     | 0.47              |
| 1:E:133:ARG:HD3    | 1:E:166:TYR:CZ   | 2.50                     | 0.47              |
| 1:G:253:THR:N      | 6:G:828:HOH:O    | 2.45                     | 0.47              |
| 1:A:56:LYS:HD3     | 1:A:121:LEU:HD13 | 1.97                     | 0.47              |
| 1:A:253:THR:CG2    | 1:A:254:ASP:O    | 2.63                     | 0.47              |
| 1:B:159:CYS:HB2    | 1:B:198:ASP:CG   | 2.40                     | 0.47              |
| 1:B:310:THR:HB     | 4:B:516:SO4:O3   | 2.15                     | 0.47              |
| 1:G:378:GLU:N      | 1:G:378:GLU:CD   | 2.70                     | 0.47              |
| 1:C:41:GLU:HB2     | 1:C:100:PHE:HA   | 1.96                     | 0.47              |
| 1:F:182:LEU:O      | 1:F:185:LEU:HB3  | 2.15                     | 0.47              |
| 1:A:281:HIS:O      | 1:A:281:HIS:ND1  | 2.49                     | 0.46              |
| 1:B:208:HIS:ND1    | 5:B:519:CIT:O5   | 2.46                     | 0.46              |
| 1:H:41:GLU:OE2     | 1:H:102:SER:HB3  | 2.15                     | 0.46              |
| 1:C:239:HIS:ND1    | 4:C:512:SO4:O4   | 2.32                     | 0.46              |
| 1:D:253:THR:HG23   | 1:D:254:ASP:O    | 2.15                     | 0.46              |
| 1:F:129:ARG:HD2    | 1:F:211:GLU:OE2  | 2.14                     | 0.46              |
| 1:H:252[B]:MET:HE2 | 1:H:273:TRP:CG   | 2.50                     | 0.46              |
| 1:H:224:ARG:HG3    | 1:H:224:ARG:HH11 | 1.80                     | 0.46              |
| 1:H:274:CYS:SG     | 1:H:275:LYS:HE2  | 2.56                     | 0.46              |
| 1:B:387:ASN:HD22   | 1:B:389:SER:H    | 1.62                     | 0.46              |
| 1:G:342:LEU:HG     | 6:G:737:HOH:O    | 2.15                     | 0.46              |
| 1:H:364:TYR:CD1    | 1:H:364:TYR:C    | 2.93                     | 0.46              |
| 1:A:405:MET:HE3    | 1:A:405:MET:HA   | 1.97                     | 0.46              |
| 1:F:322:ILE:HG23   | 1:F:354:HIS:HB2  | 1.98                     | 0.46              |
| 1:H:67:ILE:HD13    | 1:H:79:TYR:OH    | 2.16                     | 0.46              |
| 1:G:288:LEU:HD21   | 1:G:321:TRP:CD1  | 2.50                     | 0.46              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:110:LYS:HB3  | 1:B:111:PRO:HD3 | 1.98                     | 0.46              |
| 1:D:253:THR:HB   | 6:D:610:HOH:O   | 2.16                     | 0.46              |
| 1:G:318:MET:CA   | 6:G:835:HOH:O   | 2.64                     | 0.46              |
| 1:H:130:GLY:C    | 1:H:165:MET:HE3 | 2.40                     | 0.46              |
| 1:A:387:ASN:HD22 | 1:A:387:ASN:C   | 2.23                     | 0.46              |
| 1:A:72:PRO:HG2   | 6:A:1054:HOH:O  | 2.16                     | 0.46              |
| 1:B:387:ASN:ND2  | 1:B:389:SER:H   | 2.14                     | 0.46              |
| 1:B:247:ALA:O    | 6:B:697:HOH:O   | 2.21                     | 0.45              |
| 1:G:27:MET:HE2   | 1:G:59:GLY:O    | 2.15                     | 0.45              |
| 1:G:232:PRO:HB3  | 3:G:502:ARB:O2  | 2.16                     | 0.45              |
| 1:H:146:ASN:OD1  | 1:H:146:ASN:N   | 2.43                     | 0.45              |
| 1:H:221:ARG:HA   | 6:H:637:HOH:O   | 2.16                     | 0.45              |
| 5:D:515:CIT:C1   | 5:D:515:CIT:O5  | 2.64                     | 0.45              |
| 1:G:40:THR:O     | 1:G:44:VAL:HG23 | 2.16                     | 0.45              |
| 1:H:130:GLY:CA   | 6:H:634:HOH:O   | 2.64                     | 0.45              |
| 1:C:294:GLY:HA2  | 1:C:297:SER:HB3 | 1.97                     | 0.45              |
| 1:G:26:PRO:HB3   | 1:G:62:TYR:CE2  | 2.51                     | 0.45              |
| 1:G:315:ARG:O    | 1:G:316:THR:C   | 2.58                     | 0.45              |
| 1:G:392:ARG:HB2  | 1:G:431:GLY:HA2 | 1.98                     | 0.45              |
| 1:H:32:TRP:CE3   | 1:H:36:GLY:HA2  | 2.51                     | 0.45              |
| 1:H:55:LEU:HB3   | 1:H:60:TRP:HB2  | 1.98                     | 0.45              |
| 1:H:322:ILE:HG23 | 1:H:354:HIS:HB2 | 1.99                     | 0.45              |
| 1:H:224:ARG:HG3  | 1:H:224:ARG:NH1 | 2.31                     | 0.45              |
| 1:B:441:SER:HB2  | 1:B:442:PRO:HD2 | 1.98                     | 0.45              |
| 2:D:503:GOL:O2   | 4:D:513:SO4:O1  | 2.23                     | 0.45              |
| 1:H:16:MET:HB3   | 1:H:18:HIS:CD2  | 2.51                     | 0.45              |
| 1:H:344:LEU:O    | 6:H:724:HOH:O   | 2.21                     | 0.45              |
| 2:A:501:GOL:C3   | 6:A:1086:HOH:O  | 2.63                     | 0.45              |
| 1:C:259:ARG:NH2  | 1:C:261:GLU:OE2 | 2.50                     | 0.45              |
| 1:H:126:HIS:CD2  | 6:H:737:HOH:O   | 2.69                     | 0.45              |
| 1:B:424:HIS:HB2  | 6:B:764:HOH:O   | 2.16                     | 0.45              |
| 1:B:146:ASN:OD1  | 1:B:146:ASN:N   | 2.37                     | 0.45              |
| 1:C:110:LYS:HB3  | 1:C:111:PRO:HD3 | 1.99                     | 0.45              |
| 1:F:27:MET:HA    | 1:F:328:LEU:O   | 2.16                     | 0.45              |
| 1:F:412:ASP:C    | 1:F:412:ASP:OD1 | 2.60                     | 0.45              |
| 1:G:373:THR:OG1  | 1:G:382:PHE:O   | 2.18                     | 0.45              |
| 1:D:347:ASN:C    | 1:D:347:ASN:OD1 | 2.58                     | 0.45              |
| 1:E:200:VAL:O    | 1:E:207:THR:HA  | 2.17                     | 0.45              |
| 1:B:406:GLU:CB   | 1:B:407:PRO:CD  | 2.91                     | 0.44              |
| 1:D:349:GLU:OE2  | 1:D:416:LYS:HG2 | 2.16                     | 0.44              |
| 1:F:255:ASP:OD1  | 3:F:502:ARB:O2  | 2.26                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:137:HIS:CE1  | 1:H:137:HIS:CE1  | 3.05                     | 0.44              |
| 1:G:244:VAL:HG11 | 1:H:275:LYS:HD2  | 1.99                     | 0.44              |
| 1:G:378:GLU:O    | 1:G:380:ASN:N    | 2.51                     | 0.44              |
| 1:A:208:HIS:HE1  | 6:A:611:HOH:O    | 2.00                     | 0.44              |
| 1:A:379:GLY:N    | 6:A:1021:HOH:O   | 2.37                     | 0.44              |
| 1:H:16:MET:HB3   | 1:H:18:HIS:HD2   | 1.82                     | 0.44              |
| 1:H:193:PHE:CD1  | 1:H:227:VAL:CG1  | 3.01                     | 0.44              |
| 1:C:236:PRO:HG2  | 1:C:239:HIS:HD2  | 1.83                     | 0.44              |
| 1:D:221:ARG:NH2  | 4:D:514:SO4:O3   | 2.42                     | 0.44              |
| 1:H:195:LYS:NZ   | 6:H:737:HOH:O    | 2.51                     | 0.44              |
| 1:H:219:ILE:O    | 1:H:220:ASP:C    | 2.61                     | 0.44              |
| 1:H:160:PRO:HG3  | 1:H:204:LEU:HG   | 1.98                     | 0.44              |
| 1:H:239:HIS:O    | 1:H:243:PHE:CD2  | 2.70                     | 0.44              |
| 1:A:290:LEU:HD21 | 1:A:317:MET:CE   | 2.48                     | 0.44              |
| 1:A:409:LYS:HD2  | 1:A:444:VAL:HG23 | 2.00                     | 0.44              |
| 1:B:392:ARG:HE   | 1:E:338:ASP:HA   | 1.83                     | 0.44              |
| 1:C:16:MET:HE2   | 6:C:892:HOH:O    | 2.16                     | 0.44              |
| 1:D:387:ASN:C    | 1:D:387:ASN:ND2  | 2.75                     | 0.44              |
| 6:A:1139:HOH:O   | 2:E:504:GOL:H31  | 2.18                     | 0.43              |
| 1:G:66:ASP:OD1   | 3:G:502:ARB:O4   | 2.33                     | 0.43              |
| 1:H:253:THR:CG2  | 1:H:254:ASP:O    | 2.65                     | 0.43              |
| 1:B:359:GLY:O    | 1:B:360:ALA:C    | 2.61                     | 0.43              |
| 1:B:376:ASP:C    | 1:B:376:ASP:OD1  | 2.61                     | 0.43              |
| 1:E:17:HIS:NE2   | 4:E:506:SO4:O4   | 2.50                     | 0.43              |
| 1:G:55:LEU:HB3   | 1:G:60:TRP:CD1   | 2.53                     | 0.43              |
| 1:G:73:GLY:O     | 1:G:74:ALA:C     | 2.61                     | 0.43              |
| 1:G:258:ASP:OD1  | 1:G:258:ASP:N    | 2.50                     | 0.43              |
| 1:H:114:ASP:C    | 1:H:116:ILE:H    | 2.25                     | 0.43              |
| 1:A:379:GLY:CA   | 6:A:1021:HOH:O   | 2.66                     | 0.43              |
| 1:C:365:ARG:HG3  | 1:C:370:VAL:HG22 | 1.99                     | 0.43              |
| 5:C:519:CIT:H41  | 6:C:666:HOH:O    | 2.17                     | 0.43              |
| 5:C:519:CIT:O1   | 5:C:519:CIT:O6   | 2.37                     | 0.43              |
| 1:D:145:THR:HB   | 1:D:147:VAL:H    | 1.83                     | 0.43              |
| 1:G:253:THR:C    | 1:G:254:ASP:O    | 2.57                     | 0.43              |
| 1:H:241:THR:O    | 1:H:242:LEU:C    | 2.60                     | 0.43              |
| 1:C:279:LEU:HD23 | 1:C:279:LEU:C    | 2.43                     | 0.43              |
| 1:F:432:PRO:O    | 1:F:433:HIS:HB2  | 2.17                     | 0.43              |
| 1:G:426:LEU:HD12 | 6:G:714:HOH:O    | 2.17                     | 0.43              |
| 1:A:209:THR:N    | 5:A:515:CIT:O6   | 2.50                     | 0.43              |
| 1:F:294:GLY:O    | 1:F:304:ASP:HA   | 2.19                     | 0.43              |
| 1:F:313:GLU:OE2  | 1:F:433:HIS:HD2  | 2.00                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:56:LYS:N     | 1:B:57:PRO:CD    | 2.82                     | 0.43              |
| 1:E:126:HIS:HA   | 1:E:195:LYS:O    | 2.19                     | 0.43              |
| 1:H:180:ASP:OD2  | 1:H:221:ARG:NH1  | 2.42                     | 0.43              |
| 1:H:193:PHE:CD1  | 1:H:227:VAL:HG12 | 2.54                     | 0.43              |
| 1:B:17:HIS:HE1   | 4:B:505:SO4:O2   | 2.01                     | 0.43              |
| 1:C:432:PRO:O    | 1:C:433:HIS:HB2  | 2.19                     | 0.43              |
| 1:E:110:LYS:HB3  | 1:E:111:PRO:HD3  | 2.01                     | 0.43              |
| 1:E:145:THR:CG2  | 1:E:147:VAL:HG13 | 2.48                     | 0.43              |
| 1:E:210:GLU:HB2  | 5:E:517:CIT:H41  | 2.00                     | 0.43              |
| 1:E:248:ASN:ND2  | 6:E:733:HOH:O    | 2.51                     | 0.43              |
| 1:H:235:ALA:HB2  | 1:H:251:ARG:O    | 2.17                     | 0.43              |
| 1:F:199:ILE:HG21 | 1:F:230:LEU:HD22 | 2.00                     | 0.43              |
| 1:H:23:LYS:HA    | 1:H:279:LEU:HD23 | 2.00                     | 0.43              |
| 1:A:210:GLU:H    | 5:A:515:CIT:H41  | 1.84                     | 0.43              |
| 1:H:113:ALA:O    | 1:H:117:HIS:CE1  | 2.72                     | 0.43              |
| 1:H:168:VAL:HG12 | 1:H:214:MET:HE1  | 2.01                     | 0.43              |
| 1:H:294:GLY:O    | 1:H:304:ASP:HA   | 2.18                     | 0.43              |
| 1:A:56:LYS:N     | 1:A:57:PRO:CD    | 2.82                     | 0.43              |
| 1:F:142:ILE:HG22 | 1:F:143:LEU:O    | 2.18                     | 0.43              |
| 1:G:118:ASN:HB3  | 6:G:779:HOH:O    | 2.19                     | 0.43              |
| 1:H:89:GLU:OE2   | 1:H:89:GLU:HA    | 2.19                     | 0.43              |
| 1:H:216:ARG:NE   | 6:H:743:HOH:O    | 2.51                     | 0.43              |
| 1:C:406:GLU:HB2  | 1:C:407:PRO:HD2  | 2.01                     | 0.42              |
| 1:C:409:LYS:HD2  | 1:C:443:ALA:HA   | 2.00                     | 0.42              |
| 1:F:169:ASP:OD1  | 1:F:169:ASP:C    | 2.62                     | 0.42              |
| 1:C:258:ASP:OD1  | 1:C:258:ASP:N    | 2.52                     | 0.42              |
| 1:D:14:ALA:HA    | 1:D:19:TYR:HD2   | 1.83                     | 0.42              |
| 1:F:442:PRO:HA   | 6:F:714:HOH:O    | 2.19                     | 0.42              |
| 1:H:67:ILE:HA    | 1:H:126:HIS:ND1  | 2.34                     | 0.42              |
| 1:H:92:ARG:CD    | 1:H:181:SER:OG   | 2.63                     | 0.42              |
| 1:C:406:GLU:HB2  | 1:C:407:PRO:CD   | 2.49                     | 0.42              |
| 1:H:174:GLY:N    | 2:H:502:GOL:C3   | 2.83                     | 0.42              |
| 1:B:89:GLU:HG3   | 6:B:892:HOH:O    | 2.19                     | 0.42              |
| 1:B:200:VAL:HB   | 1:B:232:PRO:O    | 2.20                     | 0.42              |
| 1:C:364:TYR:CD1  | 1:C:364:TYR:C    | 2.95                     | 0.42              |
| 1:D:70:TYR:O     | 1:D:72:PRO:HD3   | 2.20                     | 0.42              |
| 1:H:277:VAL:HG21 | 1:H:324:PHE:CZ   | 2.55                     | 0.42              |
| 1:D:311:LYS:HG2  | 1:D:340:TRP:CE2  | 2.55                     | 0.42              |
| 1:E:409:LYS:O    | 1:E:440:LEU:HA   | 2.20                     | 0.42              |
| 1:E:200:VAL:HB   | 1:E:232:PRO:O    | 2.19                     | 0.42              |
| 5:E:517:CIT:C2   | 6:E:670:HOH:O    | 2.66                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:G:259:ARG:O    | 1:G:260:TRP:C      | 2.63                     | 0.42              |
| 1:G:359:GLY:O    | 1:G:360:ALA:C      | 2.62                     | 0.42              |
| 1:G:396:SER:HB3  | 1:G:427:ALA:HB2    | 2.01                     | 0.42              |
| 1:G:411:ARG:O    | 1:G:438:VAL:HA     | 2.20                     | 0.42              |
| 1:H:289:PRO:O    | 1:H:307:THR:OG1    | 2.37                     | 0.42              |
| 1:D:324:PHE:O    | 1:D:325:ARG:HB2    | 2.20                     | 0.42              |
| 1:E:210:GLU:CB   | 5:E:517:CIT:H41    | 2.49                     | 0.42              |
| 1:G:409:LYS:HG2  | 6:G:648:HOH:O      | 2.20                     | 0.42              |
| 1:H:50:TYR:O     | 1:H:51:MET:C       | 2.63                     | 0.42              |
| 1:A:66:ASP:HA    | 1:A:126:HIS:HB2    | 2.01                     | 0.42              |
| 1:C:54:TYR:OH    | 2:C:504:GOL:H2     | 2.19                     | 0.42              |
| 1:C:173:GLU:HG3  | 6:C:970:HOH:O      | 2.19                     | 0.42              |
| 1:H:176:GLN:O    | 1:H:177:ALA:C      | 2.62                     | 0.42              |
| 1:G:79:TYR:O     | 6:G:762:HOH:O      | 2.22                     | 0.42              |
| 1:H:216:ARG:CD   | 6:H:743:HOH:O      | 2.67                     | 0.42              |
| 1:D:210:GLU:HG2  | 5:D:515:CIT:H21    | 2.02                     | 0.41              |
| 1:F:251:ARG:HA   | 1:F:284:ASP:HB3    | 2.02                     | 0.41              |
| 1:G:347:ASN:ND2  | 1:G:350:VAL:H      | 2.13                     | 0.41              |
| 1:H:180:ASP:N    | 1:H:180:ASP:OD1    | 2.51                     | 0.41              |
| 1:H:277:VAL:HG11 | 6:H:761:HOH:O      | 2.20                     | 0.41              |
| 1:H:347:ASN:OD1  | 1:H:349:GLU:N      | 2.52                     | 0.41              |
| 1:C:208:HIS:HD1  | 5:C:519:CIT:C6     | 2.30                     | 0.41              |
| 1:E:50:TYR:CD2   | 1:E:334:LEU:HB3    | 2.55                     | 0.41              |
| 1:E:237:LEU:HD13 | 1:F:238:ASP:HA     | 2.02                     | 0.41              |
| 1:F:268:GLU:HG3  | 6:F:852:HOH:O      | 2.21                     | 0.41              |
| 1:H:159:CYS:HA   | 1:H:160:PRO:HD3    | 1.86                     | 0.41              |
| 1:E:54:TYR:OH    | 4:E:507:SO4:O4     | 2.35                     | 0.41              |
| 1:E:287:MET:O    | 1:E:289:PRO:HD3    | 2.19                     | 0.41              |
| 1:G:55:LEU:HB3   | 1:G:60:TRP:HB2     | 2.01                     | 0.41              |
| 1:G:314:GLN:C    | 6:G:804:HOH:O      | 2.62                     | 0.41              |
| 1:H:122:LYS:HB2  | 6:H:744:HOH:O      | 2.20                     | 0.41              |
| 1:A:204:LEU:HD11 | 1:C:156:ASN:HD21   | 1.85                     | 0.41              |
| 1:B:184:GLN:O    | 1:B:188[A]:GLN:HG3 | 2.21                     | 0.41              |
| 1:E:210:GLU:HG2  | 5:E:517:CIT:C4     | 2.51                     | 0.41              |
| 1:G:263:LEU:C    | 1:G:263:LEU:HD12   | 2.45                     | 0.41              |
| 1:G:318:MET:HG3  | 1:G:344:LEU:HD22   | 2.02                     | 0.41              |
| 1:G:330:PHE:CD2  | 1:G:334:LEU:CD2    | 3.03                     | 0.41              |
| 1:G:343:SER:N    | 6:G:737:HOH:O      | 2.52                     | 0.41              |
| 1:C:210:GLU:HG2  | 5:C:519:CIT:H21    | 2.02                     | 0.41              |
| 1:D:198:ASP:CG   | 1:D:198:ASP:O      | 2.62                     | 0.41              |
| 1:D:416:LYS:HE2  | 6:D:935:HOH:O      | 2.20                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:406:GLU:CG   | 1:G:407:PRO:O    | 2.68                     | 0.41              |
| 1:H:148:GLY:O    | 1:H:149:ALA:C    | 2.63                     | 0.41              |
| 1:H:199:ILE:HD11 | 1:H:212:ILE:HG13 | 2.03                     | 0.41              |
| 1:F:236:PRO:HG2  | 1:F:239:HIS:HD2  | 1.86                     | 0.41              |
| 1:G:195:LYS:HA   | 1:G:229:SER:HB3  | 2.02                     | 0.41              |
| 1:G:263:LEU:O    | 1:G:264:TYR:C    | 2.61                     | 0.41              |
| 1:G:270:CYS:O    | 1:G:271:TYR:C    | 2.60                     | 0.41              |
| 1:G:385:MET:O    | 1:G:435:SER:HA   | 2.20                     | 0.41              |
| 1:A:229:SER:HB2  | 1:A:249:MET:HG3  | 2.01                     | 0.41              |
| 2:B:503:GOL:H2   | 4:B:514:SO4:O2   | 2.20                     | 0.41              |
| 1:F:279:LEU:C    | 1:F:279:LEU:HD23 | 2.46                     | 0.41              |
| 1:G:116:ILE:O    | 1:G:121:LEU:HB2  | 2.20                     | 0.41              |
| 1:G:126:HIS:HE2  | 3:G:502:ARB:H51  | 1.86                     | 0.41              |
| 1:G:408:MET:CA   | 6:G:713:HOH:O    | 2.67                     | 0.41              |
| 1:H:40:THR:O     | 1:H:44:VAL:HG23  | 2.21                     | 0.41              |
| 1:A:20:GLN:HE21  | 1:A:23:LYS:HE3   | 1.85                     | 0.41              |
| 1:G:227:VAL:HA   | 1:G:248:ASN:HD22 | 1.86                     | 0.41              |
| 1:G:265:ASP:HB3  | 6:G:765:HOH:O    | 2.21                     | 0.41              |
| 1:H:279:LEU:CD2  | 1:H:279:LEU:C    | 2.94                     | 0.41              |
| 1:D:235:ALA:HA   | 1:D:236:PRO:HD3  | 1.92                     | 0.41              |
| 1:E:282:TRP:O    | 1:E:283:PRO:C    | 2.64                     | 0.41              |
| 1:G:253:THR:HB   | 6:G:828:HOH:O    | 2.20                     | 0.41              |
| 1:G:325:ARG:HD3  | 6:G:824:HOH:O    | 2.20                     | 0.41              |
| 5:G:510:CIT:O3   | 5:G:510:CIT:C2   | 2.65                     | 0.41              |
| 1:A:217:LYS:HE3  | 6:A:1106:HOH:O   | 2.21                     | 0.41              |
| 5:C:519:CIT:O6   | 5:C:519:CIT:C1   | 2.69                     | 0.41              |
| 1:G:386:PHE:CE1  | 1:G:435:SER:HB2  | 2.56                     | 0.41              |
| 1:H:204:LEU:HB2  | 1:H:205:TYR:CD2  | 2.56                     | 0.41              |
| 1:B:387:ASN:HD22 | 1:B:387:ASN:C    | 2.27                     | 0.40              |
| 1:D:359:GLY:O    | 1:D:360:ALA:C    | 2.63                     | 0.40              |
| 1:E:156:ASN:O    | 1:E:156:ASN:CG   | 2.63                     | 0.40              |
| 1:G:266:MET:O    | 1:G:267:PHE:C    | 2.64                     | 0.40              |
| 1:H:174:GLY:N    | 2:H:502:GOL:H31  | 2.36                     | 0.40              |
| 1:H:273:TRP:HE3  | 1:H:276:LEU:HD23 | 1.86                     | 0.40              |
| 1:A:272:LYS:CD   | 6:B:774:HOH:O    | 2.70                     | 0.40              |
| 1:G:387:ASN:HB3  | 1:G:431:GLY:O    | 2.21                     | 0.40              |
| 1:H:176:GLN:HB3  | 2:H:502:GOL:H2   | 2.02                     | 0.40              |
| 1:F:278:GLY:O    | 1:F:279:LEU:C    | 2.64                     | 0.40              |
| 1:G:235:ALA:HA   | 1:G:236:PRO:HD3  | 1.93                     | 0.40              |
| 1:H:61:GLU:HB2   | 6:H:744:HOH:O    | 2.21                     | 0.40              |
| 1:H:359:GLY:O    | 6:H:764:HOH:O    | 2.22                     | 0.40              |

*Continued on next page...*

Continued from previous page...

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

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------------|--------------------------|-------------------|
| 6:A:836:HOH:O | 6:B:1011:HOH:O[4_445] | 2.02                     | 0.18              |

## 5.3 Torsion angles ⓘ

### 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%)   | 417 (96%)  | 15 (4%)  | 0        | 100         | 100 |
| 1   | B     | 430/448 (96%)   | 412 (96%)  | 18 (4%)  | 0        | 100         | 100 |
| 1   | C     | 432/448 (96%)   | 419 (97%)  | 13 (3%)  | 0        | 100         | 100 |
| 1   | D     | 434/448 (97%)   | 415 (96%)  | 18 (4%)  | 1 (0%)   | 43          | 51  |
| 1   | E     | 430/448 (96%)   | 411 (96%)  | 19 (4%)  | 0        | 100         | 100 |
| 1   | F     | 428/448 (96%)   | 406 (95%)  | 21 (5%)  | 1 (0%)   | 43          | 51  |
| 1   | G     | 433/448 (97%)   | 393 (91%)  | 35 (8%)  | 5 (1%)   | 10          | 8   |
| 1   | H     | 431/448 (96%)   | 384 (89%)  | 41 (10%) | 6 (1%)   | 9           | 7   |
| All | All   | 3450/3584 (96%) | 3257 (94%) | 180 (5%) | 13 (0%)  | 30          | 34  |

All (13) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 371/382 (97%)   | 358 (96%)  | 13 (4%)  | 32          | 43 |
| 1   | B     | 370/382 (97%)   | 352 (95%)  | 18 (5%)  | 22          | 29 |
| 1   | C     | 371/382 (97%)   | 352 (95%)  | 19 (5%)  | 21          | 27 |
| 1   | D     | 371/382 (97%)   | 352 (95%)  | 19 (5%)  | 21          | 27 |
| 1   | E     | 369/382 (97%)   | 349 (95%)  | 20 (5%)  | 20          | 25 |
| 1   | F     | 368/382 (96%)   | 347 (94%)  | 21 (6%)  | 18          | 23 |
| 1   | G     | 372/382 (97%)   | 337 (91%)  | 35 (9%)  | 8           | 9  |
| 1   | H     | 371/382 (97%)   | 332 (90%)  | 39 (10%) | 6           | 6  |
| All | All   | 2963/3056 (97%) | 2779 (94%) | 184 (6%) | 16          | 20 |

All (184) residues with a non-rotameric sidechain are listed below:

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

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 203    | LYS  |
| 1   | A     | 237    | LEU  |
| 1   | A     | 253    | THR  |
| 1   | A     | 298    | VAL  |
| 1   | A     | 383    | VAL  |
| 1   | A     | 405    | MET  |
| 1   | A     | 413    | LEU  |
| 1   | A     | 419    | LEU  |
| 1   | A     | 421    | LEU  |
| 1   | A     | 429    | GLU  |
| 1   | B     | 45     | LYS  |
| 1   | B     | 71     | GLU  |
| 1   | B     | 89     | GLU  |
| 1   | B     | 121    | LEU  |
| 1   | B     | 145    | THR  |
| 1   | B     | 199    | ILE  |
| 1   | B     | 209    | THR  |
| 1   | B     | 232    | PRO  |
| 1   | B     | 237    | LEU  |
| 1   | B     | 253    | THR  |
| 1   | B     | 298    | VAL  |
| 1   | B     | 381    | GLN  |
| 1   | B     | 406    | GLU  |
| 1   | B     | 413    | LEU  |
| 1   | B     | 417[A] | GLU  |
| 1   | B     | 417[B] | GLU  |
| 1   | B     | 419    | LEU  |
| 1   | B     | 430    | LEU  |
| 1   | C     | 15     | SER  |
| 1   | C     | 16     | MET  |
| 1   | C     | 71     | GLU  |
| 1   | C     | 89     | GLU  |
| 1   | C     | 121    | LEU  |
| 1   | C     | 154    | ASP  |
| 1   | C     | 199    | ILE  |
| 1   | C     | 203    | LYS  |
| 1   | C     | 237    | LEU  |
| 1   | C     | 253    | THR  |
| 1   | C     | 298    | VAL  |
| 1   | C     | 383    | VAL  |
| 1   | C     | 391    | LYS  |
| 1   | C     | 402    | LEU  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 409 | LYS  |
| 1   | C     | 413 | LEU  |
| 1   | C     | 419 | LEU  |
| 1   | C     | 430 | LEU  |
| 1   | C     | 441 | SER  |
| 1   | D     | 15  | SER  |
| 1   | D     | 53  | LYS  |
| 1   | D     | 71  | GLU  |
| 1   | D     | 121 | LEU  |
| 1   | D     | 145 | THR  |
| 1   | D     | 237 | LEU  |
| 1   | D     | 249 | MET  |
| 1   | D     | 253 | THR  |
| 1   | D     | 298 | VAL  |
| 1   | D     | 383 | VAL  |
| 1   | D     | 387 | ASN  |
| 1   | D     | 391 | LYS  |
| 1   | D     | 402 | LEU  |
| 1   | D     | 413 | LEU  |
| 1   | D     | 417 | GLU  |
| 1   | D     | 419 | LEU  |
| 1   | D     | 421 | LEU  |
| 1   | D     | 422 | VAL  |
| 1   | D     | 430 | LEU  |
| 1   | E     | 15  | SER  |
| 1   | E     | 71  | GLU  |
| 1   | E     | 121 | LEU  |
| 1   | E     | 147 | VAL  |
| 1   | E     | 199 | ILE  |
| 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     | 409 | LYS  |
| 1   | E     | 413 | LEU  |
| 1   | E     | 419 | LEU  |
| 1   | E     | 421 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 422 | VAL  |
| 1   | E     | 430 | LEU  |
| 1   | F     | 71  | GLU  |
| 1   | F     | 101 | PRO  |
| 1   | F     | 104 | LYS  |
| 1   | F     | 116 | ILE  |
| 1   | F     | 121 | LEU  |
| 1   | F     | 147 | VAL  |
| 1   | F     | 172 | LYS  |
| 1   | F     | 188 | GLN  |
| 1   | F     | 203 | LYS  |
| 1   | F     | 237 | LEU  |
| 1   | F     | 298 | VAL  |
| 1   | F     | 383 | VAL  |
| 1   | F     | 391 | LYS  |
| 1   | F     | 402 | LEU  |
| 1   | F     | 405 | MET  |
| 1   | F     | 413 | LEU  |
| 1   | F     | 419 | LEU  |
| 1   | F     | 421 | LEU  |
| 1   | F     | 422 | VAL  |
| 1   | F     | 430 | LEU  |
| 1   | F     | 433 | HIS  |
| 1   | G     | 15  | SER  |
| 1   | G     | 16  | MET  |
| 1   | G     | 34  | CYS  |
| 1   | G     | 71  | GLU  |
| 1   | G     | 121 | LEU  |
| 1   | G     | 199 | ILE  |
| 1   | G     | 249 | MET  |
| 1   | G     | 253 | THR  |
| 1   | G     | 258 | ASP  |
| 1   | G     | 263 | LEU  |
| 1   | G     | 298 | VAL  |
| 1   | G     | 309 | PHE  |
| 1   | G     | 339 | GLU  |
| 1   | G     | 347 | ASN  |
| 1   | G     | 350 | VAL  |
| 1   | G     | 363 | VAL  |
| 1   | G     | 365 | ARG  |
| 1   | G     | 371 | VAL  |
| 1   | G     | 378 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 381 | GLN  |
| 1   | G     | 383 | VAL  |
| 1   | G     | 387 | ASN  |
| 1   | G     | 394 | VAL  |
| 1   | G     | 400 | LYS  |
| 1   | G     | 402 | LEU  |
| 1   | G     | 406 | GLU  |
| 1   | G     | 408 | MET  |
| 1   | G     | 416 | LYS  |
| 1   | G     | 419 | LEU  |
| 1   | G     | 421 | LEU  |
| 1   | G     | 425 | GLN  |
| 1   | G     | 430 | LEU  |
| 1   | G     | 436 | ILE  |
| 1   | G     | 438 | VAL  |
| 1   | G     | 441 | SER  |
| 1   | H     | 15  | SER  |
| 1   | H     | 16  | MET  |
| 1   | H     | 20  | GLN  |
| 1   | H     | 26  | PRO  |
| 1   | H     | 34  | CYS  |
| 1   | H     | 71  | GLU  |
| 1   | H     | 75  | ASN  |
| 1   | H     | 91  | SER  |
| 1   | H     | 107 | LYS  |
| 1   | H     | 116 | ILE  |
| 1   | H     | 121 | LEU  |
| 1   | H     | 146 | ASN  |
| 1   | H     | 147 | VAL  |
| 1   | H     | 154 | ASP  |
| 1   | H     | 171 | ARG  |
| 1   | H     | 181 | SER  |
| 1   | H     | 188 | GLN  |
| 1   | H     | 209 | THR  |
| 1   | H     | 237 | LEU  |
| 1   | H     | 249 | MET  |
| 1   | H     | 253 | THR  |
| 1   | H     | 279 | LEU  |
| 1   | H     | 298 | VAL  |
| 1   | H     | 303 | THR  |
| 1   | H     | 316 | THR  |
| 1   | H     | 361 | ARG  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 366 | GLU  |
| 1   | H     | 370 | VAL  |
| 1   | H     | 383 | VAL  |
| 1   | H     | 388 | ILE  |
| 1   | H     | 402 | LEU  |
| 1   | H     | 405 | MET  |
| 1   | H     | 409 | LYS  |
| 1   | H     | 413 | LEU  |
| 1   | H     | 419 | LEU  |
| 1   | H     | 421 | LEU  |
| 1   | H     | 430 | LEU  |
| 1   | H     | 441 | SER  |
| 1   | H     | 444 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | GLN  |
| 1   | A     | 156 | ASN  |
| 1   | A     | 208 | HIS  |
| 1   | A     | 248 | ASN  |
| 1   | A     | 269 | GLN  |
| 1   | A     | 355 | GLN  |
| 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     | 68  | GLN  |
| 1   | C     | 156 | ASN  |
| 1   | C     | 248 | ASN  |
| 1   | C     | 355 | GLN  |
| 1   | C     | 356 | ASN  |
| 1   | C     | 387 | ASN  |
| 1   | D     | 20  | GLN  |
| 1   | D     | 156 | ASN  |
| 1   | D     | 248 | ASN  |
| 1   | D     | 355 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 381 | GLN  |
| 1   | D     | 387 | ASN  |
| 1   | E     | 18  | HIS  |
| 1   | E     | 20  | GLN  |
| 1   | E     | 156 | ASN  |
| 1   | E     | 184 | GLN  |
| 1   | E     | 208 | HIS  |
| 1   | E     | 248 | ASN  |
| 1   | E     | 387 | ASN  |
| 1   | F     | 137 | HIS  |
| 1   | F     | 246 | ASN  |
| 1   | F     | 248 | ASN  |
| 1   | F     | 355 | GLN  |
| 1   | F     | 381 | GLN  |
| 1   | F     | 387 | ASN  |
| 1   | F     | 433 | HIS  |
| 1   | G     | 156 | ASN  |
| 1   | G     | 208 | HIS  |
| 1   | G     | 248 | ASN  |
| 1   | G     | 314 | GLN  |
| 1   | G     | 347 | ASN  |
| 1   | G     | 381 | GLN  |
| 1   | G     | 387 | ASN  |
| 1   | H     | 18  | HIS  |
| 1   | H     | 20  | GLN  |
| 1   | H     | 75  | ASN  |
| 1   | H     | 98  | ASN  |
| 1   | H     | 126 | HIS  |
| 1   | H     | 137 | HIS  |
| 1   | H     | 170 | HIS  |
| 1   | H     | 246 | ASN  |
| 1   | H     | 248 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

116 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | SO4  | A     | 513 | -    | 4,4,4        | 0.96 | 0           | 6,6,6       | 1.10 | 0           |
| 2   | GOL  | H     | 501 | -    | 5,5,5        | 0.33 | 0           | 5,5,5       | 1.45 | 1 (20%)     |
| 4   | SO4  | F     | 507 | -    | 4,4,4        | 0.48 | 0           | 6,6,6       | 0.13 | 0           |
| 3   | ARB  | F     | 502 | -    | 10,10,10     | 0.93 | 0           | 14,14,14    | 2.30 | 7 (50%)     |
| 4   | SO4  | A     | 507 | -    | 4,4,4        | 0.51 | 0           | 6,6,6       | 0.78 | 0           |
| 2   | GOL  | E     | 501 | -    | 5,5,5        | 0.30 | 0           | 5,5,5       | 0.64 | 0           |
| 2   | GOL  | E     | 502 | -    | 5,5,5        | 0.43 | 0           | 5,5,5       | 0.21 | 0           |
| 4   | SO4  | D     | 514 | -    | 4,4,4        | 0.51 | 0           | 6,6,6       | 0.63 | 0           |
| 4   | SO4  | A     | 504 | -    | 4,4,4        | 0.53 | 0           | 6,6,6       | 1.02 | 0           |
| 4   | SO4  | A     | 510 | -    | 4,4,4        | 0.84 | 0           | 6,6,6       | 1.01 | 0           |
| 4   | SO4  | F     | 509 | -    | 4,4,4        | 0.54 | 0           | 6,6,6       | 0.18 | 0           |
| 4   | SO4  | E     | 513 | -    | 4,4,4        | 0.71 | 0           | 6,6,6       | 0.38 | 0           |
| 2   | GOL  | B     | 501 | -    | 5,5,5        | 0.64 | 0           | 5,5,5       | 1.52 | 2 (40%)     |
| 4   | SO4  | B     | 509 | -    | 4,4,4        | 0.80 | 0           | 6,6,6       | 0.68 | 0           |
| 2   | GOL  | C     | 505 | -    | 5,5,5        | 1.16 | 0           | 5,5,5       | 1.31 | 1 (20%)     |
| 4   | SO4  | E     | 511 | -    | 4,4,4        | 0.57 | 0           | 6,6,6       | 0.46 | 0           |
| 2   | GOL  | E     | 503 | -    | 5,5,5        | 0.43 | 0           | 5,5,5       | 1.19 | 1 (20%)     |
| 4   | SO4  | B     | 511 | -    | 4,4,4        | 0.55 | 0           | 6,6,6       | 0.46 | 0           |
| 5   | CIT  | D     | 515 | -    | 12,12,12     | 2.09 | 2 (16%)     | 17,17,17    | 1.92 | 6 (35%)     |
| 4   | SO4  | C     | 516 | -    | 4,4,4        | 0.48 | 0           | 6,6,6       | 0.40 | 0           |
| 4   | SO4  | G     | 506 | -    | 4,4,4        | 0.50 | 0           | 6,6,6       | 0.23 | 0           |
| 4   | SO4  | B     | 515 | -    | 4,4,4        | 0.63 | 0           | 6,6,6       | 0.46 | 0           |
| 4   | SO4  | A     | 509 | -    | 4,4,4        | 0.66 | 0           | 6,6,6       | 0.55 | 0           |
| 2   | GOL  | E     | 504 | -    | 5,5,5        | 0.31 | 0           | 5,5,5       | 0.77 | 0           |
| 4   | SO4  | A     | 511 | -    | 4,4,4        | 0.40 | 0           | 6,6,6       | 0.40 | 0           |
| 3   | ARB  | E     | 505 | -    | 10,10,10     | 0.59 | 0           | 14,14,14    | 2.37 | 7 (50%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | ARB  | A     | 502 | -    | 10,10,10     | 1.24 | 1 (10%)  | 14,14,14    | 2.18 | 9 (64%)  |
| 4   | SO4  | B     | 508 | -    | 4,4,4        | 0.53 | 0        | 6,6,6       | 0.91 | 0        |
| 4   | SO4  | F     | 505 | -    | 4,4,4        | 0.50 | 0        | 6,6,6       | 0.61 | 0        |
| 4   | SO4  | F     | 511 | -    | 4,4,4        | 0.44 | 0        | 6,6,6       | 0.29 | 0        |
| 2   | GOL  | C     | 503 | -    | 5,5,5        | 0.42 | 0        | 5,5,5       | 0.65 | 0        |
| 4   | SO4  | E     | 509 | -    | 4,4,4        | 0.69 | 0        | 6,6,6       | 0.47 | 0        |
| 4   | SO4  | E     | 508 | -    | 4,4,4        | 0.67 | 0        | 6,6,6       | 0.45 | 0        |
| 4   | SO4  | D     | 510 | -    | 4,4,4        | 0.54 | 0        | 6,6,6       | 0.78 | 0        |
| 4   | SO4  | E     | 516 | -    | 4,4,4        | 0.52 | 0        | 6,6,6       | 0.36 | 0        |
| 2   | GOL  | B     | 503 | -    | 5,5,5        | 0.74 | 0        | 5,5,5       | 1.22 | 1 (20%)  |
| 4   | SO4  | C     | 511 | -    | 4,4,4        | 0.51 | 0        | 6,6,6       | 0.68 | 0        |
| 3   | ARB  | B     | 504 | -    | 10,10,10     | 1.04 | 1 (10%)  | 14,14,14    | 2.11 | 6 (42%)  |
| 4   | SO4  | H     | 505 | -    | 4,4,4        | 0.51 | 0        | 6,6,6       | 0.45 | 0        |
| 4   | SO4  | F     | 504 | -    | 4,4,4        | 0.64 | 0        | 6,6,6       | 0.63 | 0        |
| 5   | CIT  | A     | 515 | -    | 12,12,12     | 3.42 | 6 (50%)  | 17,17,17    | 2.51 | 5 (29%)  |
| 3   | ARB  | D     | 504 | -    | 10,10,10     | 1.09 | 1 (10%)  | 14,14,14    | 1.83 | 5 (35%)  |
| 4   | SO4  | D     | 505 | -    | 4,4,4        | 0.55 | 0        | 6,6,6       | 0.57 | 0        |
| 5   | CIT  | B     | 519 | -    | 12,12,12     | 3.86 | 2 (16%)  | 17,17,17    | 4.39 | 6 (35%)  |
| 3   | ARB  | G     | 502 | -    | 10,10,10     | 1.22 | 1 (10%)  | 14,14,14    | 2.20 | 8 (57%)  |
| 2   | GOL  | G     | 501 | -    | 5,5,5        | 0.44 | 0        | 5,5,5       | 1.23 | 0        |
| 4   | SO4  | D     | 508 | -    | 4,4,4        | 0.52 | 0        | 6,6,6       | 0.44 | 0        |
| 4   | SO4  | B     | 513 | -    | 4,4,4        | 0.60 | 0        | 6,6,6       | 0.42 | 0        |
| 4   | SO4  | B     | 507 | -    | 4,4,4        | 0.49 | 0        | 6,6,6       | 0.41 | 0        |
| 4   | SO4  | D     | 506 | -    | 4,4,4        | 0.56 | 0        | 6,6,6       | 0.65 | 0        |
| 4   | SO4  | C     | 515 | -    | 4,4,4        | 0.52 | 0        | 6,6,6       | 0.30 | 0        |
| 4   | SO4  | B     | 505 | -    | 4,4,4        | 0.57 | 0        | 6,6,6       | 0.42 | 0        |
| 4   | SO4  | F     | 512 | -    | 4,4,4        | 0.54 | 0        | 6,6,6       | 0.34 | 0        |
| 4   | SO4  | C     | 508 | -    | 4,4,4        | 0.57 | 0        | 6,6,6       | 0.21 | 0        |
| 4   | SO4  | C     | 514 | -    | 4,4,4        | 0.56 | 0        | 6,6,6       | 0.54 | 0        |
| 3   | ARB  | C     | 506 | -    | 10,10,10     | 0.97 | 1 (10%)  | 14,14,14    | 2.03 | 6 (42%)  |
| 4   | SO4  | A     | 514 | -    | 4,4,4        | 0.63 | 0        | 6,6,6       | 0.45 | 0        |
| 4   | SO4  | A     | 506 | -    | 4,4,4        | 0.71 | 0        | 6,6,6       | 0.61 | 0        |
| 2   | GOL  | D     | 501 | -    | 5,5,5        | 0.32 | 0        | 5,5,5       | 1.05 | 0        |
| 4   | SO4  | B     | 516 | -    | 4,4,4        | 0.70 | 0        | 6,6,6       | 0.58 | 0        |
| 4   | SO4  | C     | 509 | -    | 4,4,4        | 0.67 | 0        | 6,6,6       | 1.57 | 2 (33%)  |
| 4   | SO4  | G     | 503 | -    | 4,4,4        | 0.40 | 0        | 6,6,6       | 1.12 | 0        |
| 4   | SO4  | A     | 505 | -    | 4,4,4        | 0.46 | 0        | 6,6,6       | 0.53 | 0        |
| 4   | SO4  | F     | 503 | -    | 4,4,4        | 0.53 | 0        | 6,6,6       | 0.26 | 0        |
| 3   | ARB  | H     | 503 | -    | 10,10,10     | 1.10 | 1 (10%)  | 14,14,14    | 1.49 | 3 (21%)  |
| 5   | CIT  | C     | 519 | -    | 12,12,12     | 2.10 | 4 (33%)  | 17,17,17    | 2.52 | 7 (41%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | SO4  | G     | 507 | -    | 4,4,4        | 0.53 | 0        | 6,6,6       | 0.35 | 0        |
| 4   | SO4  | C     | 518 | -    | 4,4,4        | 0.43 | 0        | 6,6,6       | 0.29 | 0        |
| 4   | SO4  | A     | 508 | -    | 4,4,4        | 0.58 | 0        | 6,6,6       | 0.19 | 0        |
| 4   | SO4  | E     | 512 | -    | 4,4,4        | 0.58 | 0        | 6,6,6       | 0.89 | 0        |
| 4   | SO4  | G     | 505 | -    | 4,4,4        | 0.46 | 0        | 6,6,6       | 0.18 | 0        |
| 4   | SO4  | B     | 512 | -    | 4,4,4        | 0.53 | 0        | 6,6,6       | 0.51 | 0        |
| 4   | SO4  | B     | 518 | -    | 4,4,4        | 0.43 | 0        | 6,6,6       | 0.30 | 0        |
| 4   | SO4  | E     | 506 | -    | 4,4,4        | 0.52 | 0        | 6,6,6       | 0.25 | 0        |
| 4   | SO4  | B     | 506 | -    | 4,4,4        | 0.75 | 0        | 6,6,6       | 0.83 | 0        |
| 2   | GOL  | B     | 502 | -    | 5,5,5        | 0.60 | 0        | 5,5,5       | 0.76 | 0        |
| 4   | SO4  | C     | 517 | -    | 4,4,4        | 0.63 | 0        | 6,6,6       | 0.39 | 0        |
| 4   | SO4  | D     | 512 | -    | 4,4,4        | 0.52 | 0        | 6,6,6       | 0.37 | 0        |
| 4   | SO4  | F     | 508 | -    | 4,4,4        | 0.59 | 0        | 6,6,6       | 0.46 | 0        |
| 2   | GOL  | C     | 502 | -    | 5,5,5        | 0.40 | 0        | 5,5,5       | 0.47 | 0        |
| 4   | SO4  | G     | 504 | -    | 4,4,4        | 0.65 | 0        | 6,6,6       | 0.32 | 0        |
| 4   | SO4  | B     | 517 | -    | 4,4,4        | 0.63 | 0        | 6,6,6       | 0.45 | 0        |
| 4   | SO4  | E     | 514 | -    | 4,4,4        | 0.48 | 0        | 6,6,6       | 0.43 | 0        |
| 5   | CIT  | G     | 510 | -    | 12,12,12     | 3.76 | 4 (33%)  | 17,17,17    | 3.14 | 8 (47%)  |
| 4   | SO4  | H     | 507 | -    | 4,4,4        | 0.47 | 0        | 6,6,6       | 0.36 | 0        |
| 4   | SO4  | C     | 507 | -    | 4,4,4        | 0.70 | 0        | 6,6,6       | 0.61 | 0        |
| 2   | GOL  | H     | 502 | -    | 5,5,5        | 0.28 | 0        | 5,5,5       | 1.05 | 0        |
| 4   | SO4  | C     | 510 | -    | 4,4,4        | 0.49 | 0        | 6,6,6       | 0.61 | 0        |
| 4   | SO4  | E     | 515 | -    | 4,4,4        | 0.60 | 0        | 6,6,6       | 0.57 | 0        |
| 5   | CIT  | E     | 517 | -    | 12,12,12     | 1.95 | 1 (8%)   | 17,17,17    | 3.47 | 7 (41%)  |
| 2   | GOL  | D     | 503 | -    | 5,5,5        | 0.42 | 0        | 5,5,5       | 1.87 | 2 (40%)  |
| 4   | SO4  | A     | 512 | -    | 4,4,4        | 0.69 | 0        | 6,6,6       | 0.66 | 0        |
| 4   | SO4  | D     | 509 | -    | 4,4,4        | 0.54 | 0        | 6,6,6       | 0.50 | 0        |
| 2   | GOL  | F     | 501 | -    | 5,5,5        | 0.35 | 0        | 5,5,5       | 0.71 | 0        |
| 4   | SO4  | D     | 507 | -    | 4,4,4        | 0.65 | 0        | 6,6,6       | 0.41 | 0        |
| 4   | SO4  | E     | 507 | -    | 4,4,4        | 0.40 | 0        | 6,6,6       | 0.73 | 0        |
| 2   | GOL  | D     | 502 | -    | 5,5,5        | 0.42 | 0        | 5,5,5       | 0.57 | 0        |
| 4   | SO4  | F     | 506 | -    | 4,4,4        | 0.60 | 0        | 6,6,6       | 0.31 | 0        |
| 4   | SO4  | G     | 509 | -    | 4,4,4        | 0.56 | 0        | 6,6,6       | 0.52 | 0        |
| 4   | SO4  | D     | 513 | -    | 4,4,4        | 0.48 | 0        | 6,6,6       | 0.44 | 0        |
| 4   | SO4  | G     | 508 | -    | 4,4,4        | 0.55 | 0        | 6,6,6       | 0.38 | 0        |
| 4   | SO4  | F     | 513 | -    | 4,4,4        | 0.57 | 0        | 6,6,6       | 0.63 | 0        |
| 4   | SO4  | H     | 508 | -    | 4,4,4        | 0.49 | 0        | 6,6,6       | 0.48 | 0        |
| 4   | SO4  | D     | 511 | -    | 4,4,4        | 0.53 | 0        | 6,6,6       | 0.55 | 0        |
| 4   | SO4  | C     | 512 | -    | 4,4,4        | 0.72 | 0        | 6,6,6       | 1.17 | 0        |
| 4   | SO4  | H     | 506 | -    | 4,4,4        | 0.62 | 0        | 6,6,6       | 0.60 | 0        |
| 2   | GOL  | A     | 501 | -    | 5,5,5        | 0.41 | 0        | 5,5,5       | 0.64 | 0        |
| 4   | SO4  | B     | 514 | -    | 4,4,4        | 0.54 | 0        | 6,6,6       | 0.39 | 0        |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | SO4  | F     | 510 | -    | 4,4,4        | 0.58 | 0        | 6,6,6       | 0.54 | 0        |
| 4   | SO4  | H     | 504 | -    | 4,4,4        | 0.48 | 0        | 6,6,6       | 0.29 | 0        |
| 4   | SO4  | C     | 513 | -    | 4,4,4        | 0.75 | 0        | 6,6,6       | 0.70 | 0        |
| 4   | SO4  | A     | 503 | -    | 4,4,4        | 0.79 | 0        | 6,6,6       | 0.39 | 0        |
| 2   | GOL  | C     | 504 | -    | 5,5,5        | 0.72 | 0        | 5,5,5       | 2.75 | 2 (40%)  |
| 2   | GOL  | C     | 501 | -    | 5,5,5        | 0.40 | 0        | 5,5,5       | 0.93 | 0        |
| 4   | SO4  | E     | 510 | -    | 4,4,4        | 0.84 | 0        | 6,6,6       | 0.67 | 0        |
| 4   | SO4  | B     | 510 | -    | 4,4,4        | 0.63 | 0        | 6,6,6       | 0.39 | 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  | C     | 502 | -    | -       | 2/4/4/4    | -       |
| 2   | GOL  | H     | 501 | -    | -       | 0/4/4/4    | -       |
| 2   | GOL  | E     | 504 | -    | -       | 2/4/4/4    | -       |
| 5   | CIT  | G     | 510 | -    | -       | 5/16/16/16 | -       |
| 3   | ARB  | C     | 506 | -    | -       | -          | 0/1/1/1 |
| 2   | GOL  | H     | 502 | -    | -       | 4/4/4/4    | -       |
| 3   | ARB  | A     | 502 | -    | -       | -          | 0/1/1/1 |
| 3   | ARB  | E     | 505 | -    | -       | -          | 0/1/1/1 |
| 5   | CIT  | E     | 517 | -    | -       | 7/16/16/16 | -       |
| 3   | ARB  | F     | 502 | -    | -       | -          | 0/1/1/1 |
| 2   | GOL  | D     | 503 | -    | -       | 2/4/4/4    | -       |
| 2   | GOL  | D     | 501 | -    | -       | 2/4/4/4    | -       |
| 2   | GOL  | E     | 501 | -    | -       | 4/4/4/4    | -       |
| 2   | GOL  | E     | 502 | -    | -       | 2/4/4/4    | -       |
| 2   | GOL  | C     | 503 | -    | -       | 0/4/4/4    | -       |
| 2   | GOL  | F     | 501 | -    | -       | 2/4/4/4    | -       |
| 2   | GOL  | D     | 502 | -    | -       | 1/4/4/4    | -       |
| 2   | GOL  | B     | 503 | -    | -       | 2/4/4/4    | -       |
| 3   | ARB  | B     | 504 | -    | -       | -          | 0/1/1/1 |
| 2   | GOL  | B     | 501 | -    | -       | 2/4/4/4    | -       |
| 2   | GOL  | C     | 505 | -    | -       | 1/4/4/4    | -       |
| 3   | ARB  | H     | 503 | -    | -       | -          | 0/1/1/1 |
| 5   | CIT  | A     | 515 | -    | -       | 7/16/16/16 | -       |
| 5   | CIT  | C     | 519 | -    | -       | 4/16/16/16 | -       |

*Continued on next page...*

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 2   | GOL  | E     | 503 | -    | -       | 1/4/4/4     | -       |
| 3   | ARB  | D     | 504 | -    | -       | -           | 0/1/1/1 |
| 5   | CIT  | B     | 519 | -    | -       | 10/16/16/16 | -       |
| 2   | GOL  | A     | 501 | -    | -       | 4/4/4/4     | -       |
| 3   | ARB  | G     | 502 | -    | -       | -           | 0/1/1/1 |
| 5   | CIT  | D     | 515 | -    | -       | 8/16/16/16  | -       |
| 2   | GOL  | B     | 502 | -    | -       | 4/4/4/4     | -       |
| 2   | GOL  | G     | 501 | -    | -       | 2/4/4/4     | -       |
| 2   | GOL  | C     | 504 | -    | -       | 3/4/4/4     | -       |
| 2   | GOL  | C     | 501 | -    | -       | 2/4/4/4     | -       |

All (25) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 5   | B     | 519 | CIT  | C3-C6 | -11.75 | 1.41        | 1.53     |
| 5   | G     | 510 | CIT  | C3-C6 | -10.68 | 1.42        | 1.53     |
| 5   | A     | 515 | CIT  | C3-C6 | -9.71  | 1.43        | 1.53     |
| 5   | E     | 517 | CIT  | C3-C6 | -5.66  | 1.47        | 1.53     |
| 5   | B     | 519 | CIT  | C4-C3 | -5.19  | 1.47        | 1.54     |
| 5   | G     | 510 | CIT  | C2-C3 | 4.94   | 1.60        | 1.54     |
| 5   | D     | 515 | CIT  | C3-C6 | -4.68  | 1.48        | 1.53     |
| 5   | C     | 519 | CIT  | C2-C3 | -4.12  | 1.48        | 1.54     |
| 5   | D     | 515 | CIT  | C2-C3 | -4.07  | 1.48        | 1.54     |
| 5   | G     | 510 | CIT  | C4-C3 | -3.99  | 1.49        | 1.54     |
| 5   | A     | 515 | CIT  | O6-C6 | -3.55  | 1.17        | 1.30     |
| 5   | C     | 519 | CIT  | O3-C5 | 3.28   | 1.32        | 1.22     |
| 3   | A     | 502 | ARB  | O1-C1 | 2.49   | 1.47        | 1.39     |
| 3   | G     | 502 | ARB  | O1-C1 | 2.46   | 1.47        | 1.39     |
| 5   | A     | 515 | CIT  | O1-C1 | 2.45   | 1.30        | 1.22     |
| 5   | A     | 515 | CIT  | C4-C3 | -2.40  | 1.51        | 1.54     |
| 5   | C     | 519 | CIT  | O4-C5 | -2.40  | 1.22        | 1.30     |
| 5   | C     | 519 | CIT  | C3-C6 | -2.38  | 1.51        | 1.53     |
| 3   | B     | 504 | ARB  | O5-C5 | -2.27  | 1.39        | 1.43     |
| 5   | G     | 510 | CIT  | O6-C6 | -2.25  | 1.22        | 1.30     |
| 3   | D     | 504 | ARB  | C1-C2 | 2.23   | 1.57        | 1.52     |
| 5   | A     | 515 | CIT  | O3-C5 | 2.22   | 1.29        | 1.22     |
| 3   | H     | 503 | ARB  | C4-C3 | 2.19   | 1.55        | 1.52     |
| 3   | C     | 506 | ARB  | C3-C2 | -2.15  | 1.46        | 1.52     |
| 5   | A     | 515 | CIT  | C2-C3 | 2.14   | 1.56        | 1.54     |

All (102) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 5   | B     | 519 | CIT  | O7-C3-C6 | -11.97 | 91.98       | 108.96   |
| 5   | B     | 519 | CIT  | O5-C6-C3 | -8.87  | 104.92      | 122.09   |
| 5   | A     | 515 | CIT  | O7-C3-C6 | -8.18  | 97.35       | 108.96   |
| 5   | E     | 517 | CIT  | O6-C6-C3 | 8.07   | 128.63      | 113.14   |
| 5   | E     | 517 | CIT  | O5-C6-C3 | -7.81  | 106.97      | 122.09   |
| 5   | B     | 519 | CIT  | O6-C6-C3 | 6.71   | 126.02      | 113.14   |
| 5   | G     | 510 | CIT  | O7-C3-C6 | -6.50  | 99.73       | 108.96   |
| 5   | C     | 519 | CIT  | C3-C4-C5 | 6.44   | 131.52      | 113.92   |
| 5   | G     | 510 | CIT  | O7-C3-C2 | 6.07   | 123.22      | 109.38   |
| 5   | G     | 510 | CIT  | C3-C2-C1 | 5.07   | 127.77      | 113.92   |
| 3   | E     | 505 | ARB  | O4-C4-C3 | 4.94   | 120.39      | 110.15   |
| 2   | C     | 504 | GOL  | O2-C2-C3 | -4.90  | 88.89       | 109.18   |
| 5   | E     | 517 | CIT  | C4-C3-C6 | -4.48  | 100.12      | 110.03   |
| 5   | B     | 519 | CIT  | C4-C3-C2 | 4.29   | 120.33      | 109.31   |
| 3   | G     | 502 | ARB  | O3-C3-C4 | -4.17  | 101.54      | 110.05   |
| 3   | C     | 506 | ARB  | C5-C4-C3 | 4.11   | 115.62      | 109.64   |
| 5   | D     | 515 | CIT  | C3-C2-C1 | 4.09   | 125.12      | 113.92   |
| 5   | C     | 519 | CIT  | C4-C3-C6 | -4.06  | 101.05      | 110.03   |
| 3   | F     | 502 | ARB  | O3-C3-C4 | 4.01   | 118.23      | 110.05   |
| 5   | G     | 510 | CIT  | O5-C6-C3 | -4.00  | 114.35      | 122.09   |
| 5   | G     | 510 | CIT  | C4-C3-C6 | -3.97  | 101.25      | 110.03   |
| 3   | F     | 502 | ARB  | O2-C2-C1 | 3.85   | 118.14      | 109.25   |
| 3   | B     | 504 | ARB  | O4-C4-C5 | -3.77  | 100.58      | 109.22   |
| 3   | B     | 504 | ARB  | C5-O5-C1 | 3.76   | 120.27      | 112.46   |
| 3   | D     | 504 | ARB  | C5-O5-C1 | 3.69   | 120.13      | 112.46   |
| 5   | G     | 510 | CIT  | O6-C6-C3 | 3.67   | 120.17      | 113.14   |
| 3   | G     | 502 | ARB  | C4-C3-C2 | 3.66   | 117.29      | 110.86   |
| 5   | E     | 517 | CIT  | O7-C3-C6 | -3.65  | 103.79      | 108.96   |
| 5   | E     | 517 | CIT  | C3-C4-C5 | 3.48   | 123.45      | 113.92   |
| 3   | H     | 503 | ARB  | C5-C4-C3 | 3.48   | 114.71      | 109.64   |
| 5   | B     | 519 | CIT  | C3-C2-C1 | 3.43   | 123.29      | 113.92   |
| 2   | C     | 504 | GOL  | O3-C3-C2 | -3.33  | 95.37       | 110.38   |
| 5   | E     | 517 | CIT  | C2-C3-C6 | 3.29   | 117.32      | 110.03   |
| 3   | H     | 503 | ARB  | C4-C3-C2 | 3.23   | 116.55      | 110.86   |
| 3   | E     | 505 | ARB  | C5-O5-C1 | 3.23   | 119.17      | 112.46   |
| 5   | C     | 519 | CIT  | C2-C3-C6 | 3.19   | 117.10      | 110.03   |
| 5   | D     | 515 | CIT  | O4-C5-C4 | 3.16   | 124.35      | 114.35   |
| 2   | D     | 503 | GOL  | C3-C2-C1 | -3.12  | 100.34      | 111.80   |
| 3   | E     | 505 | ARB  | O3-C3-C4 | 3.09   | 116.35      | 110.05   |
| 5   | A     | 515 | CIT  | O5-C6-C3 | 3.08   | 128.06      | 122.09   |
| 5   | C     | 519 | CIT  | O6-C6-C3 | 3.08   | 119.05      | 113.14   |
| 5   | C     | 519 | CIT  | O7-C3-C2 | -3.07  | 102.38      | 109.38   |
| 5   | B     | 519 | CIT  | O2-C1-C2 | 3.06   | 124.05      | 114.35   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | A     | 502 | ARB  | O4-C4-C3 | 3.02  | 116.41      | 110.15   |
| 3   | A     | 502 | ARB  | O5-C1-C2 | 3.01  | 118.71      | 109.94   |
| 3   | F     | 502 | ARB  | O3-C3-C2 | -2.97 | 103.38      | 110.38   |
| 5   | A     | 515 | CIT  | C3-C2-C1 | 2.95  | 122.00      | 113.92   |
| 3   | E     | 505 | ARB  | O5-C1-C2 | 2.95  | 118.54      | 109.94   |
| 3   | F     | 502 | ARB  | O4-C4-C3 | 2.88  | 116.12      | 110.15   |
| 5   | C     | 519 | CIT  | C4-C3-C2 | 2.87  | 116.68      | 109.31   |
| 3   | B     | 504 | ARB  | O2-C2-C1 | 2.85  | 115.83      | 109.25   |
| 3   | F     | 502 | ARB  | O5-C1-C2 | 2.84  | 118.21      | 109.94   |
| 3   | C     | 506 | ARB  | O2-C2-C3 | 2.82  | 117.03      | 110.38   |
| 3   | C     | 506 | ARB  | O3-C3-C2 | -2.79 | 103.80      | 110.38   |
| 3   | B     | 504 | ARB  | O4-C4-C3 | 2.77  | 115.89      | 110.15   |
| 3   | F     | 502 | ARB  | C5-O5-C1 | 2.77  | 118.21      | 112.46   |
| 5   | C     | 519 | CIT  | O7-C3-C6 | 2.70  | 112.78      | 108.96   |
| 3   | D     | 504 | ARB  | O3-C3-C4 | -2.69 | 104.56      | 110.05   |
| 5   | D     | 515 | CIT  | O7-C3-C6 | -2.67 | 105.18      | 108.96   |
| 3   | A     | 502 | ARB  | O2-C2-C1 | 2.66  | 115.39      | 109.25   |
| 5   | G     | 510 | CIT  | C2-C3-C6 | 2.65  | 115.90      | 110.03   |
| 3   | A     | 502 | ARB  | O3-C3-C2 | -2.63 | 104.17      | 110.38   |
| 5   | A     | 515 | CIT  | O7-C3-C2 | 2.61  | 115.33      | 109.38   |
| 3   | E     | 505 | ARB  | O4-C4-C5 | -2.59 | 103.30      | 109.22   |
| 2   | H     | 501 | GOL  | C3-C2-C1 | -2.56 | 102.40      | 111.80   |
| 3   | C     | 506 | ARB  | O5-C1-C2 | 2.55  | 117.38      | 109.94   |
| 3   | G     | 502 | ARB  | O4-C4-C5 | -2.55 | 103.38      | 109.22   |
| 3   | A     | 502 | ARB  | C1-C2-C3 | 2.55  | 115.55      | 110.36   |
| 4   | C     | 509 | SO4  | O2-S-O1  | -2.54 | 91.20       | 109.06   |
| 3   | C     | 506 | ARB  | O4-C4-C5 | -2.51 | 103.48      | 109.22   |
| 5   | E     | 517 | CIT  | O3-C5-C4 | -2.48 | 115.92      | 122.95   |
| 3   | E     | 505 | ARB  | C5-C4-C3 | -2.48 | 106.03      | 109.64   |
| 3   | G     | 502 | ARB  | O4-C4-C3 | 2.45  | 115.22      | 110.15   |
| 5   | D     | 515 | CIT  | O6-C6-C3 | 2.40  | 117.74      | 113.14   |
| 3   | B     | 504 | ARB  | O3-C3-C2 | -2.40 | 104.72      | 110.38   |
| 3   | A     | 502 | ARB  | O4-C4-C5 | -2.40 | 103.73      | 109.22   |
| 3   | D     | 504 | ARB  | O5-C1-C2 | 2.39  | 116.90      | 109.94   |
| 5   | D     | 515 | CIT  | O4-C5-O3 | -2.39 | 117.19      | 123.33   |
| 4   | C     | 509 | SO4  | O4-S-O1  | 2.38  | 121.98      | 109.56   |
| 3   | D     | 504 | ARB  | O1-C1-C2 | 2.38  | 115.88      | 108.98   |
| 3   | F     | 502 | ARB  | C5-C4-C3 | -2.37 | 106.19      | 109.64   |
| 3   | G     | 502 | ARB  | O1-C1-C2 | 2.36  | 115.83      | 108.98   |
| 3   | A     | 502 | ARB  | O5-C5-C4 | 2.34  | 116.37      | 110.79   |
| 3   | A     | 502 | ARB  | C5-C4-C3 | -2.31 | 106.28      | 109.64   |
| 3   | H     | 503 | ARB  | C1-C2-C3 | 2.29  | 115.03      | 110.36   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | E     | 505 | ARB  | C1-C2-C3 | 2.29  | 115.02      | 110.36   |
| 3   | A     | 502 | ARB  | C5-O5-C1 | 2.27  | 117.18      | 112.46   |
| 3   | G     | 502 | ARB  | C5-C4-C3 | 2.27  | 112.95      | 109.64   |
| 2   | D     | 503 | GOL  | O1-C1-C2 | -2.24 | 100.28      | 110.38   |
| 2   | B     | 501 | GOL  | O2-C2-C3 | -2.16 | 100.25      | 109.18   |
| 5   | D     | 515 | CIT  | C3-C4-C5 | 2.13  | 119.75      | 113.92   |
| 5   | A     | 515 | CIT  | O6-C6-O5 | -2.12 | 117.06      | 123.86   |
| 5   | G     | 510 | CIT  | O7-C3-C4 | -2.09 | 104.60      | 109.38   |
| 2   | B     | 503 | GOL  | O3-C3-C2 | -2.07 | 101.04      | 110.38   |
| 3   | D     | 504 | ARB  | O2-C2-C3 | 2.07  | 115.25      | 110.38   |
| 2   | B     | 501 | GOL  | O1-C1-C2 | 2.07  | 119.68      | 110.38   |
| 2   | E     | 503 | GOL  | O1-C1-C2 | -2.06 | 101.09      | 110.38   |
| 3   | B     | 504 | ARB  | O5-C1-C2 | 2.06  | 115.94      | 109.94   |
| 3   | G     | 502 | ARB  | O3-C3-C2 | -2.05 | 105.54      | 110.38   |
| 2   | C     | 505 | GOL  | O3-C3-C2 | 2.03  | 119.50      | 110.38   |
| 3   | C     | 506 | ARB  | O2-C2-C1 | 2.03  | 113.92      | 109.25   |
| 3   | G     | 502 | ARB  | O2-C2-C3 | 2.02  | 115.13      | 110.38   |

There are no chirality outliers.

All (83) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | A     | 501 | GOL  | C1-C2-C3-O3 |
| 2   | B     | 501 | GOL  | O1-C1-C2-C3 |
| 2   | C     | 501 | GOL  | C1-C2-C3-O3 |
| 2   | C     | 502 | GOL  | C1-C2-C3-O3 |
| 2   | C     | 504 | GOL  | C1-C2-C3-O3 |
| 2   | D     | 501 | GOL  | O1-C1-C2-C3 |
| 2   | E     | 501 | GOL  | O1-C1-C2-C3 |
| 2   | E     | 502 | GOL  | O1-C1-C2-C3 |
| 2   | E     | 504 | GOL  | O1-C1-C2-O2 |
| 2   | E     | 504 | GOL  | O1-C1-C2-C3 |
| 2   | F     | 501 | GOL  | C1-C2-C3-O3 |
| 2   | H     | 502 | GOL  | O1-C1-C2-C3 |
| 2   | H     | 502 | GOL  | C1-C2-C3-O3 |
| 5   | A     | 515 | CIT  | O7-C3-C4-C5 |
| 5   | A     | 515 | CIT  | C2-C3-C6-O5 |
| 5   | A     | 515 | CIT  | C2-C3-C6-O6 |
| 5   | A     | 515 | CIT  | O7-C3-C6-O5 |
| 5   | A     | 515 | CIT  | O7-C3-C6-O6 |
| 5   | B     | 519 | CIT  | C2-C3-C4-C5 |
| 5   | B     | 519 | CIT  | C6-C3-C4-C5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | C     | 519 | CIT  | C1-C2-C3-O7 |
| 5   | C     | 519 | CIT  | C1-C2-C3-C4 |
| 5   | D     | 515 | CIT  | C1-C2-C3-O7 |
| 5   | D     | 515 | CIT  | C1-C2-C3-C4 |
| 5   | D     | 515 | CIT  | C2-C3-C6-O5 |
| 5   | D     | 515 | CIT  | C2-C3-C6-O6 |
| 5   | D     | 515 | CIT  | O7-C3-C6-O5 |
| 5   | D     | 515 | CIT  | O7-C3-C6-O6 |
| 5   | E     | 517 | CIT  | C2-C3-C6-O5 |
| 5   | E     | 517 | CIT  | C2-C3-C6-O6 |
| 5   | E     | 517 | CIT  | O7-C3-C6-O5 |
| 5   | E     | 517 | CIT  | O7-C3-C6-O6 |
| 5   | G     | 510 | CIT  | O7-C3-C6-O5 |
| 5   | G     | 510 | CIT  | O7-C3-C6-O6 |
| 5   | C     | 519 | CIT  | C1-C2-C3-C6 |
| 2   | A     | 501 | GOL  | O2-C2-C3-O3 |
| 2   | F     | 501 | GOL  | O2-C2-C3-O3 |
| 5   | B     | 519 | CIT  | C1-C2-C3-O7 |
| 5   | B     | 519 | CIT  | O7-C3-C4-C5 |
| 5   | D     | 515 | CIT  | C1-C2-C3-C6 |
| 2   | A     | 501 | GOL  | O1-C1-C2-C3 |
| 2   | B     | 502 | GOL  | O1-C1-C2-C3 |
| 2   | B     | 502 | GOL  | C1-C2-C3-O3 |
| 2   | B     | 503 | GOL  | O1-C1-C2-C3 |
| 2   | C     | 505 | GOL  | C1-C2-C3-O3 |
| 2   | D     | 503 | GOL  | O1-C1-C2-C3 |
| 2   | E     | 501 | GOL  | C1-C2-C3-O3 |
| 2   | G     | 501 | GOL  | O1-C1-C2-C3 |
| 5   | G     | 510 | CIT  | C4-C3-C6-O5 |
| 5   | G     | 510 | CIT  | C4-C3-C6-O6 |
| 2   | A     | 501 | GOL  | O1-C1-C2-O2 |
| 2   | B     | 502 | GOL  | O2-C2-C3-O3 |
| 2   | B     | 503 | GOL  | O1-C1-C2-O2 |
| 2   | C     | 502 | GOL  | O2-C2-C3-O3 |
| 2   | C     | 504 | GOL  | O1-C1-C2-O2 |
| 2   | D     | 501 | GOL  | O1-C1-C2-O2 |
| 2   | D     | 503 | GOL  | O1-C1-C2-O2 |
| 2   | E     | 502 | GOL  | O1-C1-C2-O2 |
| 2   | H     | 502 | GOL  | O1-C1-C2-O2 |
| 2   | H     | 502 | GOL  | O2-C2-C3-O3 |
| 5   | E     | 517 | CIT  | O7-C3-C4-C5 |
| 2   | B     | 501 | GOL  | O1-C1-C2-O2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | C     | 504 | GOL  | O2-C2-C3-O3 |
| 2   | E     | 501 | GOL  | O1-C1-C2-O2 |
| 5   | B     | 519 | CIT  | C2-C3-C6-O6 |
| 2   | C     | 501 | GOL  | O2-C2-C3-O3 |
| 2   | E     | 501 | GOL  | O2-C2-C3-O3 |
| 5   | B     | 519 | CIT  | C1-C2-C3-C4 |
| 2   | B     | 502 | GOL  | O1-C1-C2-O2 |
| 2   | E     | 503 | GOL  | O2-C2-C3-O3 |
| 2   | D     | 502 | GOL  | O1-C1-C2-O2 |
| 5   | B     | 519 | CIT  | O2-C1-C2-C3 |
| 5   | A     | 515 | CIT  | C6-C3-C4-C5 |
| 5   | C     | 519 | CIT  | O7-C3-C4-C5 |
| 2   | G     | 501 | GOL  | O1-C1-C2-O2 |
| 5   | B     | 519 | CIT  | O1-C1-C2-C3 |
| 5   | E     | 517 | CIT  | C4-C3-C6-O5 |
| 5   | E     | 517 | CIT  | C4-C3-C6-O6 |
| 5   | A     | 515 | CIT  | C2-C3-C4-C5 |
| 5   | B     | 519 | CIT  | C2-C3-C6-O5 |
| 5   | G     | 510 | CIT  | C2-C3-C6-O6 |
| 5   | D     | 515 | CIT  | O7-C3-C4-C5 |
| 5   | B     | 519 | CIT  | O7-C3-C6-O6 |

There are no ring outliers.

34 monomers are involved in 84 short contacts:

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

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | A     | 506 | SO4  | 1       | 0            |
| 2   | D     | 501 | GOL  | 2       | 0            |
| 4   | B     | 516 | SO4  | 1       | 0            |
| 5   | C     | 519 | CIT  | 9       | 0            |
| 4   | E     | 506 | SO4  | 1       | 0            |
| 4   | D     | 512 | SO4  | 1       | 0            |
| 5   | G     | 510 | CIT  | 3       | 0            |
| 2   | H     | 502 | GOL  | 4       | 0            |
| 4   | C     | 510 | SO4  | 1       | 0            |
| 5   | E     | 517 | CIT  | 9       | 0            |
| 2   | D     | 503 | GOL  | 4       | 0            |
| 4   | E     | 507 | SO4  | 1       | 0            |
| 2   | D     | 502 | GOL  | 1       | 0            |
| 4   | D     | 513 | SO4  | 1       | 0            |
| 4   | C     | 512 | SO4  | 1       | 0            |
| 2   | A     | 501 | GOL  | 8       | 0            |
| 4   | B     | 514 | SO4  | 1       | 0            |
| 2   | C     | 504 | GOL  | 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     | 431/448 (96%)   | -0.71  | 4 (0%)    | 81 79 | 10, 16, 35, 83        | 3 (0%)  |
| 1   | B     | 430/448 (95%)   | -0.52  | 3 (0%)    | 84 82 | 14, 22, 38, 74        | 2 (0%)  |
| 1   | C     | 432/448 (96%)   | -0.41  | 10 (2%)   | 61 58 | 12, 24, 55, 99        | 2 (0%)  |
| 1   | D     | 435/448 (97%)   | -0.35  | 2 (0%)    | 87 85 | 11, 26, 47, 97        | 1 (0%)  |
| 1   | E     | 431/448 (96%)   | -0.13  | 12 (2%)   | 55 52 | 18, 29, 63, 110       | 1 (0%)  |
| 1   | F     | 430/448 (95%)   | 0.23   | 10 (2%)   | 61 58 | 19, 37, 61, 98        | 0       |
| 1   | G     | 431/448 (96%)   | 1.14   | 108 (25%) | 1 1   | 17, 43, 76, 134       | 5 (1%)  |
| 1   | H     | 430/448 (95%)   | 1.71   | 152 (35%) | 1 0   | 25, 55, 77, 116       | 3 (0%)  |
| All | All   | 3450/3584 (96%) | 0.12   | 301 (8%)  | 16 13 | 10, 29, 66, 134       | 17 (0%) |

All (301) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 444 | VAL  | 10.1 |
| 1   | G     | 14  | ALA  | 9.9  |
| 1   | H     | 444 | VAL  | 8.4  |
| 1   | F     | 444 | VAL  | 8.0  |
| 1   | C     | 444 | VAL  | 7.9  |
| 1   | D     | 14  | ALA  | 7.3  |
| 1   | G     | 444 | VAL  | 7.0  |
| 1   | E     | 14  | ALA  | 6.1  |
| 1   | A     | 444 | VAL  | 5.9  |
| 1   | H     | 16  | MET  | 5.8  |
| 1   | G     | 370 | VAL  | 5.8  |
| 1   | G     | 430 | LEU  | 5.8  |
| 1   | G     | 15  | SER  | 5.6  |
| 1   | H     | 15  | SER  | 5.6  |
| 1   | A     | 14  | ALA  | 5.5  |
| 1   | G     | 428 | PHE  | 5.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 426 | LEU  | 5.1  |
| 1   | G     | 438 | VAL  | 5.0  |
| 1   | H     | 183 | PHE  | 4.9  |
| 1   | H     | 405 | MET  | 4.8  |
| 1   | G     | 388 | ILE  | 4.8  |
| 1   | H     | 189 | TRP  | 4.7  |
| 1   | B     | 15  | SER  | 4.6  |
| 1   | G     | 413 | LEU  | 4.5  |
| 1   | G     | 443 | ALA  | 4.5  |
| 1   | G     | 442 | PRO  | 4.5  |
| 1   | G     | 395 | VAL  | 4.3  |
| 1   | H     | 116 | ILE  | 4.3  |
| 1   | G     | 405 | MET  | 4.3  |
| 1   | G     | 321 | TRP  | 4.3  |
| 1   | H     | 193 | PHE  | 4.3  |
| 1   | G     | 422 | VAL  | 4.3  |
| 1   | H     | 219 | ILE  | 4.2  |
| 1   | C     | 14  | ALA  | 4.2  |
| 1   | H     | 93  | LEU  | 4.2  |
| 1   | G     | 432 | PRO  | 4.1  |
| 1   | G     | 344 | LEU  | 4.1  |
| 1   | H     | 127 | ILE  | 4.1  |
| 1   | G     | 419 | LEU  | 4.0  |
| 1   | F     | 15  | SER  | 4.0  |
| 1   | G     | 404 | CYS  | 4.0  |
| 1   | F     | 405 | MET  | 4.0  |
| 1   | H     | 196 | VAL  | 4.0  |
| 1   | G     | 364 | TYR  | 4.0  |
| 1   | H     | 125 | ILE  | 4.0  |
| 1   | C     | 405 | MET  | 4.0  |
| 1   | H     | 190 | GLY  | 4.0  |
| 1   | G     | 323 | ILE  | 3.9  |
| 1   | G     | 400 | LYS  | 3.9  |
| 1   | G     | 340 | TRP  | 3.9  |
| 1   | H     | 65  | VAL  | 3.9  |
| 1   | E     | 405 | MET  | 3.9  |
| 1   | H     | 64  | VAL  | 3.8  |
| 1   | H     | 85  | LEU  | 3.8  |
| 1   | G     | 260 | TRP  | 3.8  |
| 1   | G     | 371 | VAL  | 3.8  |
| 1   | G     | 383 | VAL  | 3.8  |
| 1   | G     | 397 | VAL  | 3.8  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 104 | LYS  | 3.8  |
| 1   | H     | 100 | PHE  | 3.8  |
| 1   | D     | 15  | SER  | 3.7  |
| 1   | G     | 372 | TRP  | 3.7  |
| 1   | G     | 350 | VAL  | 3.7  |
| 1   | G     | 363 | VAL  | 3.7  |
| 1   | H     | 39  | VAL  | 3.7  |
| 1   | G     | 341 | THR  | 3.7  |
| 1   | G     | 402 | LEU  | 3.7  |
| 1   | H     | 182 | LEU  | 3.7  |
| 1   | G     | 407 | PRO  | 3.7  |
| 1   | H     | 101 | PRO  | 3.7  |
| 1   | H     | 91  | SER  | 3.7  |
| 1   | G     | 423 | LYS  | 3.7  |
| 1   | G     | 424 | HIS  | 3.6  |
| 1   | H     | 149 | ALA  | 3.6  |
| 1   | H     | 331 | GLY  | 3.6  |
| 1   | H     | 147 | VAL  | 3.6  |
| 1   | G     | 317 | MET  | 3.5  |
| 1   | G     | 385 | MET  | 3.5  |
| 1   | H     | 240 | ALA  | 3.5  |
| 1   | E     | 15  | SER  | 3.5  |
| 1   | H     | 79  | TYR  | 3.5  |
| 1   | H     | 227 | VAL  | 3.5  |
| 1   | G     | 436 | ILE  | 3.4  |
| 1   | E     | 443 | ALA  | 3.4  |
| 1   | A     | 15  | SER  | 3.4  |
| 1   | H     | 46  | GLY  | 3.4  |
| 1   | H     | 21  | TRP  | 3.4  |
| 1   | H     | 69  | TRP  | 3.4  |
| 1   | G     | 312 | ASP  | 3.4  |
| 1   | C     | 13  | ASP  | 3.4  |
| 1   | H     | 103 | ALA  | 3.4  |
| 1   | F     | 204 | LEU  | 3.4  |
| 1   | G     | 263 | LEU  | 3.4  |
| 1   | H     | 60  | TRP  | 3.4  |
| 1   | H     | 218 | ALA  | 3.4  |
| 1   | G     | 330 | PHE  | 3.4  |
| 1   | H     | 201 | ALA  | 3.3  |
| 1   | H     | 112 | LEU  | 3.3  |
| 1   | G     | 273 | TRP  | 3.3  |
| 1   | G     | 387 | ASN  | 3.3  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 415 | ALA  | 3.3  |
| 1   | B     | 444 | VAL  | 3.3  |
| 1   | H     | 179 | TYR  | 3.3  |
| 1   | G     | 16  | MET  | 3.3  |
| 1   | G     | 437 | LEU  | 3.2  |
| 1   | G     | 425 | GLN  | 3.2  |
| 1   | H     | 244 | VAL  | 3.2  |
| 1   | F     | 205 | TYR  | 3.2  |
| 1   | H     | 19  | TYR  | 3.2  |
| 1   | H     | 58  | PHE  | 3.2  |
| 1   | C     | 443 | ALA  | 3.1  |
| 1   | H     | 194 | VAL  | 3.1  |
| 1   | H     | 45  | LYS  | 3.1  |
| 1   | H     | 203 | LYS  | 3.1  |
| 1   | G     | 410 | ALA  | 3.1  |
| 1   | H     | 97  | VAL  | 3.1  |
| 1   | B     | 405 | MET  | 3.1  |
| 1   | G     | 421 | LEU  | 3.1  |
| 1   | G     | 433 | HIS  | 3.1  |
| 1   | H     | 212 | ILE  | 3.1  |
| 1   | G     | 381 | GLN  | 3.1  |
| 1   | H     | 32  | TRP  | 3.0  |
| 1   | H     | 175 | ALA  | 3.0  |
| 1   | G     | 322 | ILE  | 3.0  |
| 1   | G     | 382 | PHE  | 3.0  |
| 1   | E     | 16  | MET  | 3.0  |
| 1   | F     | 16  | MET  | 3.0  |
| 1   | G     | 435 | SER  | 3.0  |
| 1   | H     | 130 | GLY  | 3.0  |
| 1   | G     | 320 | LEU  | 3.0  |
| 1   | H     | 143 | LEU  | 3.0  |
| 1   | H     | 111 | PRO  | 3.0  |
| 1   | H     | 35  | TYR  | 3.0  |
| 1   | H     | 340 | TRP  | 3.0  |
| 1   | H     | 414 | TRP  | 3.0  |
| 1   | H     | 37  | ALA  | 2.9  |
| 1   | H     | 36  | GLY  | 2.9  |
| 1   | H     | 226 | ILE  | 2.9  |
| 1   | H     | 293 | ILE  | 2.9  |
| 1   | H     | 70  | TYR  | 2.9  |
| 1   | F     | 158 | ILE  | 2.9  |
| 1   | H     | 67  | ILE  | 2.9  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 186 | TYR  | 2.9  |
| 1   | F     | 203 | LYS  | 2.9  |
| 1   | G     | 203 | LYS  | 2.9  |
| 1   | H     | 197 | ALA  | 2.9  |
| 1   | G     | 351 | LEU  | 2.9  |
| 1   | G     | 440 | LEU  | 2.9  |
| 1   | H     | 22  | ALA  | 2.9  |
| 1   | G     | 352 | HIS  | 2.9  |
| 1   | G     | 290 | LEU  | 2.8  |
| 1   | H     | 109 | PHE  | 2.8  |
| 1   | H     | 256 | PHE  | 2.8  |
| 1   | G     | 285 | ALA  | 2.8  |
| 1   | H     | 247 | ALA  | 2.8  |
| 1   | G     | 391 | LYS  | 2.8  |
| 1   | H     | 90  | TYR  | 2.8  |
| 1   | H     | 204 | LEU  | 2.8  |
| 1   | G     | 414 | TRP  | 2.8  |
| 1   | H     | 63  | VAL  | 2.8  |
| 1   | G     | 343 | SER  | 2.8  |
| 1   | H     | 291 | GLY  | 2.8  |
| 1   | G     | 394 | VAL  | 2.8  |
| 1   | E     | 423 | LYS  | 2.7  |
| 1   | H     | 48  | ALA  | 2.7  |
| 1   | E     | 204 | LEU  | 2.7  |
| 1   | G     | 412 | ASP  | 2.7  |
| 1   | C     | 203 | LYS  | 2.7  |
| 1   | H     | 96  | ALA  | 2.7  |
| 1   | G     | 55  | LEU  | 2.7  |
| 1   | H     | 140 | THR  | 2.7  |
| 1   | H     | 276 | LEU  | 2.7  |
| 1   | G     | 441 | SER  | 2.7  |
| 1   | H     | 44  | VAL  | 2.7  |
| 1   | H     | 217 | LYS  | 2.7  |
| 1   | H     | 123 | PHE  | 2.6  |
| 1   | E     | 400 | LYS  | 2.6  |
| 1   | H     | 107 | LYS  | 2.6  |
| 1   | H     | 84  | PRO  | 2.6  |
| 1   | H     | 110 | LYS  | 2.6  |
| 1   | G     | 375 | GLN  | 2.6  |
| 1   | G     | 360 | ALA  | 2.6  |
| 1   | H     | 257 | TRP  | 2.6  |
| 1   | H     | 328 | LEU  | 2.6  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 386 | PHE  | 2.6  |
| 1   | H     | 288 | LEU  | 2.6  |
| 1   | H     | 290 | LEU  | 2.6  |
| 1   | G     | 309 | PHE  | 2.5  |
| 1   | H     | 83  | VAL  | 2.5  |
| 1   | H     | 295 | ILE  | 2.5  |
| 1   | C     | 424 | HIS  | 2.5  |
| 1   | H     | 99  | ARG  | 2.5  |
| 1   | G     | 401 | ASP  | 2.5  |
| 1   | G     | 427 | ALA  | 2.5  |
| 1   | C     | 15  | SER  | 2.5  |
| 1   | H     | 119 | LEU  | 2.5  |
| 1   | G     | 379 | GLY  | 2.5  |
| 1   | G     | 431 | GLY  | 2.5  |
| 1   | H     | 137 | HIS  | 2.5  |
| 1   | H     | 225 | PRO  | 2.5  |
| 1   | H     | 242 | LEU  | 2.5  |
| 1   | H     | 287 | MET  | 2.5  |
| 1   | H     | 18  | HIS  | 2.5  |
| 1   | G     | 293 | ILE  | 2.5  |
| 1   | H     | 136 | VAL  | 2.5  |
| 1   | H     | 165 | MET  | 2.5  |
| 1   | G     | 409 | LYS  | 2.5  |
| 1   | H     | 243 | PHE  | 2.5  |
| 1   | F     | 443 | ALA  | 2.4  |
| 1   | C     | 391 | LYS  | 2.4  |
| 1   | H     | 17  | HIS  | 2.4  |
| 1   | H     | 126 | HIS  | 2.4  |
| 1   | G     | 417 | GLU  | 2.4  |
| 1   | H     | 406 | GLU  | 2.4  |
| 1   | G     | 274 | CYS  | 2.4  |
| 1   | H     | 50  | TYR  | 2.4  |
| 1   | G     | 361 | ARG  | 2.4  |
| 1   | H     | 52  | ALA  | 2.4  |
| 1   | H     | 171 | ARG  | 2.4  |
| 1   | H     | 187 | ALA  | 2.4  |
| 1   | G     | 369 | HIS  | 2.4  |
| 1   | H     | 108 | GLY  | 2.4  |
| 1   | H     | 191 | VAL  | 2.4  |
| 1   | G     | 316 | THR  | 2.4  |
| 1   | H     | 118 | ASN  | 2.4  |
| 1   | H     | 33  | ASP  | 2.4  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 306 | MET  | 2.4  |
| 1   | H     | 117 | HIS  | 2.4  |
| 1   | H     | 413 | LEU  | 2.3  |
| 1   | H     | 421 | LEU  | 2.3  |
| 1   | H     | 174 | GLY  | 2.3  |
| 1   | H     | 141 | PRO  | 2.3  |
| 1   | G     | 342 | LEU  | 2.3  |
| 1   | G     | 345 | LEU  | 2.3  |
| 1   | H     | 214 | MET  | 2.3  |
| 1   | H     | 200 | VAL  | 2.3  |
| 1   | G     | 355 | GLN  | 2.3  |
| 1   | H     | 40  | THR  | 2.3  |
| 1   | G     | 418 | ASP  | 2.3  |
| 1   | H     | 282 | TRP  | 2.3  |
| 1   | H     | 342 | LEU  | 2.3  |
| 1   | E     | 424 | HIS  | 2.3  |
| 1   | G     | 389 | SER  | 2.3  |
| 1   | G     | 362 | GLN  | 2.3  |
| 1   | H     | 207 | THR  | 2.3  |
| 1   | E     | 406 | GLU  | 2.2  |
| 1   | H     | 89  | GLU  | 2.2  |
| 1   | G     | 367 | ASN  | 2.2  |
| 1   | G     | 318 | MET  | 2.2  |
| 1   | G     | 420 | GLY  | 2.2  |
| 1   | H     | 329 | MET  | 2.2  |
| 1   | H     | 121 | LEU  | 2.2  |
| 1   | H     | 348 | GLU  | 2.2  |
| 1   | H     | 442 | PRO  | 2.2  |
| 1   | H     | 302 | GLY  | 2.2  |
| 1   | G     | 204 | LEU  | 2.2  |
| 1   | G     | 396 | SER  | 2.2  |
| 1   | G     | 60  | TRP  | 2.2  |
| 1   | H     | 407 | PRO  | 2.2  |
| 1   | H     | 353 | VAL  | 2.2  |
| 1   | H     | 49  | GLU  | 2.2  |
| 1   | H     | 443 | ALA  | 2.2  |
| 1   | G     | 399 | LEU  | 2.2  |
| 1   | H     | 334 | LEU  | 2.2  |
| 1   | H     | 181 | SER  | 2.2  |
| 1   | G     | 358 | TYR  | 2.2  |
| 1   | H     | 146 | ASN  | 2.2  |
| 1   | F     | 136 | VAL  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 354 | HIS  | 2.1  |
| 1   | H     | 177 | ALA  | 2.1  |
| 1   | H     | 344 | LEU  | 2.1  |
| 1   | C     | 400 | LYS  | 2.1  |
| 1   | A     | 405 | MET  | 2.1  |
| 1   | G     | 271 | TYR  | 2.1  |
| 1   | G     | 380 | ASN  | 2.1  |
| 1   | H     | 54  | TYR  | 2.1  |
| 1   | H     | 66  | ASP  | 2.1  |
| 1   | G     | 403 | GLY  | 2.1  |
| 1   | G     | 392 | ARG  | 2.1  |
| 1   | H     | 74  | ALA  | 2.1  |
| 1   | H     | 128 | MET  | 2.1  |
| 1   | H     | 206 | GLY  | 2.1  |
| 1   | H     | 29  | TRP  | 2.1  |
| 1   | H     | 172 | LYS  | 2.1  |
| 1   | H     | 423 | LYS  | 2.1  |
| 1   | G     | 261 | GLU  | 2.1  |
| 1   | H     | 94  | MET  | 2.1  |
| 1   | G     | 347 | ASN  | 2.1  |
| 1   | H     | 92  | ARG  | 2.1  |
| 1   | H     | 131 | ILE  | 2.1  |
| 1   | H     | 41  | GLU  | 2.0  |
| 1   | H     | 279 | LEU  | 2.0  |
| 1   | H     | 351 | LEU  | 2.0  |
| 1   | H     | 42  | ASP  | 2.0  |
| 1   | G     | 348 | GLU  | 2.0  |
| 1   | H     | 202 | SER  | 2.0  |
| 1   | H     | 326 | SER  | 2.0  |
| 1   | H     | 176 | GLN  | 2.0  |
| 1   | G     | 319 | THR  | 2.0  |
| 1   | H     | 307 | THR  | 2.0  |
| 1   | E     | 420 | GLY  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | SO4  | B     | 512 | 5/5   | 0.57 | 0.18 | 94,106,111,116             | 0     |
| 4   | SO4  | H     | 505 | 5/5   | 0.64 | 0.17 | 92,113,123,129             | 0     |
| 4   | SO4  | C     | 516 | 5/5   | 0.65 | 0.14 | 111,116,121,126            | 0     |
| 4   | SO4  | F     | 503 | 5/5   | 0.66 | 0.14 | 97,105,115,117             | 0     |
| 4   | SO4  | F     | 507 | 5/5   | 0.69 | 0.19 | 122,124,130,137            | 0     |
| 4   | SO4  | C     | 515 | 5/5   | 0.71 | 0.14 | 97,102,106,109             | 0     |
| 4   | SO4  | F     | 512 | 5/5   | 0.72 | 0.13 | 82,88,100,103              | 0     |
| 4   | SO4  | A     | 514 | 5/5   | 0.72 | 0.19 | 76,91,105,108              | 0     |
| 4   | SO4  | B     | 515 | 5/5   | 0.75 | 0.13 | 89,95,97,102               | 0     |
| 4   | SO4  | D     | 514 | 5/5   | 0.76 | 0.13 | 73,86,96,103               | 0     |
| 4   | SO4  | E     | 512 | 5/5   | 0.76 | 0.16 | 77,78,87,92                | 0     |
| 4   | SO4  | H     | 504 | 5/5   | 0.76 | 0.16 | 86,96,99,111               | 0     |
| 4   | SO4  | D     | 512 | 5/5   | 0.76 | 0.14 | 94,95,103,107              | 0     |
| 4   | SO4  | H     | 508 | 5/5   | 0.76 | 0.13 | 90,96,107,110              | 0     |
| 4   | SO4  | G     | 506 | 5/5   | 0.77 | 0.14 | 85,87,103,110              | 0     |
| 4   | SO4  | B     | 516 | 5/5   | 0.77 | 0.15 | 67,73,74,94                | 0     |
| 4   | SO4  | B     | 510 | 5/5   | 0.77 | 0.15 | 75,91,105,106              | 0     |
| 4   | SO4  | H     | 507 | 5/5   | 0.77 | 0.15 | 86,101,114,127             | 0     |
| 4   | SO4  | E     | 516 | 5/5   | 0.77 | 0.12 | 92,99,110,113              | 0     |
| 4   | SO4  | F     | 504 | 5/5   | 0.78 | 0.20 | 87,90,100,100              | 0     |
| 4   | SO4  | E     | 515 | 5/5   | 0.78 | 0.20 | 86,91,115,116              | 0     |
| 2   | GOL  | B     | 502 | 6/6   | 0.79 | 0.20 | 65,74,76,81                | 0     |
| 4   | SO4  | A     | 505 | 5/5   | 0.80 | 0.13 | 71,72,81,82                | 0     |
| 4   | SO4  | G     | 507 | 5/5   | 0.80 | 0.13 | 75,84,96,105               | 0     |
| 4   | SO4  | B     | 513 | 5/5   | 0.80 | 0.14 | 68,71,82,83                | 0     |
| 4   | SO4  | E     | 511 | 5/5   | 0.80 | 0.14 | 63,86,95,95                | 0     |
| 4   | SO4  | A     | 512 | 5/5   | 0.80 | 0.14 | 71,78,105,108              | 0     |
| 4   | SO4  | D     | 509 | 5/5   | 0.80 | 0.14 | 63,82,90,102               | 0     |
| 4   | SO4  | B     | 514 | 5/5   | 0.81 | 0.15 | 68,74,85,99                | 0     |
| 4   | SO4  | G     | 509 | 5/5   | 0.81 | 0.15 | 75,83,99,102               | 0     |
| 4   | SO4  | F     | 509 | 5/5   | 0.81 | 0.13 | 94,96,105,113              | 0     |
| 4   | SO4  | D     | 513 | 5/5   | 0.82 | 0.14 | 75,91,102,109              | 0     |
| 4   | SO4  | G     | 504 | 5/5   | 0.82 | 0.15 | 66,80,88,90                | 0     |
| 4   | SO4  | B     | 505 | 5/5   | 0.82 | 0.12 | 67,83,85,87                | 0     |
| 4   | SO4  | C     | 518 | 5/5   | 0.83 | 0.12 | 86,87,96,100               | 0     |
| 4   | SO4  | B     | 511 | 5/5   | 0.83 | 0.12 | 73,76,88,99                | 0     |
| 4   | SO4  | F     | 511 | 5/5   | 0.83 | 0.10 | 89,98,104,104              | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | SO4  | D     | 511 | 5/5   | 0.83 | 0.14 | 70,75,87,97                 | 0     |
| 4   | SO4  | F     | 505 | 5/5   | 0.83 | 0.13 | 79,91,98,108                | 0     |
| 4   | SO4  | F     | 506 | 5/5   | 0.83 | 0.15 | 70,70,87,88                 | 0     |
| 2   | GOL  | C     | 503 | 6/6   | 0.84 | 0.17 | 50,60,63,66                 | 0     |
| 4   | SO4  | E     | 514 | 5/5   | 0.84 | 0.14 | 77,82,93,94                 | 0     |
| 5   | CIT  | A     | 515 | 13/13 | 0.84 | 0.16 | 31,43,56,58                 | 0     |
| 4   | SO4  | F     | 510 | 5/5   | 0.85 | 0.12 | 60,61,72,86                 | 0     |
| 4   | SO4  | E     | 513 | 5/5   | 0.85 | 0.18 | 73,95,101,108               | 0     |
| 3   | ARB  | H     | 503 | 10/10 | 0.85 | 0.14 | 52,62,67,67                 | 0     |
| 4   | SO4  | B     | 518 | 5/5   | 0.85 | 0.15 | 99,101,110,114              | 0     |
| 2   | GOL  | F     | 501 | 6/6   | 0.85 | 0.22 | 51,61,68,74                 | 0     |
| 4   | SO4  | A     | 508 | 5/5   | 0.85 | 0.10 | 75,77,84,91                 | 0     |
| 5   | CIT  | E     | 517 | 13/13 | 0.85 | 0.15 | 39,62,77,81                 | 0     |
| 2   | GOL  | D     | 502 | 6/6   | 0.86 | 0.20 | 42,57,59,59                 | 0     |
| 4   | SO4  | D     | 506 | 5/5   | 0.86 | 0.14 | 54,69,81,86                 | 0     |
| 2   | GOL  | E     | 502 | 6/6   | 0.86 | 0.20 | 63,67,70,78                 | 0     |
| 4   | SO4  | B     | 517 | 5/5   | 0.86 | 0.10 | 65,76,82,86                 | 0     |
| 4   | SO4  | E     | 506 | 5/5   | 0.87 | 0.13 | 80,86,91,93                 | 0     |
| 2   | GOL  | E     | 503 | 6/6   | 0.87 | 0.15 | 49,57,62,65                 | 0     |
| 4   | SO4  | E     | 508 | 5/5   | 0.88 | 0.11 | 53,63,76,84                 | 0     |
| 4   | SO4  | G     | 505 | 5/5   | 0.88 | 0.12 | 73,73,76,76                 | 5     |
| 4   | SO4  | C     | 511 | 5/5   | 0.88 | 0.13 | 63,77,82,89                 | 0     |
| 4   | SO4  | C     | 514 | 5/5   | 0.88 | 0.15 | 73,86,97,108                | 0     |
| 4   | SO4  | G     | 508 | 5/5   | 0.88 | 0.12 | 59,72,82,86                 | 0     |
| 5   | CIT  | D     | 515 | 13/13 | 0.88 | 0.15 | 32,55,69,86                 | 0     |
| 2   | GOL  | H     | 501 | 6/6   | 0.88 | 0.15 | 55,57,63,68                 | 0     |
| 5   | CIT  | G     | 510 | 13/13 | 0.88 | 0.16 | 36,59,73,76                 | 0     |
| 4   | SO4  | C     | 513 | 5/5   | 0.89 | 0.20 | 55,62,71,72                 | 0     |
| 4   | SO4  | F     | 513 | 5/5   | 0.89 | 0.12 | 74,77,87,96                 | 0     |
| 4   | SO4  | H     | 506 | 5/5   | 0.89 | 0.12 | 59,72,79,80                 | 0     |
| 4   | SO4  | B     | 508 | 5/5   | 0.89 | 0.12 | 59,67,76,91                 | 0     |
| 4   | SO4  | B     | 509 | 5/5   | 0.89 | 0.21 | 50,60,63,75                 | 0     |
| 4   | SO4  | F     | 508 | 5/5   | 0.89 | 0.10 | 66,73,90,92                 | 0     |
| 4   | SO4  | E     | 510 | 5/5   | 0.89 | 0.17 | 52,58,73,73                 | 0     |
| 4   | SO4  | A     | 503 | 5/5   | 0.89 | 0.15 | 44,57,70,74                 | 0     |
| 2   | GOL  | B     | 503 | 6/6   | 0.89 | 0.13 | 32,35,41,47                 | 0     |
| 4   | SO4  | A     | 511 | 5/5   | 0.90 | 0.11 | 65,73,84,89                 | 0     |
| 4   | SO4  | D     | 508 | 5/5   | 0.90 | 0.11 | 67,84,93,94                 | 0     |
| 2   | GOL  | E     | 504 | 6/6   | 0.90 | 0.14 | 49,51,55,64                 | 0     |
| 2   | GOL  | H     | 502 | 6/6   | 0.90 | 0.11 | 54,56,62,63                 | 0     |
| 5   | CIT  | B     | 519 | 13/13 | 0.90 | 0.15 | 41,53,72,75                 | 0     |
| 4   | SO4  | C     | 509 | 5/5   | 0.90 | 0.17 | 41,46,57,63                 | 5     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | SO4  | C     | 517 | 5/5   | 0.90 | 0.13 | 68,76,103,106               | 0     |
| 4   | SO4  | A     | 509 | 5/5   | 0.90 | 0.18 | 53,59,70,74                 | 0     |
| 4   | SO4  | E     | 509 | 5/5   | 0.91 | 0.16 | 59,61,73,74                 | 0     |
| 4   | SO4  | C     | 512 | 5/5   | 0.91 | 0.15 | 55,58,63,71                 | 0     |
| 2   | GOL  | C     | 502 | 6/6   | 0.91 | 0.15 | 48,53,54,57                 | 0     |
| 4   | SO4  | C     | 507 | 5/5   | 0.91 | 0.16 | 58,59,70,75                 | 0     |
| 5   | CIT  | C     | 519 | 13/13 | 0.91 | 0.13 | 26,43,64,66                 | 0     |
| 4   | SO4  | B     | 506 | 5/5   | 0.91 | 0.18 | 35,44,51,56                 | 5     |
| 2   | GOL  | G     | 501 | 6/6   | 0.91 | 0.11 | 40,47,52,54                 | 0     |
| 4   | SO4  | D     | 510 | 5/5   | 0.91 | 0.09 | 62,64,72,76                 | 0     |
| 2   | GOL  | B     | 501 | 6/6   | 0.92 | 0.12 | 29,35,40,43                 | 0     |
| 4   | SO4  | D     | 505 | 5/5   | 0.92 | 0.14 | 49,60,66,67                 | 0     |
| 4   | SO4  | C     | 508 | 5/5   | 0.93 | 0.13 | 45,56,57,70                 | 0     |
| 4   | SO4  | A     | 513 | 5/5   | 0.93 | 0.15 | 43,47,49,55                 | 0     |
| 4   | SO4  | D     | 507 | 5/5   | 0.93 | 0.17 | 46,55,60,71                 | 0     |
| 2   | GOL  | D     | 501 | 6/6   | 0.93 | 0.10 | 33,35,37,39                 | 0     |
| 3   | ARB  | G     | 502 | 10/10 | 0.93 | 0.11 | 32,39,44,50                 | 0     |
| 2   | GOL  | D     | 503 | 6/6   | 0.93 | 0.10 | 37,41,42,48                 | 0     |
| 2   | GOL  | C     | 505 | 6/6   | 0.94 | 0.11 | 23,31,37,43                 | 0     |
| 3   | ARB  | F     | 502 | 10/10 | 0.94 | 0.10 | 32,43,48,55                 | 0     |
| 2   | GOL  | C     | 501 | 6/6   | 0.95 | 0.08 | 28,33,40,44                 | 0     |
| 4   | SO4  | A     | 510 | 5/5   | 0.95 | 0.13 | 31,37,42,62                 | 0     |
| 3   | ARB  | B     | 504 | 10/10 | 0.95 | 0.08 | 19,22,30,32                 | 0     |
| 4   | SO4  | B     | 507 | 5/5   | 0.95 | 0.08 | 62,68,74,82                 | 0     |
| 2   | GOL  | C     | 504 | 6/6   | 0.95 | 0.10 | 34,42,47,47                 | 0     |
| 2   | GOL  | E     | 501 | 6/6   | 0.95 | 0.10 | 37,45,50,61                 | 0     |
| 4   | SO4  | C     | 510 | 5/5   | 0.95 | 0.12 | 44,52,62,68                 | 0     |
| 3   | ARB  | C     | 506 | 10/10 | 0.96 | 0.07 | 19,25,35,36                 | 0     |
| 4   | SO4  | A     | 504 | 5/5   | 0.96 | 0.12 | 42,49,59,62                 | 0     |
| 3   | ARB  | D     | 504 | 10/10 | 0.96 | 0.07 | 19,25,28,32                 | 0     |
| 3   | ARB  | E     | 505 | 10/10 | 0.96 | 0.07 | 24,28,36,40                 | 0     |
| 2   | GOL  | A     | 501 | 6/6   | 0.97 | 0.08 | 25,32,38,41                 | 0     |
| 3   | ARB  | A     | 502 | 10/10 | 0.97 | 0.06 | 15,20,26,29                 | 0     |
| 4   | SO4  | E     | 507 | 5/5   | 0.97 | 0.10 | 45,47,54,58                 | 0     |
| 4   | SO4  | A     | 507 | 5/5   | 0.97 | 0.12 | 34,43,45,47                 | 0     |
| 4   | SO4  | G     | 503 | 5/5   | 0.99 | 0.04 | 28,29,36,39                 | 0     |
| 4   | SO4  | A     | 506 | 5/5   | 1.00 | 0.03 | 24,27,28,31                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.