



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:02 PM UTC

PDB ID : 2Q4H / pdb\_00002q4h  
Title : Ensemble refinement of the crystal structure of GALT-like protein from Arabidopsis thaliana At5g18200  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 1.83 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

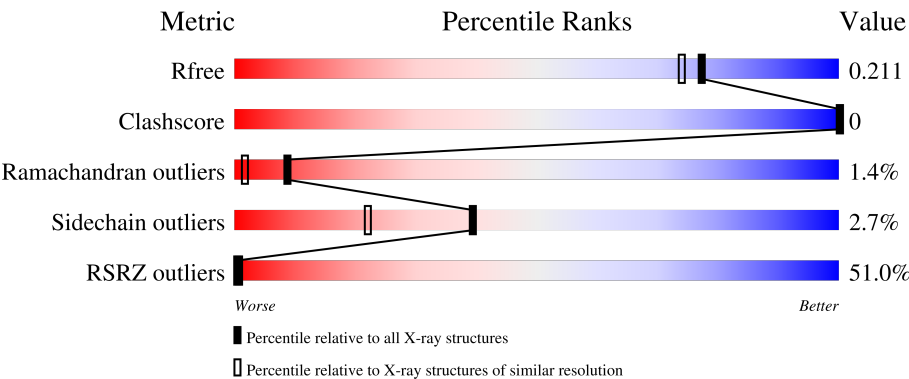
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 1.83 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 1296 (1.84-1.84)                                      |
| Clashscore            | 190562                      | 1329 (1.84-1.84)                                      |
| Ramachandran outliers | 187476                      | 1318 (1.84-1.84)                                      |
| Sidechain outliers    | 187428                      | 1318 (1.84-1.84)                                      |
| RSRZ outliers         | 180081                      | 1296 (1.84-1.84)                                      |

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   | 1-A   | 351    | <div><div>44%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>87%</div><div>11%</div></div>              |
| 1   | 1-B   | 351    | <div><div>46%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>82%</div><div>5%</div><div>13%</div></div> |
| 1   | 2-A   | 351    | <div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>86%</div><div></div><div>11%</div></div>      |
| 1   | 2-B   | 351    | <div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>83%</div><div></div><div>13%</div></div>      |

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| Mol | Chain | Length | Quality of chain                                                                               |
|-----|-------|--------|------------------------------------------------------------------------------------------------|
| 1   | 3-A   | 351    |  87% 5% 11%  |
| 1   | 3-B   | 351    |  82% 5% 13%  |
| 1   | 4-A   | 351    |  86% 5% 11%  |
| 1   | 4-B   | 351    |  82% 5% 13%  |
| 1   | 5-A   | 351    |  86% 5% 11%  |
| 1   | 5-B   | 351    |  82% 5% 13%  |
| 1   | 6-A   | 351    |  85% 5% 11%  |
| 1   | 6-B   | 351    |  83% 5% 13%  |
| 1   | 7-A   | 351    |  86% 5% 11%  |
| 1   | 7-B   | 351    |  83% 5% 13%  |
| 1   | 8-A   | 351    |  87% 5% 11%  |
| 1   | 8-B   | 351    |  82% 5% 13% |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 43592 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.

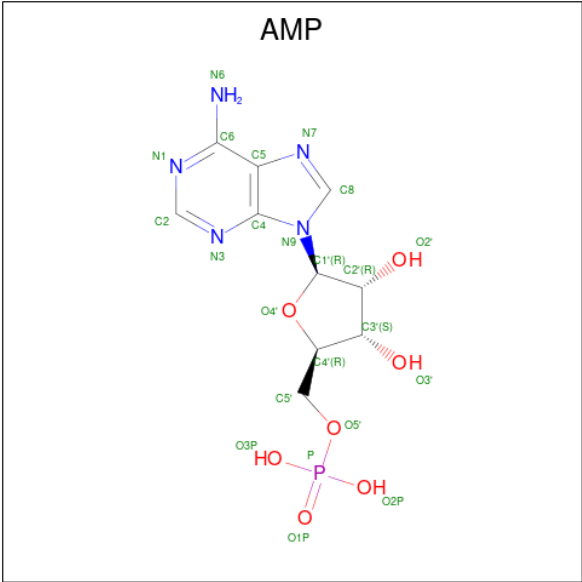
- Molecule 1 is a protein called Probable galactose-1-phosphate uridyl transferase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | 1-A   | 311      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2461  | 1577 | 417 | 454 | 13 |         |         |       |
| 1   | 2-A   | 311      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2461  | 1577 | 417 | 454 | 13 |         |         |       |
| 1   | 3-A   | 311      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2461  | 1577 | 417 | 454 | 13 |         |         |       |
| 1   | 4-A   | 311      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2461  | 1577 | 417 | 454 | 13 |         |         |       |
| 1   | 5-A   | 311      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2461  | 1577 | 417 | 454 | 13 |         |         |       |
| 1   | 6-A   | 311      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2461  | 1577 | 417 | 454 | 13 |         |         |       |
| 1   | 7-A   | 311      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2461  | 1577 | 417 | 454 | 13 |         |         |       |
| 1   | 8-A   | 311      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2461  | 1577 | 417 | 454 | 13 |         |         |       |
| 1   | 1-B   | 305      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2416  | 1550 | 408 | 445 | 13 |         |         |       |
| 1   | 2-B   | 305      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2416  | 1550 | 408 | 445 | 13 |         |         |       |
| 1   | 3-B   | 305      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2416  | 1550 | 408 | 445 | 13 |         |         |       |
| 1   | 4-B   | 305      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2416  | 1550 | 408 | 445 | 13 |         |         |       |
| 1   | 5-B   | 305      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2416  | 1550 | 408 | 445 | 13 |         |         |       |
| 1   | 6-B   | 305      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2416  | 1550 | 408 | 445 | 13 |         |         |       |
| 1   | 7-B   | 305      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2416  | 1550 | 408 | 445 | 13 |         |         |       |
| 1   | 8-B   | 305      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2416  | 1550 | 408 | 445 | 13 |         |         |       |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | 1-A   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 2-A   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 3-A   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 4-A   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 5-A   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 6-A   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 7-A   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 8-A   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 1-B   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 2-B   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 3-B   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 4-B   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 5-B   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 6-B   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 7-B   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | 8-B   | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 3   | 1-A   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 2-A   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 3-A   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 4-A   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 5-A   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 6-A   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 7-A   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 8-A   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 1-B   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 2-B   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 3-B   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 4-B   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 5-B   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 6-B   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 3   | 7-B   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |
| 3   | 8-B   | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 22    | 10 | 5 | 6 | 1 |         |         |

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | 1-A   | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | 2-A   | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | 3-A   | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | 4-A   | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | 5-A   | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | 6-A   | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | 7-A   | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | 8-A   | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | 1-A   | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

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| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 4   | 2-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 3-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 4-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 5-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 6-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 7-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 8-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 1-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 2-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 3-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 4-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 5-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 6-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 7-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 8-A   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 1-B   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 2-B   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 3-B   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 4-B   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 5-B   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |
| 4   | 6-B   | 1        | Total<br>4 | C<br>2 | O<br>2 | 0       | 0       |

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| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | 7-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 8-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 1-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 2-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 3-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 4-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 5-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 6-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 7-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 8-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 1-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 2-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 3-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 4-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 5-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 6-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 7-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | 8-B   | 1        | Total C O<br>4 2 2 | 0       | 0       |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5   | 1-A   | 273      | Total O<br>273 273 | 0       | 0       |

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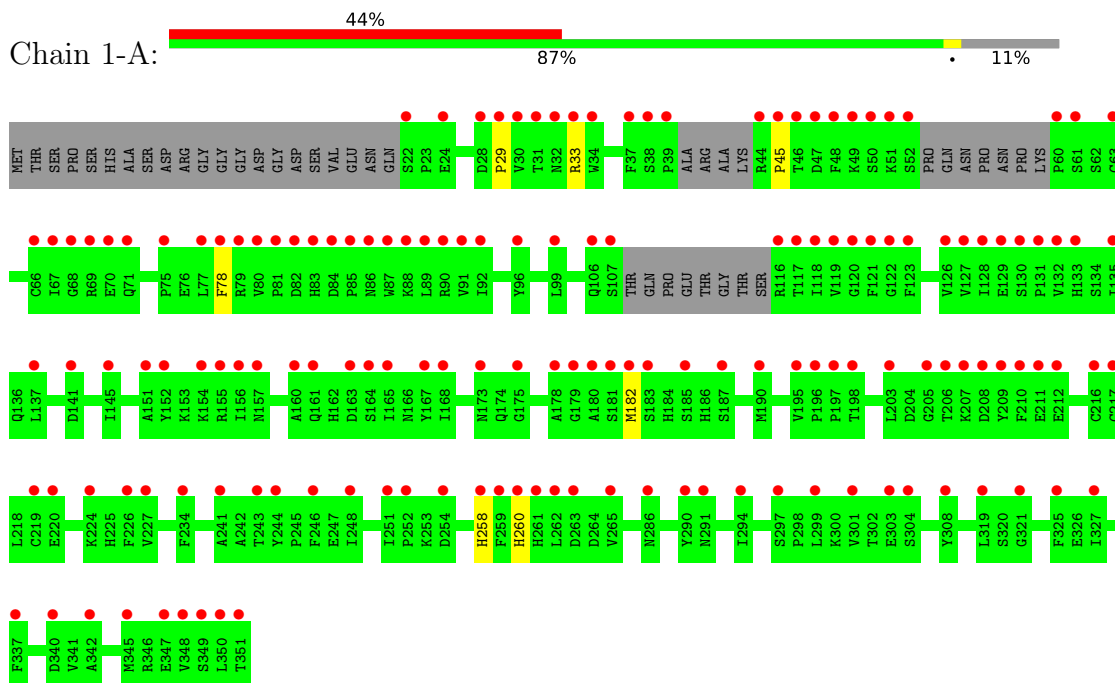
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | 2-A   | 274      | Total<br>274 | O<br>274 | 0       | 0       |
| 5   | 3-A   | 270      | Total<br>270 | O<br>270 | 0       | 0       |
| 5   | 4-A   | 272      | Total<br>272 | O<br>272 | 0       | 0       |
| 5   | 5-A   | 270      | Total<br>270 | O<br>270 | 0       | 0       |
| 5   | 6-A   | 270      | Total<br>270 | O<br>270 | 0       | 0       |
| 5   | 7-A   | 270      | Total<br>270 | O<br>270 | 0       | 0       |
| 5   | 8-A   | 271      | Total<br>271 | O<br>271 | 0       | 0       |
| 5   | 1-B   | 227      | Total<br>227 | O<br>227 | 0       | 0       |
| 5   | 2-B   | 226      | Total<br>226 | O<br>226 | 0       | 0       |
| 5   | 3-B   | 230      | Total<br>230 | O<br>230 | 0       | 0       |
| 5   | 4-B   | 228      | Total<br>228 | O<br>228 | 0       | 0       |
| 5   | 5-B   | 230      | Total<br>230 | O<br>230 | 0       | 0       |
| 5   | 6-B   | 230      | Total<br>230 | O<br>230 | 0       | 0       |
| 5   | 7-B   | 230      | Total<br>230 | O<br>230 | 0       | 0       |
| 5   | 8-B   | 229      | Total<br>229 | O<br>229 | 0       | 0       |

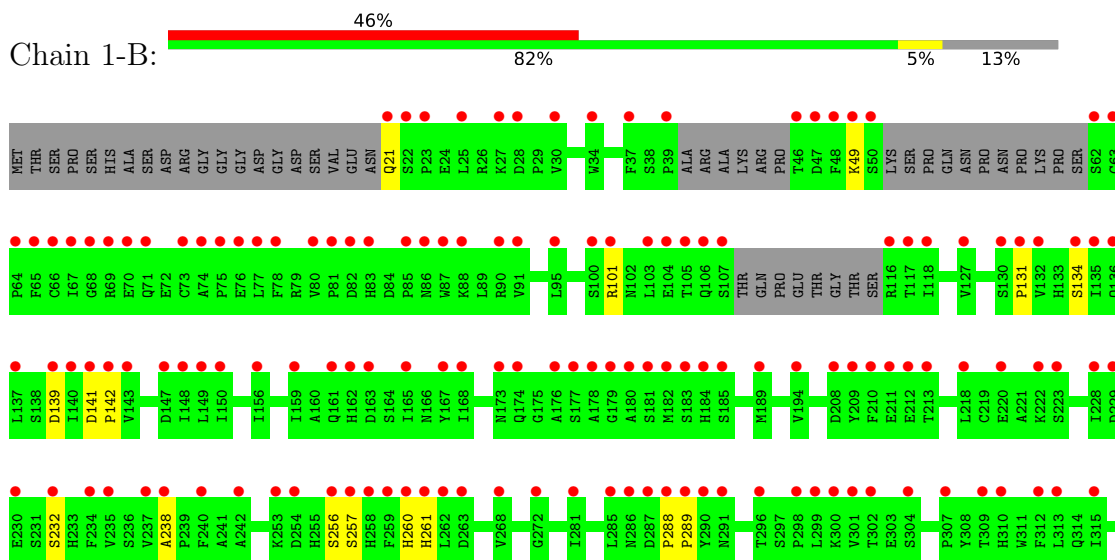
### 3 Residue-property plots

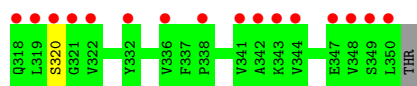
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Probable galactose-1-phosphate uridyl transferase



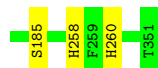
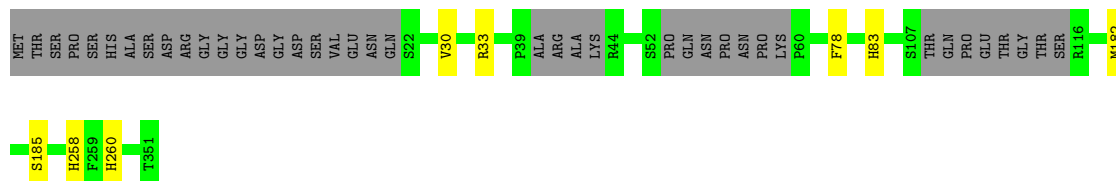
- Molecule 1: Probable galactose-1-phosphate uridyl transferase





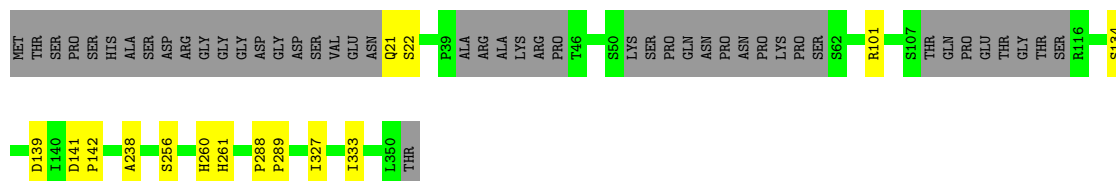
- Molecule 1: Probable galactose-1-phosphate uridyl transferase

Chain 2-A: 86% 11%



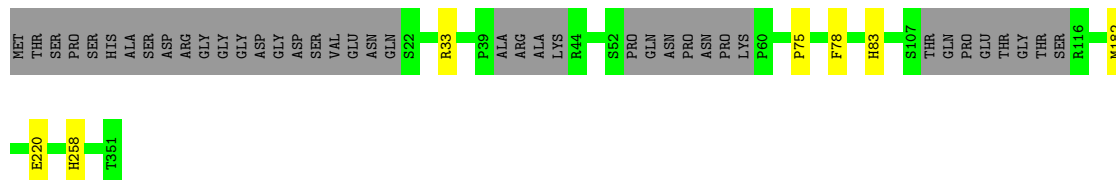
- Molecule 1: Probable galactose-1-phosphate uridyl transferase

Chain 2-B: 83% 13%



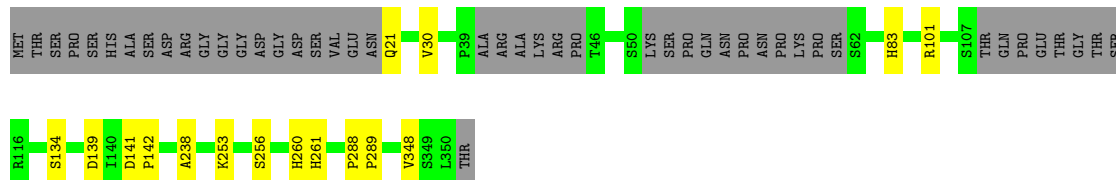
- Molecule 1: Probable galactose-1-phosphate uridyl transferase

Chain 3-A: 87% 11%



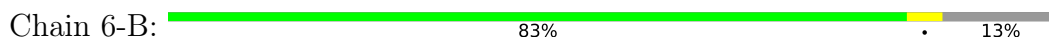
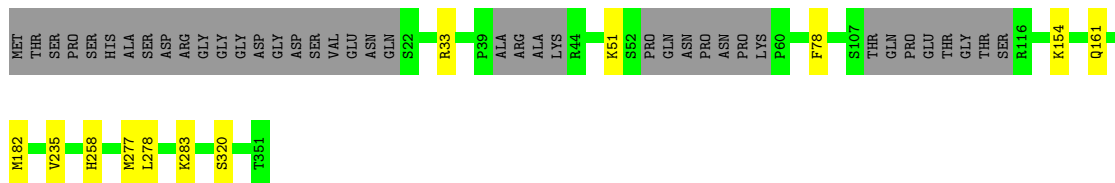
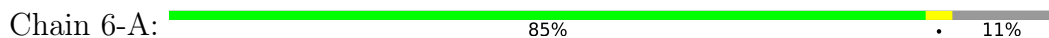
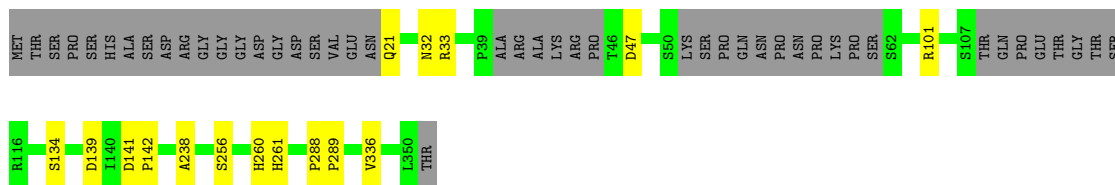
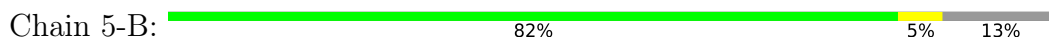
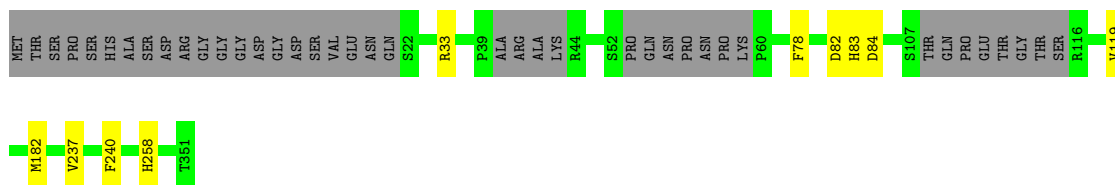
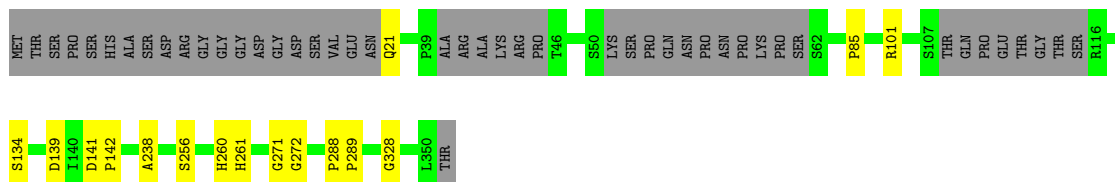
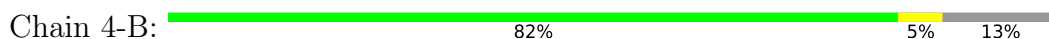
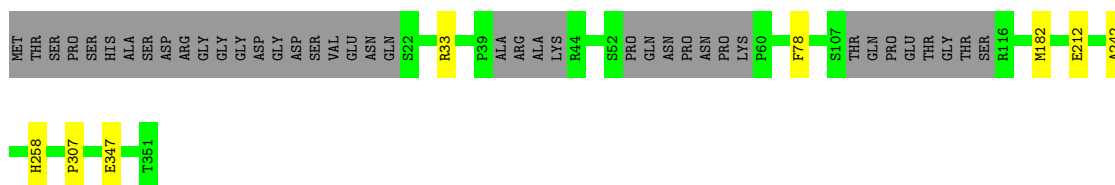
- Molecule 1: Probable galactose-1-phosphate uridyl transferase

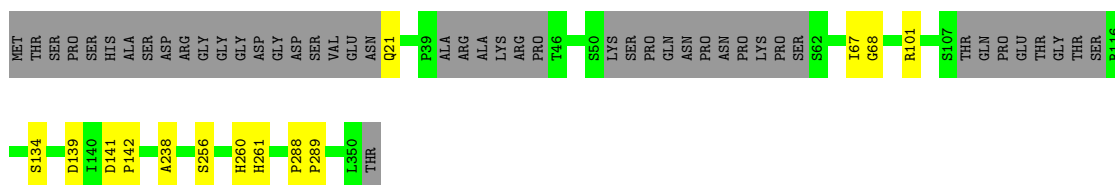
Chain 3-B: 82% 5% 13%



- Molecule 1: Probable galactose-1-phosphate uridyl transferase

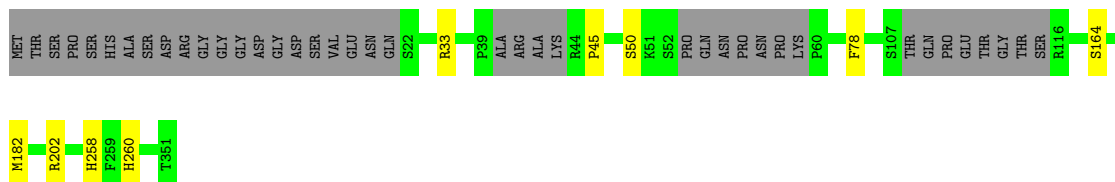
Chain 4-A: 86% 11%





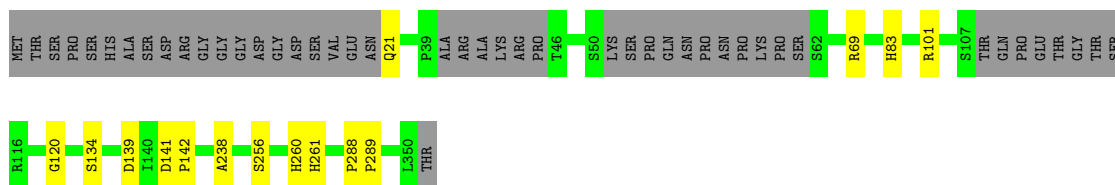
- Molecule 1: Probable galactose-1-phosphate uridyl transferase

Chain 7-A: 86% 11%



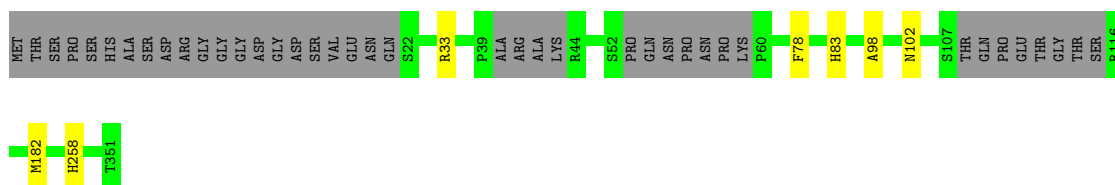
- Molecule 1: Probable galactose-1-phosphate uridyl transferase

Chain 7-B: 83% 13%



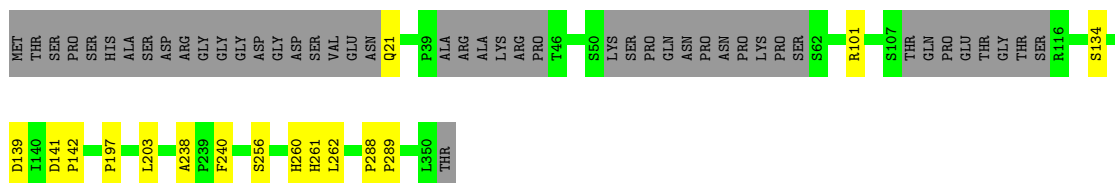
- Molecule 1: Probable galactose-1-phosphate uridyl transferase

Chain 8-A: 87% 11%



- Molecule 1: Probable galactose-1-phosphate uridyl transferase

Chain 8-B: 82% 5% 13%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 62.04Å 95.65Å 110.92Å<br>90.00° 90.00° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 31.28 – 1.83<br>31.28 – 1.83                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.9 (31.28-1.83)<br>98.1 (31.28-1.83)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.87 (at 1.83Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.154 , 0.218<br>0.155 , 0.211                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2903 reflections (4.96%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 22.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.147                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.04 , 50.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.85                                                        | EDS              |
| Total number of atoms                                                   | 43592                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 20.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, ZN, EDO

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   | 1-A   | 0.35         | 0/2529  | 0.43        | 0/3434         |
| 1   | 1-B   | 0.34         | 0/2482  | 0.43        | 1/3372 (0.0%)  |
| 1   | 2-A   | 0.35         | 0/2529  | 0.43        | 0/3434         |
| 1   | 2-B   | 0.34         | 0/2482  | 0.43        | 1/3372 (0.0%)  |
| 1   | 3-A   | 0.35         | 0/2529  | 0.43        | 0/3434         |
| 1   | 3-B   | 0.34         | 0/2482  | 0.43        | 1/3372 (0.0%)  |
| 1   | 4-A   | 0.35         | 0/2529  | 0.43        | 0/3434         |
| 1   | 4-B   | 0.34         | 0/2482  | 0.43        | 1/3372 (0.0%)  |
| 1   | 5-A   | 0.35         | 0/2529  | 0.43        | 0/3434         |
| 1   | 5-B   | 0.34         | 0/2482  | 0.43        | 1/3372 (0.0%)  |
| 1   | 6-A   | 0.35         | 0/2529  | 0.43        | 0/3434         |
| 1   | 6-B   | 0.34         | 0/2482  | 0.43        | 1/3372 (0.0%)  |
| 1   | 7-A   | 0.35         | 0/2529  | 0.43        | 0/3434         |
| 1   | 7-B   | 0.34         | 0/2482  | 0.43        | 1/3372 (0.0%)  |
| 1   | 8-A   | 0.35         | 0/2529  | 0.43        | 0/3434         |
| 1   | 8-B   | 0.34         | 0/2482  | 0.43        | 1/3372 (0.0%)  |
| All | All   | 0.34         | 0/40088 | 0.43        | 8/54448 (0.0%) |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | 1-B   | 238 | ALA  | N-CA-C | -7.00 | 99.47       | 109.62   |
| 1   | 2-B   | 238 | ALA  | N-CA-C | -7.00 | 99.47       | 109.62   |
| 1   | 3-B   | 238 | ALA  | N-CA-C | -7.00 | 99.47       | 109.62   |
| 1   | 4-B   | 238 | ALA  | N-CA-C | -7.00 | 99.47       | 109.62   |
| 1   | 5-B   | 238 | ALA  | N-CA-C | -7.00 | 99.47       | 109.62   |
| 1   | 6-B   | 238 | ALA  | N-CA-C | -7.00 | 99.47       | 109.62   |
| 1   | 7-B   | 238 | ALA  | N-CA-C | -7.00 | 99.47       | 109.62   |
| 1   | 8-B   | 238 | ALA  | N-CA-C | -7.00 | 99.47       | 109.62   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1-A   | 2461  | 0        | 2421     | 0       | 0            |
| 1   | 1-B   | 2416  | 0        | 2369     | 0       | 0            |
| 1   | 2-A   | 2461  | 0        | 2420     | 0       | 0            |
| 1   | 2-B   | 2416  | 0        | 2369     | 0       | 0            |
| 1   | 3-A   | 2461  | 0        | 2419     | 0       | 0            |
| 1   | 3-B   | 2416  | 0        | 2370     | 0       | 0            |
| 1   | 4-A   | 2461  | 0        | 2421     | 0       | 0            |
| 1   | 4-B   | 2416  | 0        | 2369     | 0       | 0            |
| 1   | 5-A   | 2461  | 0        | 2421     | 0       | 0            |
| 1   | 5-B   | 2416  | 0        | 2369     | 0       | 0            |
| 1   | 6-A   | 2461  | 0        | 2420     | 0       | 0            |
| 1   | 6-B   | 2416  | 0        | 2370     | 0       | 0            |
| 1   | 7-A   | 2461  | 0        | 2420     | 0       | 0            |
| 1   | 7-B   | 2416  | 0        | 2370     | 0       | 0            |
| 1   | 8-A   | 2461  | 0        | 2421     | 0       | 0            |
| 1   | 8-B   | 2416  | 0        | 2370     | 0       | 0            |
| 2   | 1-A   | 2     | 0        | 0        | 0       | 0            |
| 2   | 1-B   | 2     | 0        | 0        | 0       | 0            |
| 2   | 2-A   | 2     | 0        | 0        | 0       | 0            |
| 2   | 2-B   | 2     | 0        | 0        | 0       | 0            |
| 2   | 3-A   | 2     | 0        | 0        | 0       | 0            |
| 2   | 3-B   | 2     | 0        | 0        | 0       | 0            |
| 2   | 4-A   | 2     | 0        | 0        | 0       | 0            |
| 2   | 4-B   | 2     | 0        | 0        | 0       | 0            |
| 2   | 5-A   | 2     | 0        | 0        | 0       | 0            |
| 2   | 5-B   | 2     | 0        | 0        | 0       | 0            |
| 2   | 6-A   | 2     | 0        | 0        | 0       | 0            |
| 2   | 6-B   | 2     | 0        | 0        | 0       | 0            |
| 2   | 7-A   | 2     | 0        | 0        | 0       | 0            |
| 2   | 7-B   | 2     | 0        | 0        | 0       | 0            |
| 2   | 8-A   | 2     | 0        | 0        | 0       | 0            |
| 2   | 8-B   | 2     | 0        | 0        | 0       | 0            |
| 3   | 1-A   | 22    | 0        | 12       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | 1-B   | 22    | 0        | 12       | 0       | 0            |
| 3   | 2-A   | 22    | 0        | 12       | 0       | 0            |
| 3   | 2-B   | 22    | 0        | 12       | 0       | 0            |
| 3   | 3-A   | 22    | 0        | 12       | 0       | 0            |
| 3   | 3-B   | 22    | 0        | 12       | 0       | 0            |
| 3   | 4-A   | 22    | 0        | 12       | 0       | 0            |
| 3   | 4-B   | 22    | 0        | 12       | 0       | 0            |
| 3   | 5-A   | 22    | 0        | 11       | 0       | 0            |
| 3   | 5-B   | 22    | 0        | 11       | 0       | 0            |
| 3   | 6-A   | 22    | 0        | 11       | 0       | 0            |
| 3   | 6-B   | 22    | 0        | 11       | 0       | 0            |
| 3   | 7-A   | 22    | 0        | 11       | 0       | 0            |
| 3   | 7-B   | 22    | 0        | 12       | 0       | 0            |
| 3   | 8-A   | 22    | 0        | 11       | 0       | 0            |
| 3   | 8-B   | 22    | 0        | 11       | 0       | 0            |
| 4   | 1-A   | 12    | 0        | 18       | 0       | 0            |
| 4   | 1-B   | 12    | 0        | 18       | 0       | 0            |
| 4   | 2-A   | 12    | 0        | 18       | 0       | 0            |
| 4   | 2-B   | 12    | 0        | 18       | 0       | 0            |
| 4   | 3-A   | 12    | 0        | 18       | 0       | 0            |
| 4   | 3-B   | 12    | 0        | 18       | 0       | 0            |
| 4   | 4-A   | 12    | 0        | 18       | 0       | 0            |
| 4   | 4-B   | 12    | 0        | 18       | 0       | 0            |
| 4   | 5-A   | 12    | 0        | 18       | 0       | 0            |
| 4   | 5-B   | 12    | 0        | 18       | 0       | 0            |
| 4   | 6-A   | 12    | 0        | 18       | 0       | 0            |
| 4   | 6-B   | 12    | 0        | 18       | 0       | 0            |
| 4   | 7-A   | 12    | 0        | 18       | 0       | 0            |
| 4   | 7-B   | 12    | 0        | 18       | 0       | 0            |
| 4   | 8-A   | 12    | 0        | 18       | 0       | 0            |
| 4   | 8-B   | 12    | 0        | 18       | 0       | 0            |
| 5   | 1-A   | 273   | 0        | 0        | 0       | 0            |
| 5   | 1-B   | 227   | 0        | 0        | 0       | 0            |
| 5   | 2-A   | 274   | 0        | 0        | 0       | 0            |
| 5   | 2-B   | 226   | 0        | 0        | 0       | 0            |
| 5   | 3-A   | 270   | 0        | 0        | 0       | 0            |
| 5   | 3-B   | 230   | 0        | 0        | 0       | 0            |
| 5   | 4-A   | 272   | 0        | 0        | 0       | 0            |
| 5   | 4-B   | 228   | 0        | 0        | 0       | 0            |
| 5   | 5-A   | 270   | 0        | 0        | 0       | 0            |
| 5   | 5-B   | 230   | 0        | 0        | 0       | 0            |
| 5   | 6-A   | 270   | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | 6-B   | 230   | 0        | 0        | 0       | 0            |
| 5   | 7-A   | 270   | 0        | 0        | 0       | 0            |
| 5   | 7-B   | 230   | 0        | 0        | 0       | 0            |
| 5   | 8-A   | 271   | 0        | 0        | 0       | 0            |
| 5   | 8-B   | 229   | 0        | 0        | 0       | 0            |
| All | All   | 43592 | 0        | 38792    | 0       | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|---------|----------|-------------|---|
| 1   | 1-A   | 303/351 (86%) | 275 (91%) | 25 (8%) | 3 (1%)   | 12          | 4 |
| 1   | 1-B   | 297/351 (85%) | 270 (91%) | 22 (7%) | 5 (2%)   | 7           | 1 |
| 1   | 2-A   | 303/351 (86%) | 279 (92%) | 20 (7%) | 4 (1%)   | 9           | 2 |
| 1   | 2-B   | 297/351 (85%) | 276 (93%) | 18 (6%) | 3 (1%)   | 12          | 4 |
| 1   | 3-A   | 303/351 (86%) | 282 (93%) | 18 (6%) | 3 (1%)   | 12          | 4 |
| 1   | 3-B   | 297/351 (85%) | 271 (91%) | 22 (7%) | 4 (1%)   | 9           | 2 |
| 1   | 4-A   | 303/351 (86%) | 279 (92%) | 20 (7%) | 4 (1%)   | 9           | 2 |
| 1   | 4-B   | 297/351 (85%) | 266 (90%) | 27 (9%) | 4 (1%)   | 9           | 2 |
| 1   | 5-A   | 303/351 (86%) | 275 (91%) | 22 (7%) | 6 (2%)   | 6           | 0 |
| 1   | 5-B   | 297/351 (85%) | 267 (90%) | 26 (9%) | 4 (1%)   | 9           | 2 |
| 1   | 6-A   | 303/351 (86%) | 268 (88%) | 27 (9%) | 8 (3%)   | 4           | 0 |
| 1   | 6-B   | 297/351 (85%) | 267 (90%) | 28 (9%) | 2 (1%)   | 18          | 7 |
| 1   | 7-A   | 303/351 (86%) | 273 (90%) | 25 (8%) | 5 (2%)   | 7           | 1 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|----------|----------|-------------|---|
| 1   | 7-B   | 297/351 (85%)   | 276 (93%)  | 18 (6%)  | 3 (1%)   | 12          | 4 |
| 1   | 8-A   | 303/351 (86%)   | 290 (96%)  | 10 (3%)  | 3 (1%)   | 12          | 4 |
| 1   | 8-B   | 297/351 (85%)   | 266 (90%)  | 27 (9%)  | 4 (1%)   | 9           | 2 |
| All | All   | 4800/5616 (86%) | 4380 (91%) | 355 (7%) | 65 (1%)  | 9           | 2 |

All (65) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-B   | 320 | SER  |
| 1   | 2-A   | 30  | VAL  |
| 1   | 3-A   | 75  | PRO  |
| 1   | 3-A   | 220 | GLU  |
| 1   | 3-B   | 30  | VAL  |
| 1   | 3-B   | 83  | HIS  |
| 1   | 4-A   | 242 | ALA  |
| 1   | 4-B   | 85  | PRO  |
| 1   | 5-A   | 84  | ASP  |
| 1   | 6-A   | 320 | SER  |
| 1   | 8-A   | 83  | HIS  |
| 1   | 8-B   | 197 | PRO  |
| 1   | 8-B   | 262 | LEU  |
| 1   | 1-A   | 29  | PRO  |
| 1   | 1-B   | 49  | LYS  |
| 1   | 1-B   | 232 | SER  |
| 1   | 2-A   | 185 | SER  |
| 1   | 2-B   | 327 | ILE  |
| 1   | 3-B   | 348 | VAL  |
| 1   | 4-A   | 347 | GLU  |
| 1   | 4-B   | 271 | GLY  |
| 1   | 4-B   | 272 | GLY  |
| 1   | 5-A   | 82  | ASP  |
| 1   | 5-B   | 32  | ASN  |
| 1   | 5-B   | 47  | ASP  |
| 1   | 7-A   | 164 | SER  |
| 1   | 7-B   | 120 | GLY  |
| 1   | 8-A   | 98  | ALA  |
| 1   | 1-A   | 260 | HIS  |
| 1   | 2-A   | 83  | HIS  |
| 1   | 2-A   | 260 | HIS  |
| 1   | 4-B   | 328 | GLY  |
| 1   | 5-A   | 119 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5-A   | 240 | PHE  |
| 1   | 5-B   | 336 | VAL  |
| 1   | 6-A   | 51  | LYS  |
| 1   | 6-A   | 154 | LYS  |
| 1   | 6-A   | 161 | GLN  |
| 1   | 6-A   | 277 | MET  |
| 1   | 6-A   | 283 | LYS  |
| 1   | 7-B   | 83  | HIS  |
| 1   | 8-A   | 102 | ASN  |
| 1   | 4-A   | 212 | GLU  |
| 1   | 4-A   | 307 | PRO  |
| 1   | 5-A   | 83  | HIS  |
| 1   | 5-B   | 33  | ARG  |
| 1   | 6-A   | 278 | LEU  |
| 1   | 7-A   | 50  | SER  |
| 1   | 7-A   | 202 | ARG  |
| 1   | 1-B   | 257 | SER  |
| 1   | 2-B   | 22  | SER  |
| 1   | 2-B   | 333 | ILE  |
| 1   | 3-A   | 83  | HIS  |
| 1   | 3-B   | 253 | LYS  |
| 1   | 6-A   | 235 | VAL  |
| 1   | 6-B   | 68  | GLY  |
| 1   | 8-B   | 203 | LEU  |
| 1   | 8-B   | 240 | PHE  |
| 1   | 7-A   | 45  | PRO  |
| 1   | 7-A   | 260 | HIS  |
| 1   | 7-B   | 69  | ARG  |
| 1   | 6-B   | 67  | ILE  |
| 1   | 1-A   | 45  | PRO  |
| 1   | 1-B   | 131 | PRO  |
| 1   | 5-A   | 237 | 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   | 1-A   | 280/312 (90%)   | 276 (99%)  | 4 (1%)   | 59          | 45 |
| 1   | 1-B   | 274/312 (88%)   | 263 (96%)  | 11 (4%)  | 28          | 11 |
| 1   | 2-A   | 280/312 (90%)   | 276 (99%)  | 4 (1%)   | 59          | 45 |
| 1   | 2-B   | 274/312 (88%)   | 263 (96%)  | 11 (4%)  | 28          | 11 |
| 1   | 3-A   | 280/312 (90%)   | 276 (99%)  | 4 (1%)   | 59          | 45 |
| 1   | 3-B   | 274/312 (88%)   | 263 (96%)  | 11 (4%)  | 28          | 11 |
| 1   | 4-A   | 280/312 (90%)   | 276 (99%)  | 4 (1%)   | 59          | 45 |
| 1   | 4-B   | 274/312 (88%)   | 263 (96%)  | 11 (4%)  | 28          | 11 |
| 1   | 5-A   | 280/312 (90%)   | 276 (99%)  | 4 (1%)   | 59          | 45 |
| 1   | 5-B   | 274/312 (88%)   | 263 (96%)  | 11 (4%)  | 28          | 11 |
| 1   | 6-A   | 280/312 (90%)   | 276 (99%)  | 4 (1%)   | 59          | 45 |
| 1   | 6-B   | 274/312 (88%)   | 263 (96%)  | 11 (4%)  | 28          | 11 |
| 1   | 7-A   | 280/312 (90%)   | 276 (99%)  | 4 (1%)   | 59          | 45 |
| 1   | 7-B   | 274/312 (88%)   | 263 (96%)  | 11 (4%)  | 28          | 11 |
| 1   | 8-A   | 280/312 (90%)   | 276 (99%)  | 4 (1%)   | 59          | 45 |
| 1   | 8-B   | 274/312 (88%)   | 263 (96%)  | 11 (4%)  | 28          | 11 |
| All | All   | 4432/4992 (89%) | 4312 (97%) | 120 (3%) | 39          | 22 |

All (120) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 33  | ARG  |
| 1   | 1-A   | 78  | PHE  |
| 1   | 1-A   | 182 | MET  |
| 1   | 1-A   | 258 | HIS  |
| 1   | 1-B   | 21  | GLN  |
| 1   | 1-B   | 101 | ARG  |
| 1   | 1-B   | 134 | SER  |
| 1   | 1-B   | 139 | ASP  |
| 1   | 1-B   | 141 | ASP  |
| 1   | 1-B   | 142 | PRO  |
| 1   | 1-B   | 256 | SER  |
| 1   | 1-B   | 260 | HIS  |
| 1   | 1-B   | 261 | HIS  |
| 1   | 1-B   | 288 | PRO  |
| 1   | 1-B   | 289 | PRO  |
| 1   | 2-A   | 33  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2-A   | 78  | PHE  |
| 1   | 2-A   | 182 | MET  |
| 1   | 2-A   | 258 | HIS  |
| 1   | 2-B   | 21  | GLN  |
| 1   | 2-B   | 101 | ARG  |
| 1   | 2-B   | 134 | SER  |
| 1   | 2-B   | 139 | ASP  |
| 1   | 2-B   | 141 | ASP  |
| 1   | 2-B   | 142 | PRO  |
| 1   | 2-B   | 256 | SER  |
| 1   | 2-B   | 260 | HIS  |
| 1   | 2-B   | 261 | HIS  |
| 1   | 2-B   | 288 | PRO  |
| 1   | 2-B   | 289 | PRO  |
| 1   | 3-A   | 33  | ARG  |
| 1   | 3-A   | 78  | PHE  |
| 1   | 3-A   | 182 | MET  |
| 1   | 3-A   | 258 | HIS  |
| 1   | 3-B   | 21  | GLN  |
| 1   | 3-B   | 101 | ARG  |
| 1   | 3-B   | 134 | SER  |
| 1   | 3-B   | 139 | ASP  |
| 1   | 3-B   | 141 | ASP  |
| 1   | 3-B   | 142 | PRO  |
| 1   | 3-B   | 256 | SER  |
| 1   | 3-B   | 260 | HIS  |
| 1   | 3-B   | 261 | HIS  |
| 1   | 3-B   | 288 | PRO  |
| 1   | 3-B   | 289 | PRO  |
| 1   | 4-A   | 33  | ARG  |
| 1   | 4-A   | 78  | PHE  |
| 1   | 4-A   | 182 | MET  |
| 1   | 4-A   | 258 | HIS  |
| 1   | 4-B   | 21  | GLN  |
| 1   | 4-B   | 101 | ARG  |
| 1   | 4-B   | 134 | SER  |
| 1   | 4-B   | 139 | ASP  |
| 1   | 4-B   | 141 | ASP  |
| 1   | 4-B   | 142 | PRO  |
| 1   | 4-B   | 256 | SER  |
| 1   | 4-B   | 260 | HIS  |
| 1   | 4-B   | 261 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 4-B   | 288 | PRO  |
| 1   | 4-B   | 289 | PRO  |
| 1   | 5-A   | 33  | ARG  |
| 1   | 5-A   | 78  | PHE  |
| 1   | 5-A   | 182 | MET  |
| 1   | 5-A   | 258 | HIS  |
| 1   | 5-B   | 21  | GLN  |
| 1   | 5-B   | 101 | ARG  |
| 1   | 5-B   | 134 | SER  |
| 1   | 5-B   | 139 | ASP  |
| 1   | 5-B   | 141 | ASP  |
| 1   | 5-B   | 142 | PRO  |
| 1   | 5-B   | 256 | SER  |
| 1   | 5-B   | 260 | HIS  |
| 1   | 5-B   | 261 | HIS  |
| 1   | 5-B   | 288 | PRO  |
| 1   | 5-B   | 289 | PRO  |
| 1   | 6-A   | 33  | ARG  |
| 1   | 6-A   | 78  | PHE  |
| 1   | 6-A   | 182 | MET  |
| 1   | 6-A   | 258 | HIS  |
| 1   | 6-B   | 21  | GLN  |
| 1   | 6-B   | 101 | ARG  |
| 1   | 6-B   | 134 | SER  |
| 1   | 6-B   | 139 | ASP  |
| 1   | 6-B   | 141 | ASP  |
| 1   | 6-B   | 142 | PRO  |
| 1   | 6-B   | 256 | SER  |
| 1   | 6-B   | 260 | HIS  |
| 1   | 6-B   | 261 | HIS  |
| 1   | 6-B   | 288 | PRO  |
| 1   | 6-B   | 289 | PRO  |
| 1   | 7-A   | 33  | ARG  |
| 1   | 7-A   | 78  | PHE  |
| 1   | 7-A   | 182 | MET  |
| 1   | 7-A   | 258 | HIS  |
| 1   | 7-B   | 21  | GLN  |
| 1   | 7-B   | 101 | ARG  |
| 1   | 7-B   | 134 | SER  |
| 1   | 7-B   | 139 | ASP  |
| 1   | 7-B   | 141 | ASP  |
| 1   | 7-B   | 142 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 7-B   | 256 | SER  |
| 1   | 7-B   | 260 | HIS  |
| 1   | 7-B   | 261 | HIS  |
| 1   | 7-B   | 288 | PRO  |
| 1   | 7-B   | 289 | PRO  |
| 1   | 8-A   | 33  | ARG  |
| 1   | 8-A   | 78  | PHE  |
| 1   | 8-A   | 182 | MET  |
| 1   | 8-A   | 258 | HIS  |
| 1   | 8-B   | 21  | GLN  |
| 1   | 8-B   | 101 | ARG  |
| 1   | 8-B   | 134 | SER  |
| 1   | 8-B   | 139 | ASP  |
| 1   | 8-B   | 141 | ASP  |
| 1   | 8-B   | 142 | PRO  |
| 1   | 8-B   | 256 | SER  |
| 1   | 8-B   | 260 | HIS  |
| 1   | 8-B   | 261 | HIS  |
| 1   | 8-B   | 288 | PRO  |
| 1   | 8-B   | 289 | PRO  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1-A   | 86  | ASN  |
| 1   | 1-A   | 173 | ASN  |
| 1   | 1-A   | 260 | HIS  |
| 1   | 1-A   | 261 | HIS  |
| 1   | 1-A   | 286 | ASN  |
| 1   | 1-A   | 291 | ASN  |
| 1   | 1-A   | 314 | GLN  |
| 1   | 1-B   | 106 | GLN  |
| 1   | 1-B   | 166 | ASN  |
| 1   | 1-B   | 169 | GLN  |
| 1   | 1-B   | 284 | GLN  |
| 1   | 1-B   | 286 | ASN  |
| 1   | 1-B   | 291 | ASN  |
| 1   | 1-B   | 318 | GLN  |
| 1   | 2-A   | 94  | ASN  |
| 1   | 2-A   | 158 | GLN  |
| 1   | 2-A   | 233 | HIS  |
| 1   | 2-A   | 261 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2-A   | 318 | GLN  |
| 1   | 2-B   | 32  | ASN  |
| 1   | 2-B   | 83  | HIS  |
| 1   | 2-B   | 106 | GLN  |
| 1   | 2-B   | 161 | GLN  |
| 1   | 2-B   | 174 | GLN  |
| 1   | 2-B   | 186 | HIS  |
| 1   | 2-B   | 291 | ASN  |
| 1   | 2-B   | 318 | GLN  |
| 1   | 3-A   | 86  | ASN  |
| 1   | 3-A   | 162 | HIS  |
| 1   | 3-A   | 260 | HIS  |
| 1   | 3-B   | 21  | GLN  |
| 1   | 3-B   | 106 | GLN  |
| 1   | 3-B   | 136 | GLN  |
| 1   | 3-B   | 166 | ASN  |
| 1   | 3-B   | 174 | GLN  |
| 1   | 3-B   | 284 | GLN  |
| 1   | 3-B   | 286 | ASN  |
| 1   | 3-B   | 318 | GLN  |
| 1   | 4-A   | 86  | ASN  |
| 1   | 4-A   | 169 | GLN  |
| 1   | 4-A   | 186 | HIS  |
| 1   | 4-A   | 233 | HIS  |
| 1   | 4-A   | 261 | HIS  |
| 1   | 4-A   | 286 | ASN  |
| 1   | 4-A   | 310 | HIS  |
| 1   | 4-B   | 32  | ASN  |
| 1   | 4-B   | 83  | HIS  |
| 1   | 4-B   | 106 | GLN  |
| 1   | 4-B   | 157 | ASN  |
| 1   | 4-B   | 173 | ASN  |
| 1   | 4-B   | 258 | HIS  |
| 1   | 4-B   | 260 | HIS  |
| 1   | 4-B   | 279 | GLN  |
| 1   | 4-B   | 286 | ASN  |
| 1   | 4-B   | 291 | ASN  |
| 1   | 5-A   | 71  | GLN  |
| 1   | 5-A   | 86  | ASN  |
| 1   | 5-A   | 174 | GLN  |
| 1   | 5-A   | 260 | HIS  |
| 1   | 5-A   | 261 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5-A   | 279 | GLN  |
| 1   | 5-A   | 284 | GLN  |
| 1   | 5-A   | 334 | ASN  |
| 1   | 5-B   | 83  | HIS  |
| 1   | 5-B   | 106 | GLN  |
| 1   | 5-B   | 174 | GLN  |
| 1   | 5-B   | 233 | HIS  |
| 1   | 5-B   | 258 | HIS  |
| 1   | 5-B   | 291 | ASN  |
| 1   | 6-A   | 86  | ASN  |
| 1   | 6-A   | 166 | ASN  |
| 1   | 6-A   | 174 | GLN  |
| 1   | 6-A   | 188 | GLN  |
| 1   | 6-A   | 233 | HIS  |
| 1   | 6-A   | 284 | GLN  |
| 1   | 6-A   | 318 | GLN  |
| 1   | 6-B   | 21  | GLN  |
| 1   | 6-B   | 83  | HIS  |
| 1   | 6-B   | 136 | GLN  |
| 1   | 6-B   | 161 | GLN  |
| 1   | 6-B   | 258 | HIS  |
| 1   | 6-B   | 260 | HIS  |
| 1   | 7-A   | 318 | GLN  |
| 1   | 7-A   | 334 | ASN  |
| 1   | 7-B   | 83  | HIS  |
| 1   | 7-B   | 136 | GLN  |
| 1   | 7-B   | 161 | GLN  |
| 1   | 7-B   | 174 | GLN  |
| 1   | 7-B   | 260 | HIS  |
| 1   | 8-A   | 86  | ASN  |
| 1   | 8-A   | 260 | HIS  |
| 1   | 8-A   | 334 | ASN  |
| 1   | 8-B   | 136 | GLN  |
| 1   | 8-B   | 161 | GLN  |
| 1   | 8-B   | 169 | GLN  |
| 1   | 8-B   | 174 | GLN  |
| 1   | 8-B   | 261 | HIS  |
| 1   | 8-B   | 314 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 96 ligands modelled in this entry, 32 are monoatomic - leaving 64 for Mogul analysis.

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   | EDO  | 6-A   | 608 | -    | 3,3,3        | 0.58 | 0           | 2,2,2       | 0.46 | 0           |
| 4   | EDO  | 6-A   | 609 | -    | 3,3,3        | 0.35 | 0           | 2,2,2       | 0.55 | 0           |
| 4   | EDO  | 1-B   | 610 | -    | 3,3,3        | 0.48 | 0           | 2,2,2       | 0.33 | 0           |
| 3   | AMP  | 6-A   | 601 | -    | 21,24,25     | 2.00 | 7 (33%)     | 30,35,38    | 2.35 | 12 (40%)    |
| 4   | EDO  | 2-A   | 607 | -    | 3,3,3        | 0.40 | 0           | 2,2,2       | 0.38 | 0           |
| 3   | AMP  | 8-A   | 601 | -    | 21,24,25     | 2.08 | 7 (33%)     | 30,35,38    | 2.38 | 13 (43%)    |
| 4   | EDO  | 5-A   | 608 | -    | 3,3,3        | 0.61 | 0           | 2,2,2       | 0.37 | 0           |
| 4   | EDO  | 8-B   | 610 | -    | 3,3,3        | 0.65 | 0           | 2,2,2       | 0.15 | 0           |
| 4   | EDO  | 7-A   | 607 | -    | 3,3,3        | 0.44 | 0           | 2,2,2       | 0.40 | 0           |
| 4   | EDO  | 6-A   | 607 | -    | 3,3,3        | 0.47 | 0           | 2,2,2       | 0.30 | 0           |
| 4   | EDO  | 3-A   | 608 | -    | 3,3,3        | 0.57 | 0           | 2,2,2       | 0.45 | 0           |
| 4   | EDO  | 1-A   | 609 | -    | 3,3,3        | 0.30 | 0           | 2,2,2       | 0.50 | 0           |
| 3   | AMP  | 5-A   | 601 | -    | 21,24,25     | 2.20 | 8 (38%)     | 30,35,38    | 2.49 | 15 (50%)    |
| 4   | EDO  | 1-B   | 612 | -    | 3,3,3        | 0.27 | 0           | 2,2,2       | 0.47 | 0           |
| 4   | EDO  | 8-A   | 607 | -    | 3,3,3        | 0.48 | 0           | 2,2,2       | 0.37 | 0           |
| 3   | AMP  | 5-B   | 602 | -    | 21,24,25     | 1.82 | 8 (38%)     | 30,35,38    | 2.21 | 9 (30%)     |
| 4   | EDO  | 2-B   | 612 | -    | 3,3,3        | 0.27 | 0           | 2,2,2       | 0.49 | 0           |
| 4   | EDO  | 5-B   | 611 | -    | 3,3,3        | 0.63 | 0           | 2,2,2       | 0.32 | 0           |
| 3   | AMP  | 1-A   | 601 | -    | 21,24,25     | 1.73 | 5 (23%)     | 30,35,38    | 2.07 | 10 (33%)    |
| 4   | EDO  | 7-B   | 611 | -    | 3,3,3        | 0.56 | 0           | 2,2,2       | 0.36 | 0           |
| 4   | EDO  | 2-B   | 610 | -    | 3,3,3        | 0.55 | 0           | 2,2,2       | 0.36 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | AMP  | 7-B   | 602 | -    | 21,24,25     | 1.79 | 5 (23%)  | 30,35,38    | 2.11 | 10 (33%) |
| 4   | EDO  | 5-A   | 607 | -    | 3,3,3        | 0.57 | 0        | 2,2,2       | 0.21 | 0        |
| 4   | EDO  | 4-A   | 609 | -    | 3,3,3        | 0.35 | 0        | 2,2,2       | 0.50 | 0        |
| 4   | EDO  | 1-B   | 611 | -    | 3,3,3        | 0.55 | 0        | 2,2,2       | 0.37 | 0        |
| 3   | AMP  | 7-A   | 601 | -    | 21,24,25     | 1.95 | 6 (28%)  | 30,35,38    | 2.32 | 9 (30%)  |
| 4   | EDO  | 6-B   | 610 | -    | 3,3,3        | 0.61 | 0        | 2,2,2       | 0.22 | 0        |
| 4   | EDO  | 8-B   | 612 | -    | 3,3,3        | 0.23 | 0        | 2,2,2       | 0.51 | 0        |
| 4   | EDO  | 2-A   | 608 | -    | 3,3,3        | 0.54 | 0        | 2,2,2       | 0.52 | 0        |
| 4   | EDO  | 4-B   | 611 | -    | 3,3,3        | 0.53 | 0        | 2,2,2       | 0.33 | 0        |
| 4   | EDO  | 7-A   | 608 | -    | 3,3,3        | 0.57 | 0        | 2,2,2       | 0.43 | 0        |
| 3   | AMP  | 2-A   | 601 | -    | 21,24,25     | 1.74 | 4 (19%)  | 30,35,38    | 2.13 | 10 (33%) |
| 4   | EDO  | 3-B   | 610 | -    | 3,3,3        | 0.55 | 0        | 2,2,2       | 0.21 | 0        |
| 4   | EDO  | 4-A   | 607 | -    | 3,3,3        | 0.51 | 0        | 2,2,2       | 0.39 | 0        |
| 4   | EDO  | 1-A   | 608 | -    | 3,3,3        | 0.58 | 0        | 2,2,2       | 0.50 | 0        |
| 4   | EDO  | 5-B   | 610 | -    | 3,3,3        | 0.48 | 0        | 2,2,2       | 0.32 | 0        |
| 4   | EDO  | 4-B   | 612 | -    | 3,3,3        | 0.27 | 0        | 2,2,2       | 0.50 | 0        |
| 4   | EDO  | 5-B   | 612 | -    | 3,3,3        | 0.26 | 0        | 2,2,2       | 0.53 | 0        |
| 3   | AMP  | 3-B   | 602 | -    | 21,24,25     | 1.59 | 4 (19%)  | 30,35,38    | 2.02 | 11 (36%) |
| 3   | AMP  | 8-B   | 602 | -    | 21,24,25     | 1.71 | 7 (33%)  | 30,35,38    | 2.17 | 11 (36%) |
| 4   | EDO  | 6-B   | 612 | -    | 3,3,3        | 0.90 | 0        | 2,2,2       | 0.35 | 0        |
| 3   | AMP  | 3-A   | 601 | -    | 21,24,25     | 1.76 | 5 (23%)  | 30,35,38    | 2.03 | 8 (26%)  |
| 3   | AMP  | 4-A   | 601 | -    | 21,24,25     | 1.70 | 5 (23%)  | 30,35,38    | 2.04 | 9 (30%)  |
| 4   | EDO  | 7-B   | 612 | -    | 3,3,3        | 0.31 | 0        | 2,2,2       | 0.57 | 0        |
| 4   | EDO  | 3-B   | 611 | -    | 3,3,3        | 0.55 | 0        | 2,2,2       | 0.36 | 0        |
| 3   | AMP  | 1-B   | 602 | -    | 21,24,25     | 1.54 | 4 (19%)  | 30,35,38    | 1.99 | 8 (26%)  |
| 4   | EDO  | 2-B   | 611 | -    | 3,3,3        | 0.54 | 0        | 2,2,2       | 0.36 | 0        |
| 4   | EDO  | 3-A   | 609 | -    | 3,3,3        | 0.29 | 0        | 2,2,2       | 0.47 | 0        |
| 4   | EDO  | 7-B   | 610 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.28 | 0        |
| 3   | AMP  | 2-B   | 602 | -    | 21,24,25     | 1.64 | 5 (23%)  | 30,35,38    | 2.08 | 10 (33%) |
| 4   | EDO  | 3-B   | 612 | -    | 3,3,3        | 0.25 | 0        | 2,2,2       | 0.47 | 0        |
| 4   | EDO  | 8-B   | 611 | -    | 3,3,3        | 0.56 | 0        | 2,2,2       | 0.37 | 0        |
| 4   | EDO  | 1-A   | 607 | -    | 3,3,3        | 0.46 | 0        | 2,2,2       | 0.32 | 0        |
| 4   | EDO  | 3-A   | 607 | -    | 3,3,3        | 0.44 | 0        | 2,2,2       | 0.49 | 0        |
| 4   | EDO  | 8-A   | 608 | -    | 3,3,3        | 0.58 | 0        | 2,2,2       | 0.51 | 0        |
| 4   | EDO  | 4-B   | 610 | -    | 3,3,3        | 0.62 | 0        | 2,2,2       | 0.14 | 0        |
| 3   | AMP  | 6-B   | 602 | -    | 21,24,25     | 1.81 | 6 (28%)  | 30,35,38    | 2.24 | 10 (33%) |
| 4   | EDO  | 5-A   | 609 | -    | 3,3,3        | 0.30 | 0        | 2,2,2       | 0.51 | 0        |
| 4   | EDO  | 4-A   | 608 | -    | 3,3,3        | 0.57 | 0        | 2,2,2       | 0.49 | 0        |
| 4   | EDO  | 6-B   | 611 | -    | 3,3,3        | 0.57 | 0        | 2,2,2       | 0.32 | 0        |
| 4   | EDO  | 8-A   | 609 | -    | 3,3,3        | 0.35 | 0        | 2,2,2       | 0.47 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | AMP  | 4-B   | 602 | -    | 21,24,25     | 1.75 | 5 (23%)  | 30,35,38    | 2.04 | 10 (33%) |
| 4   | EDO  | 2-A   | 609 | -    | 3,3,3        | 0.28 | 0        | 2,2,2       | 0.49 | 0        |
| 4   | EDO  | 7-A   | 609 | -    | 3,3,3        | 0.65 | 0        | 2,2,2       | 0.23 | 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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | EDO  | 6-A   | 608 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 6-A   | 609 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 1-B   | 610 | -    | -       | 1/1/1/1   | -       |
| 3   | AMP  | 6-A   | 601 | -    | -       | 2/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 2-A   | 607 | -    | -       | 0/1/1/1   | -       |
| 3   | AMP  | 8-A   | 601 | -    | -       | 1/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 5-A   | 608 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 8-B   | 610 | -    | -       | 1/1/1/1   | -       |
| 4   | EDO  | 7-A   | 607 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 6-A   | 607 | -    | -       | 1/1/1/1   | -       |
| 4   | EDO  | 3-A   | 608 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 1-A   | 609 | -    | -       | 0/1/1/1   | -       |
| 3   | AMP  | 5-A   | 601 | -    | -       | 2/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 1-B   | 612 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 8-A   | 607 | -    | -       | 1/1/1/1   | -       |
| 3   | AMP  | 5-B   | 602 | -    | -       | 2/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 2-B   | 612 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 5-B   | 611 | -    | -       | 0/1/1/1   | -       |
| 3   | AMP  | 1-A   | 601 | -    | -       | 3/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 7-B   | 611 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 2-B   | 610 | -    | -       | 0/1/1/1   | -       |
| 3   | AMP  | 7-B   | 602 | -    | -       | 2/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 5-A   | 607 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 4-A   | 609 | -    | -       | 1/1/1/1   | -       |
| 4   | EDO  | 1-B   | 611 | -    | -       | 0/1/1/1   | -       |
| 3   | AMP  | 7-A   | 601 | -    | -       | 3/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 6-B   | 610 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 8-B   | 612 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 2-A   | 608 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 4-B   | 611 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 7-A   | 608 | -    | -       | 0/1/1/1   | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | AMP  | 2-A   | 601 | -    | -       | 1/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 3-B   | 610 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 4-A   | 607 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 1-A   | 608 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 5-B   | 610 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 4-B   | 612 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 5-B   | 612 | -    | -       | 0/1/1/1   | -       |
| 3   | AMP  | 3-B   | 602 | -    | -       | 5/7/25/26 | 0/3/3/3 |
| 3   | AMP  | 8-B   | 602 | -    | -       | 3/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 6-B   | 612 | -    | -       | 0/1/1/1   | -       |
| 3   | AMP  | 3-A   | 601 | -    | -       | 4/7/25/26 | 0/3/3/3 |
| 3   | AMP  | 4-A   | 601 | -    | -       | 5/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 7-B   | 612 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 3-B   | 611 | -    | -       | 0/1/1/1   | -       |
| 3   | AMP  | 1-B   | 602 | -    | -       | 1/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 2-B   | 611 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 3-A   | 609 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 7-B   | 610 | -    | -       | 1/1/1/1   | -       |
| 3   | AMP  | 2-B   | 602 | -    | -       | 4/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 3-B   | 612 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 8-B   | 611 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 1-A   | 607 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 3-A   | 607 | -    | -       | 1/1/1/1   | -       |
| 4   | EDO  | 8-A   | 608 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 4-B   | 610 | -    | -       | 1/1/1/1   | -       |
| 3   | AMP  | 6-B   | 602 | -    | -       | 1/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 5-A   | 609 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 4-A   | 608 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 6-B   | 611 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 8-A   | 609 | -    | -       | 1/1/1/1   | -       |
| 3   | AMP  | 4-B   | 602 | -    | -       | 5/7/25/26 | 0/3/3/3 |
| 4   | EDO  | 2-A   | 609 | -    | -       | 0/1/1/1   | -       |
| 4   | EDO  | 7-A   | 609 | -    | -       | 1/1/1/1   | -       |

All (91) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | 4-A   | 601 | AMP  | C2-N3   | 4.56  | 1.42        | 1.33     |
| 3   | 8-A   | 601 | AMP  | O5'-C5' | -4.44 | 1.31        | 1.44     |
| 3   | 3-A   | 601 | AMP  | C2-N3   | 4.36  | 1.41        | 1.33     |
| 3   | 1-A   | 601 | AMP  | C2-N3   | 4.34  | 1.41        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | 2-A   | 601 | AMP  | C2-N3   | 4.33  | 1.41        | 1.33     |
| 3   | 6-A   | 601 | AMP  | C2-N3   | 4.33  | 1.41        | 1.33     |
| 3   | 5-A   | 601 | AMP  | O5'-C5' | -4.31 | 1.31        | 1.44     |
| 3   | 7-A   | 601 | AMP  | C2-N3   | 4.18  | 1.41        | 1.33     |
| 3   | 8-A   | 601 | AMP  | C2-N3   | 4.10  | 1.41        | 1.33     |
| 3   | 5-A   | 601 | AMP  | C2-N3   | 4.08  | 1.41        | 1.33     |
| 3   | 6-A   | 601 | AMP  | C2-N1   | 3.89  | 1.40        | 1.33     |
| 3   | 7-B   | 602 | AMP  | C2-N1   | 3.88  | 1.40        | 1.33     |
| 3   | 8-A   | 601 | AMP  | C2-N1   | 3.87  | 1.40        | 1.33     |
| 3   | 5-A   | 601 | AMP  | C2-N1   | 3.83  | 1.40        | 1.33     |
| 3   | 1-A   | 601 | AMP  | C2-N1   | 3.69  | 1.40        | 1.33     |
| 3   | 2-A   | 601 | AMP  | C2-N1   | 3.65  | 1.40        | 1.33     |
| 3   | 5-B   | 602 | AMP  | C8-N7   | 3.62  | 1.38        | 1.31     |
| 3   | 4-B   | 602 | AMP  | C2-N1   | 3.62  | 1.40        | 1.33     |
| 3   | 6-A   | 601 | AMP  | O5'-C5' | -3.61 | 1.33        | 1.44     |
| 3   | 7-A   | 601 | AMP  | C2-N1   | 3.61  | 1.40        | 1.33     |
| 3   | 6-B   | 602 | AMP  | C8-N7   | 3.60  | 1.38        | 1.31     |
| 3   | 5-B   | 602 | AMP  | C2-N1   | 3.55  | 1.40        | 1.33     |
| 3   | 3-A   | 601 | AMP  | C2-N1   | 3.54  | 1.40        | 1.33     |
| 3   | 7-B   | 602 | AMP  | C2-N3   | 3.45  | 1.40        | 1.33     |
| 3   | 7-B   | 602 | AMP  | C8-N7   | 3.45  | 1.38        | 1.31     |
| 3   | 4-A   | 601 | AMP  | C2-N1   | 3.44  | 1.40        | 1.33     |
| 3   | 8-B   | 602 | AMP  | O5'-C5' | -3.43 | 1.34        | 1.44     |
| 3   | 1-B   | 602 | AMP  | C2-N1   | 3.38  | 1.39        | 1.33     |
| 3   | 2-B   | 602 | AMP  | C2-N1   | 3.37  | 1.39        | 1.33     |
| 3   | 4-B   | 602 | AMP  | C8-N7   | 3.29  | 1.38        | 1.31     |
| 3   | 2-B   | 602 | AMP  | C8-N7   | 3.28  | 1.38        | 1.31     |
| 3   | 6-B   | 602 | AMP  | C2-N1   | 3.26  | 1.39        | 1.33     |
| 3   | 6-B   | 602 | AMP  | C2-N3   | 3.14  | 1.39        | 1.33     |
| 3   | 1-B   | 602 | AMP  | C2-N3   | 3.13  | 1.39        | 1.33     |
| 3   | 8-A   | 601 | AMP  | C4-N3   | 3.13  | 1.40        | 1.34     |
| 3   | 3-B   | 602 | AMP  | C2-N1   | 3.13  | 1.39        | 1.33     |
| 3   | 5-B   | 602 | AMP  | C2-N3   | 3.11  | 1.39        | 1.33     |
| 3   | 4-B   | 602 | AMP  | C2-N3   | 3.08  | 1.39        | 1.33     |
| 3   | 1-B   | 602 | AMP  | C8-N7   | 3.06  | 1.37        | 1.31     |
| 3   | 7-A   | 601 | AMP  | O5'-C5' | -3.05 | 1.35        | 1.44     |
| 3   | 8-B   | 602 | AMP  | C8-N7   | 3.04  | 1.37        | 1.31     |
| 3   | 8-B   | 602 | AMP  | C2-N3   | 3.01  | 1.39        | 1.33     |
| 3   | 6-A   | 601 | AMP  | C4-N3   | 2.99  | 1.40        | 1.34     |
| 3   | 3-B   | 602 | AMP  | C2-N3   | 2.98  | 1.39        | 1.33     |
| 3   | 7-A   | 601 | AMP  | C4-N3   | 2.94  | 1.39        | 1.34     |
| 3   | 2-A   | 601 | AMP  | C4-N3   | 2.94  | 1.39        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | 5-A   | 601 | AMP  | C4-N3   | 2.91  | 1.39        | 1.34     |
| 3   | 6-B   | 602 | AMP  | O5'-C5' | -2.91 | 1.35        | 1.44     |
| 3   | 8-B   | 602 | AMP  | C2-N1   | 2.89  | 1.39        | 1.33     |
| 3   | 3-B   | 602 | AMP  | C8-N7   | 2.82  | 1.37        | 1.31     |
| 3   | 1-A   | 601 | AMP  | C4-N3   | 2.82  | 1.39        | 1.34     |
| 3   | 2-B   | 602 | AMP  | C2-N3   | 2.74  | 1.38        | 1.33     |
| 3   | 7-B   | 602 | AMP  | C4-N3   | 2.73  | 1.39        | 1.34     |
| 3   | 4-A   | 601 | AMP  | C4-N3   | 2.71  | 1.39        | 1.34     |
| 3   | 5-A   | 601 | AMP  | C2'-C1' | -2.65 | 1.45        | 1.53     |
| 3   | 3-A   | 601 | AMP  | C4-N3   | 2.64  | 1.39        | 1.34     |
| 3   | 5-A   | 601 | AMP  | C8-N7   | 2.64  | 1.36        | 1.31     |
| 3   | 4-B   | 602 | AMP  | C4-N3   | 2.60  | 1.39        | 1.34     |
| 3   | 7-B   | 602 | AMP  | C6-N1   | 2.56  | 1.42        | 1.35     |
| 3   | 6-B   | 602 | AMP  | C4-N3   | 2.51  | 1.39        | 1.34     |
| 3   | 6-A   | 601 | AMP  | C6-N1   | 2.50  | 1.42        | 1.35     |
| 3   | 7-A   | 601 | AMP  | C6-N1   | 2.48  | 1.42        | 1.35     |
| 3   | 6-A   | 601 | AMP  | C8-N7   | 2.46  | 1.36        | 1.31     |
| 3   | 8-A   | 601 | AMP  | C8-N7   | 2.45  | 1.36        | 1.31     |
| 3   | 2-B   | 602 | AMP  | C4-N3   | 2.44  | 1.39        | 1.34     |
| 3   | 7-A   | 601 | AMP  | C8-N7   | 2.42  | 1.36        | 1.31     |
| 3   | 5-A   | 601 | AMP  | C6-N1   | 2.41  | 1.42        | 1.35     |
| 3   | 8-B   | 602 | AMP  | C4-N3   | 2.41  | 1.38        | 1.34     |
| 3   | 5-B   | 602 | AMP  | C4-N3   | 2.40  | 1.38        | 1.34     |
| 3   | 1-A   | 601 | AMP  | C6-N1   | 2.39  | 1.42        | 1.35     |
| 3   | 8-A   | 601 | AMP  | C6-N1   | 2.39  | 1.42        | 1.35     |
| 3   | 2-A   | 601 | AMP  | C6-N1   | 2.37  | 1.42        | 1.35     |
| 3   | 3-B   | 602 | AMP  | C4-N3   | 2.36  | 1.38        | 1.34     |
| 3   | 3-A   | 601 | AMP  | C6-N1   | 2.32  | 1.42        | 1.35     |
| 3   | 8-B   | 602 | AMP  | C2'-C1' | -2.32 | 1.46        | 1.53     |
| 3   | 5-A   | 601 | AMP  | C5'-C4' | 2.32  | 1.58        | 1.51     |
| 3   | 1-B   | 602 | AMP  | C4-N3   | 2.28  | 1.38        | 1.34     |
| 3   | 2-B   | 602 | AMP  | O5'-C5' | -2.23 | 1.37        | 1.44     |
| 3   | 1-A   | 601 | AMP  | C8-N7   | 2.20  | 1.35        | 1.31     |
| 3   | 4-A   | 601 | AMP  | O3'-C3' | -2.19 | 1.37        | 1.43     |
| 3   | 5-B   | 602 | AMP  | O5'-C5' | -2.19 | 1.37        | 1.44     |
| 3   | 8-A   | 601 | AMP  | C2'-C1' | -2.18 | 1.46        | 1.53     |
| 3   | 6-B   | 602 | AMP  | C1'-N9  | 2.15  | 1.52        | 1.46     |
| 3   | 4-A   | 601 | AMP  | C6-N1   | 2.14  | 1.41        | 1.35     |
| 3   | 3-A   | 601 | AMP  | C8-N7   | 2.13  | 1.35        | 1.31     |
| 3   | 5-B   | 602 | AMP  | C5-N7   | -2.11 | 1.35        | 1.39     |
| 3   | 5-B   | 602 | AMP  | C1'-N9  | 2.08  | 1.52        | 1.46     |
| 3   | 6-A   | 601 | AMP  | C2'-C1' | -2.06 | 1.47        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | 8-B   | 602 | AMP  | C6-N1   | 2.06  | 1.41        | 1.35     |
| 3   | 5-B   | 602 | AMP  | C6-N1   | 2.02  | 1.41        | 1.35     |
| 3   | 4-B   | 602 | AMP  | O5'-C5' | -2.01 | 1.38        | 1.44     |

All (165) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | 5-B   | 602 | AMP  | N3-C2-N1    | -6.17 | 119.23      | 128.58   |
| 3   | 4-B   | 602 | AMP  | N3-C2-N1    | -6.15 | 119.27      | 128.58   |
| 3   | 2-B   | 602 | AMP  | N3-C2-N1    | -6.08 | 119.38      | 128.58   |
| 3   | 6-B   | 602 | AMP  | N3-C2-N1    | -6.07 | 119.39      | 128.58   |
| 3   | 1-B   | 602 | AMP  | N3-C2-N1    | -6.04 | 119.43      | 128.58   |
| 3   | 7-B   | 602 | AMP  | N3-C2-N1    | -6.03 | 119.45      | 128.58   |
| 3   | 8-B   | 602 | AMP  | N3-C2-N1    | -6.02 | 119.47      | 128.58   |
| 3   | 3-B   | 602 | AMP  | N3-C2-N1    | -5.99 | 119.51      | 128.58   |
| 3   | 7-A   | 601 | AMP  | N3-C2-N1    | -5.92 | 119.62      | 128.58   |
| 3   | 6-A   | 601 | AMP  | N3-C2-N1    | -5.86 | 119.72      | 128.58   |
| 3   | 1-A   | 601 | AMP  | N3-C2-N1    | -5.85 | 119.72      | 128.58   |
| 3   | 5-A   | 601 | AMP  | O4'-C4'-C5' | 5.84  | 128.03      | 109.33   |
| 3   | 2-A   | 601 | AMP  | N3-C2-N1    | -5.83 | 119.76      | 128.58   |
| 3   | 3-A   | 601 | AMP  | N3-C2-N1    | -5.82 | 119.77      | 128.58   |
| 3   | 5-A   | 601 | AMP  | N3-C2-N1    | -5.82 | 119.78      | 128.58   |
| 3   | 8-A   | 601 | AMP  | N3-C2-N1    | -5.71 | 119.93      | 128.58   |
| 3   | 4-A   | 601 | AMP  | N3-C2-N1    | -5.54 | 120.20      | 128.58   |
| 3   | 8-A   | 601 | AMP  | O4'-C4'-C5' | 5.20  | 126.00      | 109.33   |
| 3   | 6-B   | 602 | AMP  | O4'-C4'-C5' | 5.04  | 125.49      | 109.33   |
| 3   | 7-A   | 601 | AMP  | O4'-C4'-C5' | 4.99  | 125.32      | 109.33   |
| 3   | 6-A   | 601 | AMP  | O4'-C4'-C5' | 4.71  | 124.41      | 109.33   |
| 3   | 5-B   | 602 | AMP  | O4'-C4'-C5' | 4.58  | 124.02      | 109.33   |
| 3   | 8-B   | 602 | AMP  | O4'-C4'-C5' | 4.54  | 123.89      | 109.33   |
| 3   | 8-A   | 601 | AMP  | N9-C8-N7    | -4.15 | 108.05      | 113.94   |
| 3   | 6-A   | 601 | AMP  | N9-C8-N7    | -4.13 | 108.08      | 113.94   |
| 3   | 7-A   | 601 | AMP  | N9-C8-N7    | -4.11 | 108.10      | 113.94   |
| 3   | 2-A   | 601 | AMP  | N9-C8-N7    | -3.98 | 108.29      | 113.94   |
| 3   | 5-A   | 601 | AMP  | N9-C8-N7    | -3.97 | 108.30      | 113.94   |
| 3   | 5-A   | 601 | AMP  | C5-C4-N3    | -3.88 | 121.37      | 126.72   |
| 3   | 1-A   | 601 | AMP  | N9-C8-N7    | -3.84 | 108.48      | 113.94   |
| 3   | 6-A   | 601 | AMP  | C5-C4-N3    | -3.81 | 121.47      | 126.72   |
| 3   | 7-B   | 602 | AMP  | N9-C8-N7    | -3.79 | 108.56      | 113.94   |
| 3   | 1-A   | 601 | AMP  | C5-C4-N3    | -3.77 | 121.52      | 126.72   |
| 3   | 7-A   | 601 | AMP  | C5-C4-N3    | -3.74 | 121.57      | 126.72   |
| 3   | 8-A   | 601 | AMP  | C5-C4-N3    | -3.72 | 121.59      | 126.72   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | 2-B   | 602 | AMP  | N9-C8-N7    | -3.71 | 108.68      | 113.94   |
| 3   | 4-B   | 602 | AMP  | N9-C8-N7    | -3.69 | 108.69      | 113.94   |
| 3   | 2-A   | 601 | AMP  | C5-C4-N3    | -3.69 | 121.64      | 126.72   |
| 3   | 4-A   | 601 | AMP  | C5-C4-N3    | -3.64 | 121.70      | 126.72   |
| 3   | 4-A   | 601 | AMP  | N9-C8-N7    | -3.63 | 108.78      | 113.94   |
| 3   | 3-A   | 601 | AMP  | C5-C4-N3    | -3.62 | 121.73      | 126.72   |
| 3   | 6-B   | 602 | AMP  | C5-C4-N3    | -3.61 | 121.74      | 126.72   |
| 3   | 5-B   | 602 | AMP  | N9-C8-N7    | -3.61 | 108.81      | 113.94   |
| 3   | 3-A   | 601 | AMP  | N9-C8-N7    | -3.54 | 108.91      | 113.94   |
| 3   | 1-B   | 602 | AMP  | N9-C8-N7    | -3.53 | 108.93      | 113.94   |
| 3   | 6-A   | 601 | AMP  | C5-N7-C8    | 3.48  | 108.92      | 103.45   |
| 3   | 5-B   | 602 | AMP  | C5-C4-N3    | -3.48 | 121.93      | 126.72   |
| 3   | 8-A   | 601 | AMP  | C5-N7-C8    | 3.46  | 108.88      | 103.45   |
| 3   | 8-A   | 601 | AMP  | C2'-C1'-N9  | 3.42  | 121.80      | 113.30   |
| 3   | 5-A   | 601 | AMP  | C5-N7-C8    | 3.40  | 108.79      | 103.45   |
| 3   | 8-B   | 602 | AMP  | C5-C4-N3    | -3.36 | 122.09      | 126.72   |
| 3   | 1-B   | 602 | AMP  | C5-C4-N3    | -3.36 | 122.09      | 126.72   |
| 3   | 6-B   | 602 | AMP  | N9-C8-N7    | -3.35 | 109.18      | 113.94   |
| 3   | 7-A   | 601 | AMP  | C5-N7-C8    | 3.31  | 108.65      | 103.45   |
| 3   | 1-A   | 601 | AMP  | C5-N7-C8    | 3.26  | 108.58      | 103.45   |
| 3   | 4-A   | 601 | AMP  | C5-N7-C8    | 3.25  | 108.56      | 103.45   |
| 3   | 8-B   | 602 | AMP  | N9-C8-N7    | -3.25 | 109.32      | 113.94   |
| 3   | 3-B   | 602 | AMP  | N9-C8-N7    | -3.24 | 109.33      | 113.94   |
| 3   | 2-A   | 601 | AMP  | C5-N7-C8    | 3.24  | 108.54      | 103.45   |
| 3   | 7-A   | 601 | AMP  | C2-N3-C4    | 3.23  | 119.73      | 111.83   |
| 3   | 5-A   | 601 | AMP  | C2-N3-C4    | 3.22  | 119.70      | 111.83   |
| 3   | 6-A   | 601 | AMP  | C2-N3-C4    | 3.22  | 119.70      | 111.83   |
| 3   | 3-B   | 602 | AMP  | C5-C4-N3    | -3.20 | 122.31      | 126.72   |
| 3   | 7-B   | 602 | AMP  | C5-C4-N3    | -3.20 | 122.31      | 126.72   |
| 3   | 1-A   | 601 | AMP  | C2-N3-C4    | 3.15  | 119.52      | 111.83   |
| 3   | 6-A   | 601 | AMP  | C2'-C1'-N9  | 3.13  | 121.09      | 113.30   |
| 3   | 2-A   | 601 | AMP  | O4'-C4'-C5' | 3.11  | 119.29      | 109.33   |
| 3   | 8-A   | 601 | AMP  | C2-N3-C4    | 3.09  | 119.39      | 111.83   |
| 3   | 2-B   | 602 | AMP  | O4'-C4'-C5' | 3.06  | 119.15      | 109.33   |
| 3   | 2-B   | 602 | AMP  | C5-C4-N3    | -3.05 | 122.52      | 126.72   |
| 3   | 2-A   | 601 | AMP  | C2-N3-C4    | 3.05  | 119.27      | 111.83   |
| 3   | 3-A   | 601 | AMP  | C5-N7-C8    | 3.04  | 108.23      | 103.45   |
| 3   | 5-B   | 602 | AMP  | C2-N3-C4    | 3.04  | 119.25      | 111.83   |
| 3   | 5-A   | 601 | AMP  | O4'-C1'-N9  | 3.03  | 113.91      | 108.09   |
| 3   | 7-A   | 601 | AMP  | C2'-C1'-N9  | 3.02  | 120.80      | 113.30   |
| 3   | 3-A   | 601 | AMP  | C2-N3-C4    | 2.99  | 119.14      | 111.83   |
| 3   | 4-B   | 602 | AMP  | C5-C4-N3    | -2.99 | 122.60      | 126.72   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3   | 6-B   | 602 | AMP  | C2-N3-C4    | 2.98 | 119.11      | 111.83   |
| 3   | 2-A   | 601 | AMP  | N3-C4-N9    | 2.96 | 132.20      | 127.17   |
| 3   | 5-A   | 601 | AMP  | C2'-C1'-N9  | 2.95 | 120.63      | 113.30   |
| 3   | 7-B   | 602 | AMP  | C2-N3-C4    | 2.92 | 118.96      | 111.83   |
| 3   | 7-B   | 602 | AMP  | C2'-C1'-N9  | 2.90 | 120.50      | 113.30   |
| 3   | 3-B   | 602 | AMP  | O4'-C4'-C5' | 2.87 | 118.54      | 109.33   |
| 3   | 4-A   | 601 | AMP  | N3-C4-N9    | 2.87 | 132.06      | 127.17   |
| 3   | 1-B   | 602 | AMP  | C2-N3-C4    | 2.87 | 118.84      | 111.83   |
| 3   | 1-A   | 601 | AMP  | N3-C4-N9    | 2.86 | 132.02      | 127.17   |
| 3   | 4-A   | 601 | AMP  | C2-N3-C4    | 2.84 | 118.76      | 111.83   |
| 3   | 3-A   | 601 | AMP  | O4'-C4'-C5' | 2.84 | 118.42      | 109.33   |
| 3   | 5-B   | 602 | AMP  | C2'-C1'-N9  | 2.83 | 120.35      | 113.30   |
| 3   | 6-A   | 601 | AMP  | N3-C4-N9    | 2.83 | 131.98      | 127.17   |
| 3   | 5-B   | 602 | AMP  | C5-N7-C8    | 2.82 | 107.89      | 103.45   |
| 3   | 6-B   | 602 | AMP  | C5-N7-C8    | 2.80 | 107.85      | 103.45   |
| 3   | 8-B   | 602 | AMP  | C2-N3-C4    | 2.80 | 118.66      | 111.83   |
| 3   | 5-A   | 601 | AMP  | N3-C4-N9    | 2.79 | 131.92      | 127.17   |
| 3   | 8-A   | 601 | AMP  | N3-C4-N9    | 2.77 | 131.88      | 127.17   |
| 3   | 4-B   | 602 | AMP  | C2-N1-C6    | 2.77 | 123.28      | 118.73   |
| 3   | 1-B   | 602 | AMP  | C5-N7-C8    | 2.71 | 107.72      | 103.45   |
| 3   | 2-B   | 602 | AMP  | C2-N3-C4    | 2.71 | 118.44      | 111.83   |
| 3   | 8-B   | 602 | AMP  | C5-N7-C8    | 2.68 | 107.66      | 103.45   |
| 3   | 7-B   | 602 | AMP  | C5-N7-C8    | 2.67 | 107.64      | 103.45   |
| 3   | 3-A   | 601 | AMP  | N3-C4-N9    | 2.66 | 131.68      | 127.17   |
| 3   | 7-A   | 601 | AMP  | N3-C4-N9    | 2.65 | 131.67      | 127.17   |
| 3   | 3-B   | 602 | AMP  | C2-N3-C4    | 2.64 | 118.28      | 111.83   |
| 3   | 3-A   | 601 | AMP  | C3'-C2'-C1' | 2.62 | 106.42      | 101.46   |
| 3   | 6-B   | 602 | AMP  | C2'-C1'-N9  | 2.62 | 119.81      | 113.30   |
| 3   | 2-A   | 601 | AMP  | C2'-C1'-N9  | 2.62 | 119.81      | 113.30   |
| 3   | 3-B   | 602 | AMP  | C2-N1-C6    | 2.62 | 123.03      | 118.73   |
| 3   | 4-B   | 602 | AMP  | C2-N3-C4    | 2.60 | 118.18      | 111.83   |
| 3   | 2-A   | 601 | AMP  | C4-N9-C8    | 2.59 | 108.45      | 105.74   |
| 3   | 2-B   | 602 | AMP  | C2-N1-C6    | 2.58 | 122.96      | 118.73   |
| 3   | 6-B   | 602 | AMP  | O4'-C1'-N9  | 2.57 | 113.03      | 108.09   |
| 3   | 2-B   | 602 | AMP  | C5-N7-C8    | 2.53 | 107.43      | 103.45   |
| 3   | 4-A   | 601 | AMP  | C3'-C2'-C1' | 2.50 | 106.20      | 101.46   |
| 3   | 4-B   | 602 | AMP  | C4-N9-C8    | 2.47 | 108.34      | 105.74   |
| 3   | 8-B   | 602 | AMP  | C2-N1-C6    | 2.47 | 122.79      | 118.73   |
| 3   | 6-B   | 602 | AMP  | C2-N1-C6    | 2.47 | 122.78      | 118.73   |
| 3   | 2-B   | 602 | AMP  | C2'-C1'-N9  | 2.45 | 119.38      | 113.30   |
| 3   | 2-B   | 602 | AMP  | C4-N9-C8    | 2.44 | 108.30      | 105.74   |
| 3   | 7-B   | 602 | AMP  | C4-N9-C8    | 2.44 | 108.30      | 105.74   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | 3-B   | 602 | AMP  | C5-N7-C8    | 2.43  | 107.27      | 103.45   |
| 3   | 1-B   | 602 | AMP  | C2-N1-C6    | 2.43  | 122.72      | 118.73   |
| 3   | 5-A   | 601 | AMP  | O4'-C1'-C2' | 2.43  | 111.81      | 106.62   |
| 3   | 8-A   | 601 | AMP  | C4-N9-C8    | 2.41  | 108.27      | 105.74   |
| 3   | 6-B   | 602 | AMP  | N3-C4-N9    | 2.40  | 131.24      | 127.17   |
| 3   | 8-B   | 602 | AMP  | O4'-C1'-N9  | 2.39  | 112.69      | 108.09   |
| 3   | 1-B   | 602 | AMP  | N3-C4-N9    | 2.38  | 131.22      | 127.17   |
| 3   | 6-A   | 601 | AMP  | C4-N9-C8    | 2.37  | 108.23      | 105.74   |
| 3   | 4-B   | 602 | AMP  | C5-N7-C8    | 2.35  | 107.14      | 103.45   |
| 3   | 7-B   | 602 | AMP  | C4'-O4'-C1' | 2.35  | 114.65      | 109.47   |
| 3   | 7-A   | 601 | AMP  | C4-N9-C8    | 2.34  | 108.20      | 105.74   |
| 3   | 5-B   | 602 | AMP  | C2-N1-C6    | 2.33  | 122.56      | 118.73   |
| 3   | 8-B   | 602 | AMP  | N3-C4-N9    | 2.31  | 131.09      | 127.17   |
| 3   | 3-B   | 602 | AMP  | N3-C4-N9    | 2.30  | 131.07      | 127.17   |
| 3   | 3-B   | 602 | AMP  | O4'-C1'-N9  | 2.28  | 112.47      | 108.09   |
| 3   | 8-A   | 601 | AMP  | O4'-C1'-C2' | 2.27  | 111.48      | 106.62   |
| 3   | 1-A   | 601 | AMP  | O4'-C4'-C5' | 2.27  | 116.60      | 109.33   |
| 3   | 8-B   | 602 | AMP  | C2'-C1'-N9  | 2.27  | 118.94      | 113.30   |
| 3   | 3-B   | 602 | AMP  | C3'-C2'-C1' | 2.24  | 105.70      | 101.46   |
| 3   | 4-A   | 601 | AMP  | C4-N9-C8    | 2.21  | 108.06      | 105.74   |
| 3   | 5-A   | 601 | AMP  | C4'-O4'-C1' | -2.21 | 104.58      | 109.47   |
| 3   | 1-A   | 601 | AMP  | C2'-C1'-N9  | 2.20  | 118.77      | 113.30   |
| 3   | 1-A   | 601 | AMP  | C4-N9-C8    | 2.20  | 108.05      | 105.74   |
| 3   | 4-B   | 602 | AMP  | C2'-C1'-N9  | 2.19  | 118.75      | 113.30   |
| 3   | 4-B   | 602 | AMP  | C4'-O4'-C1' | 2.16  | 114.25      | 109.47   |
| 3   | 5-B   | 602 | AMP  | N3-C4-N9    | 2.15  | 130.83      | 127.17   |
| 3   | 1-B   | 602 | AMP  | C4-N9-C8    | 2.15  | 108.00      | 105.74   |
| 3   | 7-B   | 602 | AMP  | N3-C4-N9    | 2.13  | 130.78      | 127.17   |
| 3   | 4-B   | 602 | AMP  | C3'-C2'-C1' | 2.13  | 105.49      | 101.46   |
| 3   | 7-B   | 602 | AMP  | C2-N1-C6    | 2.13  | 122.22      | 118.73   |
| 3   | 5-A   | 601 | AMP  | C4-N9-C8    | 2.12  | 107.97      | 105.74   |
| 3   | 4-A   | 601 | AMP  | C6-C5-C4    | 2.12  | 120.07      | 117.18   |
| 3   | 6-A   | 601 | AMP  | C6-C5-C4    | 2.11  | 120.06      | 117.18   |
| 3   | 5-A   | 601 | AMP  | C6-C5-C4    | 2.11  | 120.05      | 117.18   |
| 3   | 3-B   | 602 | AMP  | C4-N9-C8    | 2.08  | 107.92      | 105.74   |
| 3   | 5-A   | 601 | AMP  | C2'-C3'-C4' | 2.07  | 106.61      | 102.61   |
| 3   | 6-A   | 601 | AMP  | C4-C5-N7    | -2.07 | 108.22      | 110.58   |
| 3   | 5-A   | 601 | AMP  | C4-C5-N7    | -2.05 | 108.23      | 110.58   |
| 3   | 6-A   | 601 | AMP  | O4'-C1'-C2' | 2.04  | 110.98      | 106.62   |
| 3   | 2-A   | 601 | AMP  | C6-C5-C4    | 2.03  | 119.95      | 117.18   |
| 3   | 8-A   | 601 | AMP  | C6-C5-C4    | 2.03  | 119.95      | 117.18   |
| 3   | 8-A   | 601 | AMP  | C4-C5-N7    | -2.02 | 108.27      | 110.58   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | 2-B   | 602 | AMP  | C4-N9-C1' | -2.01 | 121.92      | 126.63   |
| 3   | 1-A   | 601 | AMP  | C6-C5-C4  | 2.01  | 119.92      | 117.18   |
| 3   | 8-A   | 601 | AMP  | C4-N9-C1' | -2.00 | 121.95      | 126.63   |
| 3   | 8-B   | 602 | AMP  | C4-N9-C8  | 2.00  | 107.84      | 105.74   |

There are no chirality outliers.

All (54) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | 3-A   | 601 | AMP  | O4'-C4'-C5'-O5' |
| 3   | 3-A   | 601 | AMP  | C2'-C1'-N9-C8   |
| 3   | 3-B   | 602 | AMP  | O4'-C4'-C5'-O5' |
| 3   | 3-B   | 602 | AMP  | C3'-C4'-C5'-O5' |
| 3   | 7-B   | 602 | AMP  | O4'-C4'-C5'-O5' |
| 3   | 3-A   | 601 | AMP  | C3'-C4'-C5'-O5' |
| 3   | 4-A   | 601 | AMP  | O4'-C4'-C5'-O5' |
| 3   | 4-A   | 601 | AMP  | C3'-C4'-C5'-O5' |
| 3   | 2-B   | 602 | AMP  | O4'-C4'-C5'-O5' |
| 3   | 4-B   | 602 | AMP  | O4'-C4'-C5'-O5' |
| 3   | 7-B   | 602 | AMP  | C3'-C4'-C5'-O5' |
| 3   | 3-A   | 601 | AMP  | C2'-C1'-N9-C4   |
| 4   | 3-A   | 607 | EDO  | O1-C1-C2-O2     |
| 3   | 1-B   | 602 | AMP  | O4'-C4'-C5'-O5' |
| 4   | 8-A   | 607 | EDO  | O1-C1-C2-O2     |
| 3   | 4-A   | 601 | AMP  | C2'-C1'-N9-C8   |
| 3   | 4-B   | 602 | AMP  | C3'-C4'-C5'-O5' |
| 3   | 2-B   | 602 | AMP  | C3'-C4'-C5'-O5' |
| 3   | 3-B   | 602 | AMP  | C2'-C1'-N9-C8   |
| 3   | 4-B   | 602 | AMP  | C2'-C1'-N9-C8   |
| 3   | 7-A   | 601 | AMP  | C2'-C1'-N9-C8   |
| 3   | 2-B   | 602 | AMP  | C2'-C1'-N9-C8   |
| 3   | 4-A   | 601 | AMP  | C2'-C1'-N9-C4   |
| 4   | 6-A   | 607 | EDO  | O1-C1-C2-O2     |
| 3   | 7-A   | 601 | AMP  | O4'-C4'-C5'-O5' |
| 3   | 3-B   | 602 | AMP  | C2'-C1'-N9-C4   |
| 4   | 7-A   | 609 | EDO  | O1-C1-C2-O2     |
| 3   | 5-B   | 602 | AMP  | C2'-C1'-N9-C8   |
| 3   | 1-A   | 601 | AMP  | C2'-C1'-N9-C8   |
| 3   | 4-B   | 602 | AMP  | C2'-C1'-N9-C4   |
| 3   | 6-A   | 601 | AMP  | O4'-C1'-N9-C8   |
| 3   | 8-B   | 602 | AMP  | O4'-C1'-N9-C8   |
| 4   | 4-A   | 609 | EDO  | O1-C1-C2-O2     |

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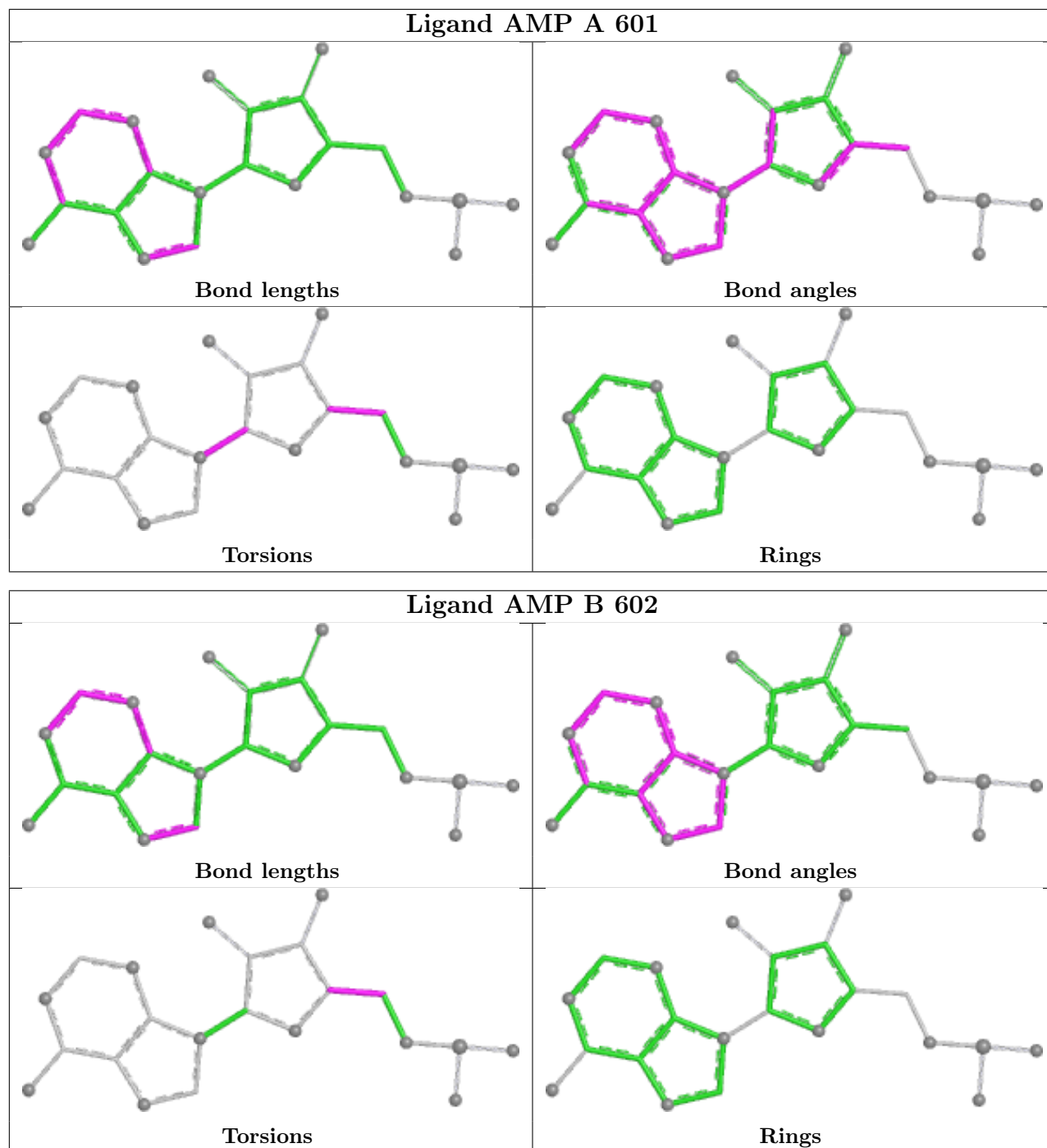
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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | 1-B   | 610 | EDO  | O1-C1-C2-O2     |
| 3   | 1-A   | 601 | AMP  | O4'-C1'-N9-C8   |
| 3   | 5-A   | 601 | AMP  | O4'-C1'-N9-C8   |
| 3   | 7-A   | 601 | AMP  | O4'-C1'-N9-C8   |
| 3   | 4-A   | 601 | AMP  | O4'-C1'-N9-C8   |
| 3   | 8-A   | 601 | AMP  | O4'-C1'-N9-C8   |
| 3   | 4-B   | 602 | AMP  | O4'-C1'-N9-C8   |
| 3   | 6-B   | 602 | AMP  | O4'-C1'-N9-C8   |
| 4   | 8-A   | 609 | EDO  | O1-C1-C2-O2     |
| 4   | 4-B   | 610 | EDO  | O1-C1-C2-O2     |
| 4   | 7-B   | 610 | EDO  | O1-C1-C2-O2     |
| 4   | 8-B   | 610 | EDO  | O1-C1-C2-O2     |
| 3   | 1-A   | 601 | AMP  | O4'-C4'-C5'-O5' |
| 3   | 2-A   | 601 | AMP  | O4'-C4'-C5'-O5' |
| 3   | 8-B   | 602 | AMP  | C2'-C1'-N9-C8   |
| 3   | 2-B   | 602 | AMP  | O4'-C1'-N9-C8   |
| 3   | 5-B   | 602 | AMP  | O4'-C1'-N9-C8   |
| 3   | 6-A   | 601 | AMP  | O4'-C4'-C5'-O5' |
| 3   | 8-B   | 602 | AMP  | O4'-C4'-C5'-O5' |
| 3   | 5-A   | 601 | AMP  | C3'-C4'-C5'-O5' |
| 3   | 3-B   | 602 | AMP  | O4'-C1'-N9-C8   |

There are no ring outliers.

No monomer is involved in short contacts.

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



## 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   | 1-A   | 311/351 (88%)  | 2.31   | 154 (49%) 0 1 | 1, 2, 4, 6            | 311 (100%) |
| 1   | 1-B   | 305/351 (86%)  | 2.43   | 160 (52%) 0 1 | 1, 2, 4, 7            | 305 (100%) |
| 1   | 2-A   | 0/351          | -      | -             | -                     | -          |
| 1   | 2-B   | 0/351          | -      | -             | -                     | -          |
| 1   | 3-A   | 0/351          | -      | -             | -                     | -          |
| 1   | 3-B   | 0/351          | -      | -             | -                     | -          |
| 1   | 4-A   | 0/351          | -      | -             | -                     | -          |
| 1   | 4-B   | 0/351          | -      | -             | -                     | -          |
| 1   | 5-A   | 0/351          | -      | -             | -                     | -          |
| 1   | 5-B   | 0/351          | -      | -             | -                     | -          |
| 1   | 6-A   | 0/351          | -      | -             | -                     | -          |
| 1   | 6-B   | 0/351          | -      | -             | -                     | -          |
| 1   | 7-A   | 0/351          | -      | -             | -                     | -          |
| 1   | 7-B   | 0/351          | -      | -             | -                     | -          |
| 1   | 8-A   | 0/351          | -      | -             | -                     | -          |
| 1   | 8-B   | 0/351          | -      | -             | -                     | -          |
| All | All   | 616/5616 (10%) | 2.37   | 314 (50%) 0 1 | 1, 2, 4, 7            | 616 (100%) |

All (314) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 1-B   | 46  | THR  | 8.5  |
| 1   | 1-A   | 52  | SER  | 8.2  |
| 1   | 1-A   | 128 | ILE  | 8.0  |
| 1   | 1-B   | 117 | THR  | 7.2  |
| 1   | 1-B   | 50  | SER  | 7.1  |
| 1   | 1-A   | 28  | ASP  | 6.9  |
| 1   | 1-B   | 134 | SER  | 6.9  |
| 1   | 1-A   | 219 | CYS  | 6.8  |
| 1   | 1-A   | 22  | SER  | 6.4  |
| 1   | 1-B   | 238 | ALA  | 6.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 1-B   | 131 | PRO  | 6.4  |
| 1   | 1-A   | 217 | CYS  | 6.4  |
| 1   | 1-B   | 178 | ALA  | 6.3  |
| 1   | 1-B   | 48  | PHE  | 6.1  |
| 1   | 1-B   | 87  | TRP  | 6.1  |
| 1   | 1-B   | 261 | HIS  | 5.9  |
| 1   | 1-B   | 136 | GLN  | 5.9  |
| 1   | 1-A   | 127 | VAL  | 5.7  |
| 1   | 1-A   | 132 | VAL  | 5.7  |
| 1   | 1-B   | 310 | HIS  | 5.7  |
| 1   | 1-B   | 39  | PRO  | 5.7  |
| 1   | 1-A   | 34  | TRP  | 5.6  |
| 1   | 1-B   | 85  | PRO  | 5.5  |
| 1   | 1-A   | 291 | ASN  | 5.5  |
| 1   | 1-A   | 290 | TYR  | 5.4  |
| 1   | 1-B   | 240 | PHE  | 5.4  |
| 1   | 1-A   | 32  | ASN  | 5.4  |
| 1   | 1-B   | 21  | GLN  | 5.3  |
| 1   | 1-A   | 39  | PRO  | 5.3  |
| 1   | 1-A   | 260 | HIS  | 5.3  |
| 1   | 1-A   | 83  | HIS  | 5.2  |
| 1   | 1-A   | 46  | THR  | 5.2  |
| 1   | 1-B   | 80  | VAL  | 5.2  |
| 1   | 1-A   | 45  | PRO  | 5.2  |
| 1   | 1-B   | 106 | GLN  | 5.2  |
| 1   | 1-A   | 131 | PRO  | 5.1  |
| 1   | 1-B   | 180 | ALA  | 5.1  |
| 1   | 1-A   | 87  | TRP  | 5.1  |
| 1   | 1-A   | 182 | MET  | 5.1  |
| 1   | 1-B   | 179 | GLY  | 5.0  |
| 1   | 1-B   | 291 | ASN  | 5.0  |
| 1   | 1-A   | 130 | SER  | 5.0  |
| 1   | 1-A   | 44  | ARG  | 5.0  |
| 1   | 1-B   | 176 | ALA  | 5.0  |
| 1   | 1-B   | 319 | LEU  | 5.0  |
| 1   | 1-B   | 116 | ARG  | 4.9  |
| 1   | 1-B   | 67  | ILE  | 4.8  |
| 1   | 1-A   | 261 | HIS  | 4.8  |
| 1   | 1-B   | 34  | TRP  | 4.8  |
| 1   | 1-A   | 86  | ASN  | 4.7  |
| 1   | 1-A   | 85  | PRO  | 4.7  |
| 1   | 1-B   | 105 | THR  | 4.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 1-B   | 68  | GLY  | 4.7  |
| 1   | 1-A   | 107 | SER  | 4.7  |
| 1   | 1-B   | 107 | SER  | 4.6  |
| 1   | 1-B   | 77  | LEU  | 4.6  |
| 1   | 1-B   | 260 | HIS  | 4.6  |
| 1   | 1-A   | 198 | THR  | 4.6  |
| 1   | 1-A   | 51  | LYS  | 4.5  |
| 1   | 1-B   | 223 | SER  | 4.5  |
| 1   | 1-B   | 234 | PHE  | 4.5  |
| 1   | 1-A   | 350 | LEU  | 4.5  |
| 1   | 1-B   | 208 | ASP  | 4.5  |
| 1   | 1-A   | 37  | PHE  | 4.5  |
| 1   | 1-A   | 120 | GLY  | 4.5  |
| 1   | 1-B   | 304 | SER  | 4.5  |
| 1   | 1-A   | 126 | VAL  | 4.4  |
| 1   | 1-B   | 168 | ILE  | 4.4  |
| 1   | 1-A   | 254 | ASP  | 4.4  |
| 1   | 1-B   | 237 | VAL  | 4.4  |
| 1   | 1-A   | 91  | VAL  | 4.3  |
| 1   | 1-B   | 229 | ASP  | 4.3  |
| 1   | 1-B   | 86  | ASN  | 4.3  |
| 1   | 1-A   | 211 | GLU  | 4.3  |
| 1   | 1-B   | 132 | VAL  | 4.3  |
| 1   | 1-B   | 37  | PHE  | 4.3  |
| 1   | 1-A   | 197 | PRO  | 4.3  |
| 1   | 1-B   | 71  | GLN  | 4.2  |
| 1   | 1-B   | 49  | LYS  | 4.2  |
| 1   | 1-A   | 84  | ASP  | 4.2  |
| 1   | 1-A   | 212 | GLU  | 4.2  |
| 1   | 1-B   | 213 | THR  | 4.2  |
| 1   | 1-A   | 78  | PHE  | 4.1  |
| 1   | 1-B   | 182 | MET  | 4.1  |
| 1   | 1-A   | 48  | PHE  | 4.0  |
| 1   | 1-A   | 38  | SER  | 4.0  |
| 1   | 1-B   | 47  | ASP  | 4.0  |
| 1   | 1-A   | 243 | THR  | 4.0  |
| 1   | 1-B   | 212 | GLU  | 4.0  |
| 1   | 1-B   | 209 | TYR  | 4.0  |
| 1   | 1-B   | 350 | LEU  | 4.0  |
| 1   | 1-A   | 82  | ASP  | 4.0  |
| 1   | 1-A   | 263 | ASP  | 4.0  |
| 1   | 1-A   | 196 | PRO  | 3.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 1-B   | 163 | ASP  | 3.9  |
| 1   | 1-B   | 83  | HIS  | 3.9  |
| 1   | 1-B   | 142 | PRO  | 3.9  |
| 1   | 1-A   | 258 | HIS  | 3.9  |
| 1   | 1-A   | 209 | TYR  | 3.8  |
| 1   | 1-A   | 262 | LEU  | 3.8  |
| 1   | 1-B   | 321 | GLY  | 3.8  |
| 1   | 1-A   | 141 | ASP  | 3.8  |
| 1   | 1-A   | 183 | SER  | 3.8  |
| 1   | 1-B   | 320 | SER  | 3.8  |
| 1   | 1-A   | 205 | GLY  | 3.8  |
| 1   | 1-B   | 177 | SER  | 3.8  |
| 1   | 1-A   | 246 | PHE  | 3.8  |
| 1   | 1-A   | 60  | PRO  | 3.7  |
| 1   | 1-A   | 180 | ALA  | 3.7  |
| 1   | 1-B   | 139 | ASP  | 3.7  |
| 1   | 1-A   | 351 | THR  | 3.7  |
| 1   | 1-A   | 301 | VAL  | 3.7  |
| 1   | 1-B   | 75  | PRO  | 3.7  |
| 1   | 1-B   | 232 | SER  | 3.7  |
| 1   | 1-A   | 106 | GLN  | 3.7  |
| 1   | 1-B   | 322 | VAL  | 3.7  |
| 1   | 1-A   | 151 | ALA  | 3.6  |
| 1   | 1-B   | 74  | ALA  | 3.6  |
| 1   | 1-A   | 304 | SER  | 3.6  |
| 1   | 1-B   | 254 | ASP  | 3.6  |
| 1   | 1-B   | 263 | ASP  | 3.6  |
| 1   | 1-A   | 33  | ARG  | 3.6  |
| 1   | 1-B   | 173 | ASN  | 3.5  |
| 1   | 1-B   | 211 | GLU  | 3.5  |
| 1   | 1-B   | 135 | ILE  | 3.5  |
| 1   | 1-B   | 289 | PRO  | 3.5  |
| 1   | 1-A   | 117 | THR  | 3.5  |
| 1   | 1-A   | 347 | GLU  | 3.5  |
| 1   | 1-A   | 116 | ARG  | 3.5  |
| 1   | 1-A   | 24  | GLU  | 3.4  |
| 1   | 1-A   | 220 | GLU  | 3.4  |
| 1   | 1-B   | 235 | VAL  | 3.4  |
| 1   | 1-B   | 81  | PRO  | 3.4  |
| 1   | 1-B   | 69  | ARG  | 3.4  |
| 1   | 1-B   | 101 | ARG  | 3.4  |
| 1   | 1-B   | 147 | ASP  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 1-B   | 299 | LEU  | 3.4  |
| 1   | 1-B   | 27  | LYS  | 3.3  |
| 1   | 1-A   | 349 | SER  | 3.3  |
| 1   | 1-B   | 141 | ASP  | 3.3  |
| 1   | 1-A   | 216 | CYS  | 3.3  |
| 1   | 1-A   | 224 | LYS  | 3.3  |
| 1   | 1-B   | 185 | SER  | 3.3  |
| 1   | 1-A   | 80  | VAL  | 3.2  |
| 1   | 1-A   | 30  | VAL  | 3.2  |
| 1   | 1-B   | 66  | CYS  | 3.2  |
| 1   | 1-A   | 181 | SER  | 3.2  |
| 1   | 1-A   | 163 | ASP  | 3.2  |
| 1   | 1-B   | 103 | LEU  | 3.1  |
| 1   | 1-B   | 256 | SER  | 3.1  |
| 1   | 1-A   | 156 | ILE  | 3.1  |
| 1   | 1-B   | 298 | PRO  | 3.1  |
| 1   | 1-A   | 173 | ASN  | 3.1  |
| 1   | 1-A   | 90  | ARG  | 3.1  |
| 1   | 1-B   | 302 | THR  | 3.1  |
| 1   | 1-B   | 290 | TYR  | 3.1  |
| 1   | 1-B   | 91  | VAL  | 3.1  |
| 1   | 1-A   | 49  | LYS  | 3.1  |
| 1   | 1-B   | 318 | GLN  | 3.1  |
| 1   | 1-B   | 159 | ILE  | 3.0  |
| 1   | 1-A   | 227 | VAL  | 3.0  |
| 1   | 1-A   | 185 | SER  | 3.0  |
| 1   | 1-B   | 73  | CYS  | 3.0  |
| 1   | 1-A   | 154 | LYS  | 3.0  |
| 1   | 1-A   | 77  | LEU  | 3.0  |
| 1   | 1-A   | 135 | ILE  | 3.0  |
| 1   | 1-B   | 218 | LEU  | 3.0  |
| 1   | 1-B   | 118 | ILE  | 3.0  |
| 1   | 1-B   | 183 | SER  | 2.9  |
| 1   | 1-B   | 332 | TYR  | 2.9  |
| 1   | 1-A   | 160 | ALA  | 2.9  |
| 1   | 1-B   | 228 | ILE  | 2.9  |
| 1   | 1-B   | 137 | LEU  | 2.9  |
| 1   | 1-B   | 349 | SER  | 2.9  |
| 1   | 1-A   | 119 | VAL  | 2.9  |
| 1   | 1-B   | 307 | PRO  | 2.9  |
| 1   | 1-A   | 157 | ASN  | 2.9  |
| 1   | 1-B   | 258 | HIS  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 1-A   | 79  | ARG  | 2.9  |
| 1   | 1-A   | 203 | LEU  | 2.9  |
| 1   | 1-A   | 133 | HIS  | 2.9  |
| 1   | 1-A   | 164 | SER  | 2.9  |
| 1   | 1-A   | 321 | GLY  | 2.9  |
| 1   | 1-B   | 288 | PRO  | 2.8  |
| 1   | 1-B   | 65  | PHE  | 2.8  |
| 1   | 1-A   | 66  | CYS  | 2.8  |
| 1   | 1-A   | 89  | LEU  | 2.8  |
| 1   | 1-B   | 262 | LEU  | 2.8  |
| 1   | 1-A   | 122 | GLY  | 2.8  |
| 1   | 1-B   | 28  | ASP  | 2.8  |
| 1   | 1-B   | 300 | LYS  | 2.8  |
| 1   | 1-A   | 29  | PRO  | 2.8  |
| 1   | 1-A   | 210 | PHE  | 2.8  |
| 1   | 1-A   | 71  | GLN  | 2.8  |
| 1   | 1-A   | 68  | GLY  | 2.8  |
| 1   | 1-A   | 327 | ILE  | 2.8  |
| 1   | 1-B   | 156 | ILE  | 2.8  |
| 1   | 1-B   | 25  | LEU  | 2.7  |
| 1   | 1-B   | 165 | ILE  | 2.7  |
| 1   | 1-B   | 309 | THR  | 2.7  |
| 1   | 1-A   | 63  | CYS  | 2.7  |
| 1   | 1-A   | 190 | MET  | 2.6  |
| 1   | 1-B   | 174 | GLN  | 2.6  |
| 1   | 1-B   | 78  | PHE  | 2.6  |
| 1   | 1-A   | 81  | PRO  | 2.6  |
| 1   | 1-B   | 76  | GLU  | 2.6  |
| 1   | 1-B   | 343 | LYS  | 2.6  |
| 1   | 1-A   | 325 | PHE  | 2.6  |
| 1   | 1-B   | 312 | PHE  | 2.6  |
| 1   | 1-B   | 342 | ALA  | 2.6  |
| 1   | 1-A   | 123 | PHE  | 2.6  |
| 1   | 1-B   | 90  | ARG  | 2.6  |
| 1   | 1-B   | 148 | ILE  | 2.6  |
| 1   | 1-B   | 230 | GLU  | 2.6  |
| 1   | 1-A   | 187 | SER  | 2.6  |
| 1   | 1-A   | 259 | PHE  | 2.5  |
| 1   | 1-A   | 47  | ASP  | 2.5  |
| 1   | 1-A   | 179 | GLY  | 2.5  |
| 1   | 1-B   | 220 | GLU  | 2.5  |
| 1   | 1-B   | 259 | PHE  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 1-A   | 299 | LEU  | 2.5  |
| 1   | 1-B   | 313 | LEU  | 2.5  |
| 1   | 1-B   | 286 | ASN  | 2.5  |
| 1   | 1-B   | 130 | SER  | 2.5  |
| 1   | 1-B   | 30  | VAL  | 2.5  |
| 1   | 1-B   | 70  | GLU  | 2.5  |
| 1   | 1-A   | 175 | GLY  | 2.5  |
| 1   | 1-A   | 69  | ARG  | 2.5  |
| 1   | 1-A   | 165 | ILE  | 2.5  |
| 1   | 1-B   | 257 | SER  | 2.5  |
| 1   | 1-A   | 340 | ASP  | 2.5  |
| 1   | 1-A   | 286 | ASN  | 2.4  |
| 1   | 1-A   | 308 | TYR  | 2.4  |
| 1   | 1-B   | 95  | LEU  | 2.4  |
| 1   | 1-A   | 345 | MET  | 2.4  |
| 1   | 1-A   | 168 | ILE  | 2.4  |
| 1   | 1-A   | 206 | THR  | 2.4  |
| 1   | 1-B   | 336 | VAL  | 2.4  |
| 1   | 1-A   | 303 | GLU  | 2.4  |
| 1   | 1-A   | 96  | TYR  | 2.4  |
| 1   | 1-B   | 210 | PHE  | 2.4  |
| 1   | 1-A   | 137 | LEU  | 2.4  |
| 1   | 1-A   | 178 | ALA  | 2.4  |
| 1   | 1-A   | 342 | ALA  | 2.4  |
| 1   | 1-B   | 23  | PRO  | 2.4  |
| 1   | 1-B   | 64  | PRO  | 2.4  |
| 1   | 1-A   | 61  | SER  | 2.4  |
| 1   | 1-A   | 208 | ASP  | 2.3  |
| 1   | 1-A   | 244 | TYR  | 2.3  |
| 1   | 1-A   | 129 | GLU  | 2.3  |
| 1   | 1-B   | 140 | ILE  | 2.3  |
| 1   | 1-B   | 194 | VAL  | 2.3  |
| 1   | 1-A   | 99  | LEU  | 2.3  |
| 1   | 1-B   | 184 | HIS  | 2.3  |
| 1   | 1-A   | 337 | PHE  | 2.3  |
| 1   | 1-A   | 50  | SER  | 2.3  |
| 1   | 1-A   | 297 | SER  | 2.3  |
| 1   | 1-B   | 149 | LEU  | 2.3  |
| 1   | 1-A   | 75  | PRO  | 2.2  |
| 1   | 1-B   | 104 | GLU  | 2.2  |
| 1   | 1-B   | 181 | SER  | 2.2  |
| 1   | 1-B   | 82  | ASP  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 1-B   | 150 | ILE  | 2.2  |
| 1   | 1-A   | 265 | VAL  | 2.2  |
| 1   | 1-B   | 344 | VAL  | 2.2  |
| 1   | 1-B   | 347 | GLU  | 2.2  |
| 1   | 1-A   | 152 | TYR  | 2.2  |
| 1   | 1-A   | 67  | ILE  | 2.2  |
| 1   | 1-A   | 294 | ILE  | 2.2  |
| 1   | 1-B   | 281 | ILE  | 2.2  |
| 1   | 1-A   | 195 | VAL  | 2.2  |
| 1   | 1-A   | 348 | VAL  | 2.2  |
| 1   | 1-A   | 70  | GLU  | 2.2  |
| 1   | 1-A   | 319 | LEU  | 2.2  |
| 1   | 1-B   | 161 | GLN  | 2.2  |
| 1   | 1-A   | 121 | PHE  | 2.2  |
| 1   | 1-A   | 251 | ILE  | 2.2  |
| 1   | 1-B   | 162 | HIS  | 2.2  |
| 1   | 1-B   | 63  | CYS  | 2.2  |
| 1   | 1-A   | 241 | ALA  | 2.2  |
| 1   | 1-A   | 207 | LYS  | 2.2  |
| 1   | 1-A   | 92  | ILE  | 2.1  |
| 1   | 1-A   | 145 | ILE  | 2.1  |
| 1   | 1-A   | 248 | ILE  | 2.1  |
| 1   | 1-B   | 143 | VAL  | 2.1  |
| 1   | 1-B   | 348 | VAL  | 2.1  |
| 1   | 1-B   | 22  | SER  | 2.1  |
| 1   | 1-A   | 155 | ARG  | 2.1  |
| 1   | 1-B   | 242 | ALA  | 2.1  |
| 1   | 1-B   | 301 | VAL  | 2.1  |
| 1   | 1-B   | 88  | LYS  | 2.1  |
| 1   | 1-A   | 161 | GLN  | 2.1  |
| 1   | 1-A   | 118 | ILE  | 2.1  |
| 1   | 1-B   | 287 | ASP  | 2.1  |
| 1   | 1-B   | 62  | SER  | 2.1  |
| 1   | 1-A   | 88  | LYS  | 2.1  |
| 1   | 1-B   | 272 | GLY  | 2.1  |
| 1   | 1-B   | 268 | VAL  | 2.1  |
| 1   | 1-B   | 285 | LEU  | 2.1  |
| 1   | 1-B   | 100 | SER  | 2.0  |
| 1   | 1-A   | 167 | TYR  | 2.0  |
| 1   | 1-B   | 167 | TYR  | 2.0  |
| 1   | 1-A   | 31  | THR  | 2.0  |
| 1   | 1-B   | 189 | MET  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 1-A   | 252 | PRO  | 2.0  |
| 1   | 1-B   | 341 | VAL  | 2.0  |
| 1   | 1-B   | 222 | LYS  | 2.0  |
| 1   | 1-B   | 253 | LYS  | 2.0  |
| 1   | 1-A   | 226 | PHE  | 2.0  |
| 1   | 1-A   | 234 | PHE  | 2.0  |
| 1   | 1-B   | 315 | ILE  | 2.0  |
| 1   | 1-B   | 296 | THR  | 2.0  |
| 1   | 1-B   | 338 | PRO  | 2.0  |
| 1   | 1-B   | 127 | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | ZN   | 1-A   | 603 | 1/1   | 0.54 | 0.26 | 11,11,11,11                | 1     |
| 2   | ZN   | 2-A   | 603 | 1/1   | -    | -    | 24,24,24,24                | 1     |
| 2   | ZN   | 3-A   | 603 | 1/1   | -    | -    | 25,25,25,25                | 1     |
| 2   | ZN   | 4-A   | 603 | 1/1   | -    | -    | 10,10,10,10                | 1     |
| 2   | ZN   | 5-A   | 603 | 1/1   | -    | -    | 23,23,23,23                | 1     |
| 2   | ZN   | 6-A   | 603 | 1/1   | -    | -    | 24,24,24,24                | 1     |
| 2   | ZN   | 7-A   | 603 | 1/1   | -    | -    | 8,8,8,8                    | 1     |
| 2   | ZN   | 8-A   | 603 | 1/1   | -    | -    | 24,24,24,24                | 1     |
| 3   | AMP  | 1-B   | 602 | 22/23 | 0.55 | 0.21 | 20,27,28,31                | 22    |
| 2   | ZN   | 2-A   | 604 | 1/1   | -    | -    | 7,7,7,7                    | 1     |
| 2   | ZN   | 3-A   | 604 | 1/1   | -    | -    | 27,27,27,27                | 1     |
| 2   | ZN   | 4-A   | 604 | 1/1   | -    | -    | 9,9,9,9                    | 1     |
| 2   | ZN   | 5-A   | 604 | 1/1   | -    | -    | 0,0,0,0                    | 1     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | ZN   | 6-A   | 604 | 1/1   | -    | -    | 30,30,30,30                 | 1     |
| 2   | ZN   | 7-A   | 604 | 1/1   | -    | -    | 26,26,26,26                 | 1     |
| 2   | ZN   | 8-A   | 604 | 1/1   | -    | -    | 2,2,2,2                     | 1     |
| 4   | EDO  | 1-A   | 609 | 4/4   | 0.64 | 0.20 | 27,28,28,29                 | 4     |
| 2   | ZN   | 2-B   | 605 | 1/1   | -    | -    | 19,19,19,19                 | 1     |
| 2   | ZN   | 3-B   | 605 | 1/1   | -    | -    | 14,14,14,14                 | 1     |
| 2   | ZN   | 4-B   | 605 | 1/1   | -    | -    | 13,13,13,13                 | 1     |
| 2   | ZN   | 5-B   | 605 | 1/1   | -    | -    | 19,19,19,19                 | 1     |
| 2   | ZN   | 6-B   | 605 | 1/1   | -    | -    | 13,13,13,13                 | 1     |
| 2   | ZN   | 7-B   | 605 | 1/1   | -    | -    | 11,11,11,11                 | 1     |
| 2   | ZN   | 8-B   | 605 | 1/1   | -    | -    | 7,7,7,7                     | 1     |
| 4   | EDO  | 1-A   | 608 | 4/4   | 0.66 | 0.26 | 28,29,30,31                 | 4     |
| 2   | ZN   | 2-B   | 606 | 1/1   | -    | -    | 18,18,18,18                 | 1     |
| 2   | ZN   | 3-B   | 606 | 1/1   | -    | -    | 24,24,24,24                 | 1     |
| 2   | ZN   | 4-B   | 606 | 1/1   | -    | -    | 23,23,23,23                 | 1     |
| 2   | ZN   | 5-B   | 606 | 1/1   | -    | -    | 24,24,24,24                 | 1     |
| 2   | ZN   | 6-B   | 606 | 1/1   | -    | -    | 13,13,13,13                 | 1     |
| 2   | ZN   | 7-B   | 606 | 1/1   | -    | -    | 12,12,12,12                 | 1     |
| 2   | ZN   | 8-B   | 606 | 1/1   | -    | -    | 25,25,25,25                 | 1     |
| 2   | ZN   | 1-B   | 605 | 1/1   | 0.75 | 0.21 | 10,10,10,10                 | 1     |
| 3   | AMP  | 2-A   | 601 | 22/23 | -    | -    | 16,21,22,26                 | 22    |
| 3   | AMP  | 3-A   | 601 | 22/23 | -    | -    | 12,21,23,26                 | 22    |
| 3   | AMP  | 4-A   | 601 | 22/23 | -    | -    | 12,21,24,24                 | 22    |
| 3   | AMP  | 5-A   | 601 | 22/23 | -    | -    | 3,21,22,23                  | 22    |
| 3   | AMP  | 6-A   | 601 | 22/23 | -    | -    | 13,21,22,24                 | 22    |
| 3   | AMP  | 7-A   | 601 | 22/23 | -    | -    | 7,21,23,24                  | 22    |
| 3   | AMP  | 8-A   | 601 | 22/23 | -    | -    | 11,21,22,23                 | 22    |
| 4   | EDO  | 1-B   | 611 | 4/4   | 0.79 | 0.16 | 30,30,30,32                 | 4     |
| 3   | AMP  | 2-B   | 602 | 22/23 | -    | -    | 21,27,28,30                 | 22    |
| 3   | AMP  | 3-B   | 602 | 22/23 | -    | -    | 19,26,28,29                 | 22    |
| 3   | AMP  | 4-B   | 602 | 22/23 | -    | -    | 20,27,28,31                 | 22    |
| 3   | AMP  | 5-B   | 602 | 22/23 | -    | -    | 19,27,28,30                 | 22    |
| 3   | AMP  | 6-B   | 602 | 22/23 | -    | -    | 20,27,28,29                 | 22    |
| 3   | AMP  | 7-B   | 602 | 22/23 | -    | -    | 19,26,28,32                 | 22    |
| 3   | AMP  | 8-B   | 602 | 22/23 | -    | -    | 19,26,28,30                 | 22    |
| 3   | AMP  | 1-A   | 601 | 22/23 | 0.81 | 0.14 | 16,21,22,27                 | 22    |
| 4   | EDO  | 2-A   | 607 | 4/4   | -    | -    | 10,11,13,13                 | 4     |
| 4   | EDO  | 3-A   | 607 | 4/4   | -    | -    | 12,12,12,13                 | 4     |
| 4   | EDO  | 4-A   | 607 | 4/4   | -    | -    | 10,11,12,13                 | 4     |
| 4   | EDO  | 5-A   | 607 | 4/4   | -    | -    | 11,12,12,13                 | 4     |
| 4   | EDO  | 6-A   | 607 | 4/4   | -    | -    | 11,12,12,13                 | 4     |
| 4   | EDO  | 7-A   | 607 | 4/4   | -    | -    | 9,11,12,13                  | 4     |

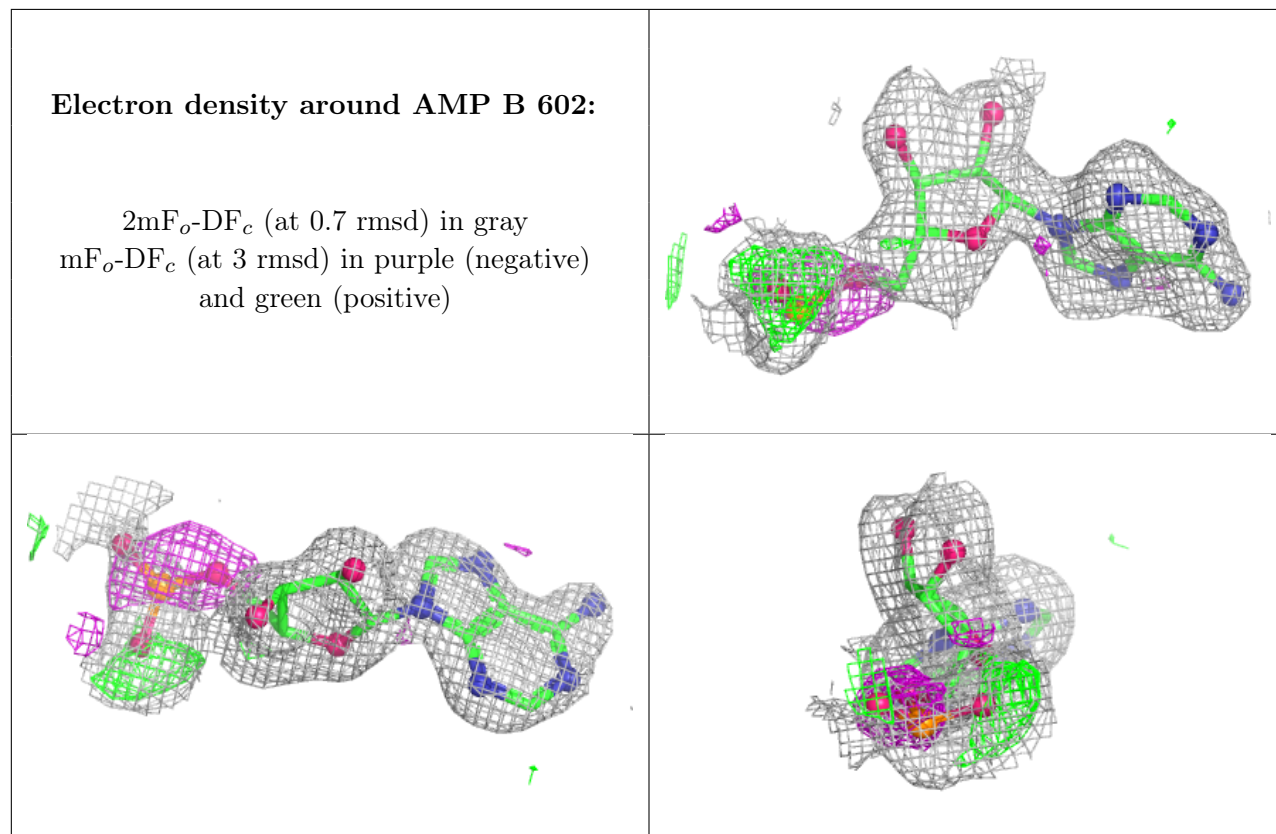
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*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | EDO  | 8-A   | 607 | 4/4   | -    | -    | 11,12,12,12                 | 4     |
| 4   | EDO  | 1-B   | 612 | 4/4   | 0.81 | 0.15 | 35,36,37,37                 | 4     |
| 4   | EDO  | 2-A   | 608 | 4/4   | -    | -    | 27,29,30,30                 | 4     |
| 4   | EDO  | 3-A   | 608 | 4/4   | -    | -    | 28,29,30,31                 | 4     |
| 4   | EDO  | 4-A   | 608 | 4/4   | -    | -    | 28,29,30,31                 | 4     |
| 4   | EDO  | 5-A   | 608 | 4/4   | -    | -    | 28,29,30,31                 | 4     |
| 4   | EDO  | 6-A   | 608 | 4/4   | -    | -    | 28,29,30,31                 | 4     |
| 4   | EDO  | 7-A   | 608 | 4/4   | -    | -    | 28,29,30,31                 | 4     |
| 4   | EDO  | 8-A   | 608 | 4/4   | -    | -    | 28,29,30,31                 | 4     |
| 4   | EDO  | 1-A   | 607 | 4/4   | 0.82 | 0.12 | 10,11,12,13                 | 4     |
| 4   | EDO  | 2-A   | 609 | 4/4   | -    | -    | 27,28,28,28                 | 4     |
| 4   | EDO  | 3-A   | 609 | 4/4   | -    | -    | 27,28,28,29                 | 4     |
| 4   | EDO  | 4-A   | 609 | 4/4   | -    | -    | 27,28,28,29                 | 4     |
| 4   | EDO  | 5-A   | 609 | 4/4   | -    | -    | 27,28,28,29                 | 4     |
| 4   | EDO  | 6-A   | 609 | 4/4   | -    | -    | 28,28,28,29                 | 4     |
| 4   | EDO  | 7-A   | 609 | 4/4   | -    | -    | 27,27,28,31                 | 4     |
| 4   | EDO  | 8-A   | 609 | 4/4   | -    | -    | 27,28,28,29                 | 4     |
| 2   | ZN   | 1-A   | 604 | 1/1   | 0.86 | 0.07 | 10,10,10,10                 | 1     |
| 4   | EDO  | 2-B   | 610 | 4/4   | -    | -    | 12,14,17,17                 | 4     |
| 4   | EDO  | 3-B   | 610 | 4/4   | -    | -    | 12,13,17,18                 | 4     |
| 4   | EDO  | 4-B   | 610 | 4/4   | -    | -    | 12,13,16,18                 | 4     |
| 4   | EDO  | 5-B   | 610 | 4/4   | -    | -    | 13,14,17,18                 | 4     |
| 4   | EDO  | 6-B   | 610 | 4/4   | -    | -    | 12,13,16,18                 | 4     |
| 4   | EDO  | 7-B   | 610 | 4/4   | -    | -    | 11,12,17,18                 | 4     |
| 4   | EDO  | 8-B   | 610 | 4/4   | -    | -    | 11,12,16,18                 | 4     |
| 4   | EDO  | 1-B   | 610 | 4/4   | 0.91 | 0.12 | 13,14,16,18                 | 4     |
| 4   | EDO  | 2-B   | 611 | 4/4   | -    | -    | 30,30,30,32                 | 4     |
| 4   | EDO  | 3-B   | 611 | 4/4   | -    | -    | 30,30,31,32                 | 4     |
| 4   | EDO  | 4-B   | 611 | 4/4   | -    | -    | 30,30,30,32                 | 4     |
| 4   | EDO  | 5-B   | 611 | 4/4   | -    | -    | 30,30,31,32                 | 4     |
| 4   | EDO  | 6-B   | 611 | 4/4   | -    | -    | 30,30,31,32                 | 4     |
| 4   | EDO  | 7-B   | 611 | 4/4   | -    | -    | 30,30,30,33                 | 4     |
| 4   | EDO  | 8-B   | 611 | 4/4   | -    | -    | 30,30,30,33                 | 4     |
| 2   | ZN   | 1-B   | 606 | 1/1   | 0.97 | 0.14 | 24,24,24,24                 | 1     |
| 4   | EDO  | 2-B   | 612 | 4/4   | -    | -    | 35,36,37,37                 | 4     |
| 4   | EDO  | 3-B   | 612 | 4/4   | -    | -    | 35,36,37,37                 | 4     |
| 4   | EDO  | 4-B   | 612 | 4/4   | -    | -    | 35,36,36,37                 | 4     |
| 4   | EDO  | 5-B   | 612 | 4/4   | -    | -    | 35,36,36,37                 | 4     |
| 4   | EDO  | 6-B   | 612 | 4/4   | -    | -    | 35,35,35,38                 | 4     |
| 4   | EDO  | 7-B   | 612 | 4/4   | -    | -    | 35,35,36,37                 | 4     |
| 4   | EDO  | 8-B   | 612 | 4/4   | -    | -    | 34,36,36,37                 | 4     |

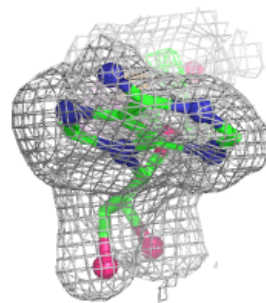
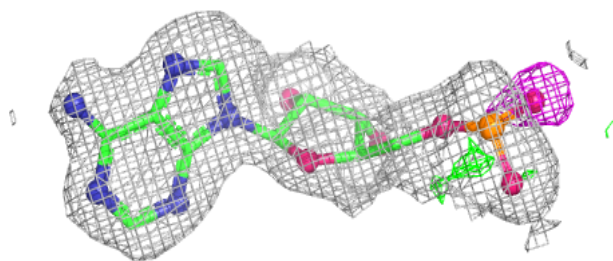
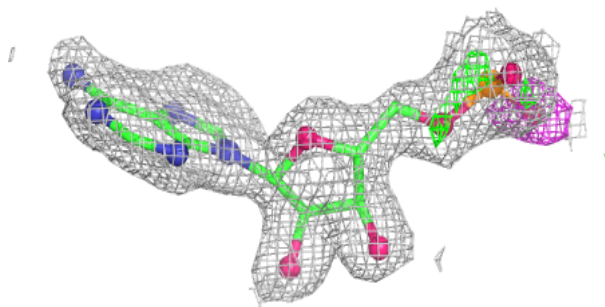
The following is a graphical depiction of the model fit to experimental electron density of all

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



**Electron density around AMP A 601:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.