



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:39 am GMT

PDB ID : 1NW4  
Title : Crystal Structure of Plasmodium falciparum Purine Nucleoside Phosphorylase  
in complex with ImmH and Sulfate  
Authors : Shi, W.; Ting, L.M.; Kicska, G.A.; Lewandowicz, A.; Tyler, P.C.; Evans, G.B.;  
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Deposited on : 2003-02-05  
Resolution : 2.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Mogul                          | : | 1.7.2 (RC1), CSD as538be (2017)                                    |
| Xtriage (Phenix)               | : | 1.9-1692   |
| EDS                            | : | trunk28620   |
| Percentile statistics          | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac                         | : | 5.8.0135   |
| CCP4                           | : | 6.5.0  |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | recalc28949  |

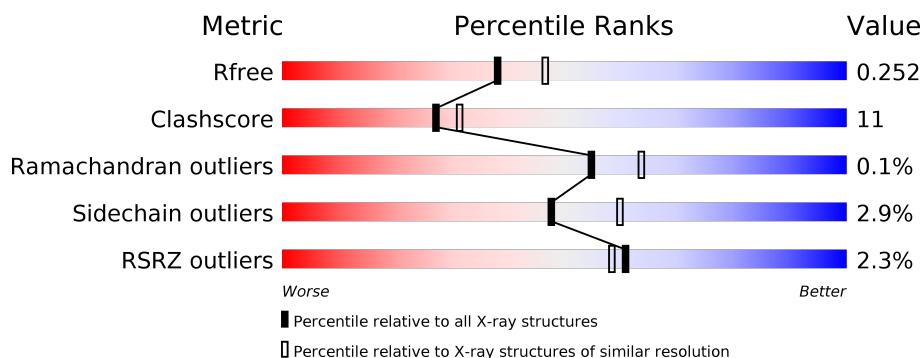
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 4002 (2.20-2.20)                                      |
| Clashscore            | 112137                      | 4730 (2.20-2.20)                                      |
| Ramachandran outliers | 110173                      | 4656 (2.20-2.20)                                      |
| Sidechain outliers    | 110143                      | 4657 (2.20-2.20)                                      |
| RSRZ outliers         | 101464                      | 4033 (2.20-2.20)                                      |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 276    | <div> <div>2%</div> <div> <div></div> <div>63%</div> <div>23%</div> <div>•</div> <div>12%</div> </div> </div> |
| 1   | B     | 276    | <div> <div>3%</div> <div> <div></div> <div>63%</div> <div>23%</div> <div>•</div> <div>12%</div> </div> </div> |
| 1   | C     | 276    | <div> <div>3%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>•</div> <div>12%</div> </div> </div> |
| 1   | D     | 276    | <div> <div>2%</div> <div> <div></div> <div>67%</div> <div>20%</div> <div>•</div> <div>12%</div> </div> </div> |
| 1   | E     | 276    | <div> <div>2%</div> <div> <div></div> <div>66%</div> <div>20%</div> <div>•</div> <div>12%</div> </div> </div> |
| 1   | F     | 276    | <div> <div>%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>•</div> <div>12%</div> </div> </div>  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | SO4  | F     | 415 | -         | -        | -       | X                |
| 4   | IPA  | A     | 510 | -         | -        | -       | X                |
| 4   | IPA  | B     | 501 | -         | -        | -       | X                |
| 4   | IPA  | B     | 508 | -         | -        | -       | X                |
| 4   | IPA  | C     | 504 | -         | -        | -       | X                |
| 4   | IPA  | D     | 514 | -         | -        | -       | X                |
| 4   | IPA  | E     | 506 | -         | -        | -       | X                |
| 4   | IPA  | E     | 513 | -         | -        | -       | X                |
| 4   | IPA  | F     | 505 | -         | -        | -       | X                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11683 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 uridine phosphorylase, putative.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 243      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1861  | 1179 | 319 | 347 | 16 |         |         |       |
| 1   | B     | 243      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1861  | 1179 | 319 | 347 | 16 |         |         |       |
| 1   | C     | 243      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1861  | 1179 | 319 | 347 | 16 |         |         |       |
| 1   | D     | 243      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1861  | 1179 | 319 | 347 | 16 |         |         |       |
| 1   | E     | 243      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1861  | 1179 | 319 | 347 | 16 |         |         |       |
| 1   | F     | 243      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1861  | 1179 | 319 | 347 | 16 |         |         |       |

There are 186 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 0       | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 1       | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 246     | LYS      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 247     | GLY      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 248     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 249     | PHE      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 250     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 251     | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 252     | TYR      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 253     | VAL      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 254     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 255     | GLN      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 256     | LYS      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 257     | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 258     | ILE      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 259     | SER      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 260     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |

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| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 261     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 262     | ASP      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 263     | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 264     | ASN      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 265     | SER      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 266     | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 267     | VAL      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 268     | ASP      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| A     | 269     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| A     | 270     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| A     | 271     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| A     | 272     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| A     | 273     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| A     | 274     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| B     | 0       | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 1       | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 246     | LYS      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 247     | GLY      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 248     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 249     | PHE      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 250     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 251     | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 252     | TYR      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 253     | VAL      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 254     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 255     | GLN      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 256     | LYS      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 257     | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 258     | ILE      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 259     | SER      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 260     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 261     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 262     | ASP      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 263     | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 264     | ASN      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 265     | SER      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 266     | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 267     | VAL      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 268     | ASP      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| B     | 269     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| B     | 270     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| B     | 271     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |

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| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| B     | 272     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| B     | 273     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| B     | 274     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| C     | 0       | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 1       | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 246     | LYS      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 247     | GLY      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 248     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 249     | PHE      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 250     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 251     | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 252     | TYR      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 253     | VAL      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 254     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 255     | GLN      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 256     | LYS      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 257     | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 258     | ILE      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 259     | SER      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 260     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 261     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 262     | ASP      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 263     | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 264     | ASN      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 265     | SER      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 266     | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 267     | VAL      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 268     | ASP      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| C     | 269     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| C     | 270     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| C     | 271     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| C     | 272     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| C     | 273     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| C     | 274     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| D     | 0       | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 1       | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 246     | LYS      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 247     | GLY      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 248     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 249     | PHE      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 250     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 251     | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |

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| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| D     | 252     | TYR      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 253     | VAL      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 254     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 255     | GLN      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 256     | LYS      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 257     | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 258     | ILE      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 259     | SER      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 260     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 261     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 262     | ASP      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 263     | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 264     | ASN      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 265     | SER      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 266     | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 267     | VAL      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 268     | ASP      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| D     | 269     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| D     | 270     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| D     | 271     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| D     | 272     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| D     | 273     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| D     | 274     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| E     | 0       | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 1       | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 246     | LYS      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 247     | GLY      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 248     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 249     | PHE      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 250     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 251     | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 252     | TYR      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 253     | VAL      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 254     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 255     | GLN      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 256     | LYS      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 257     | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 258     | ILE      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 259     | SER      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 260     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 261     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 262     | ASP      | -      | CLONING ARTIFACT | UNP Q8I3X4 |

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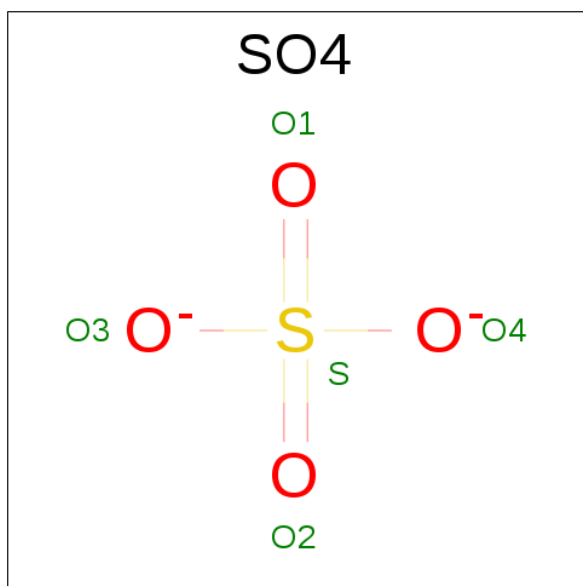
| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| E     | 263     | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 264     | ASN      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 265     | SER      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 266     | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 267     | VAL      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 268     | ASP      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| E     | 269     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| E     | 270     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| E     | 271     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| E     | 272     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| E     | 273     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| E     | 274     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| F     | 0       | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 1       | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 246     | LYS      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 247     | GLY      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 248     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 249     | PHE      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 250     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 251     | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 252     | TYR      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 253     | VAL      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 254     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 255     | GLN      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 256     | LYS      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 257     | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 258     | ILE      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 259     | SER      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 260     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 261     | GLU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 262     | ASP      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 263     | LEU      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 264     | ASN      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 265     | SER      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 266     | ALA      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 267     | VAL      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 268     | ASP      | -      | CLONING ARTIFACT | UNP Q8I3X4 |
| F     | 269     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| F     | 270     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| F     | 271     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| F     | 272     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |
| F     | 273     | HIS      | -      | EXPRESSION TAG   | UNP Q8I3X4 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F     | 274     | HIS      | -      | EXPRESSION TAG | UNP Q8I3X4 |

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



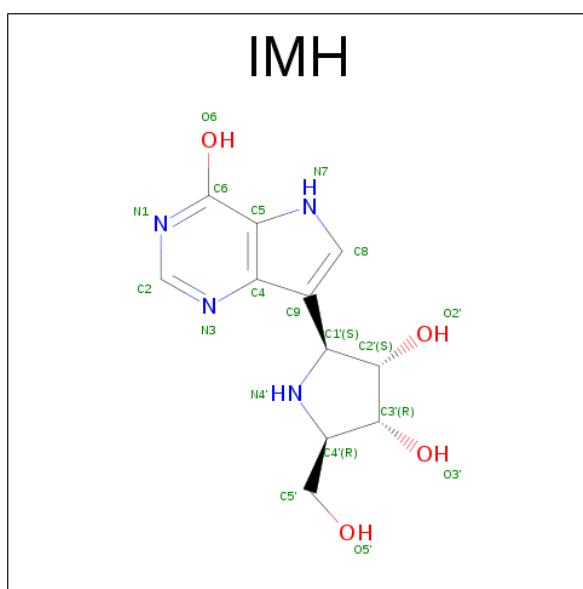
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 3 is 1,4-DIDEOXY-4-AZA-1-(S)-(9-DEAZAHYPOXANTHIN-9-YL)-D-RIBITOL (three-letter code: IMH) (formula: C<sub>11</sub>H<sub>14</sub>N<sub>4</sub>O<sub>4</sub>).



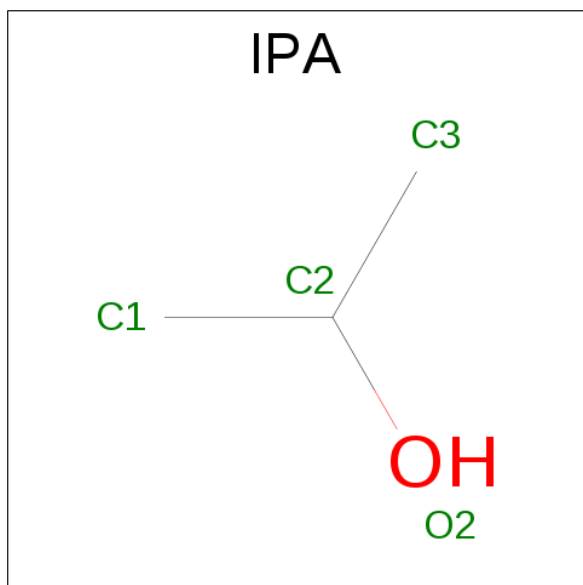
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 11 | 4 | 4 |         |         |
| 3   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 11 | 4 | 4 |         |         |
| 3   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 11 | 4 | 4 |         |         |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 11 | 4 | 4 |         |         |
| 3   | E     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 11 | 4 | 4 |         |         |
| 3   | F     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 19    | 11 | 4 | 4 |         |         |

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



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

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| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | A     | 1        | Total C O<br>4 3 1 | 0       | 0       |
| 4   | A     | 1        | Total C O<br>4 3 1 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>4 3 1 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>4 3 1 | 0       | 0       |
| 4   | E     | 1        | Total C O<br>4 3 1 | 0       | 0       |
| 4   | D     | 1        | Total C O<br>4 3 1 | 0       | 0       |
| 4   | B     | 1        | Total C O<br>4 3 1 | 0       | 0       |

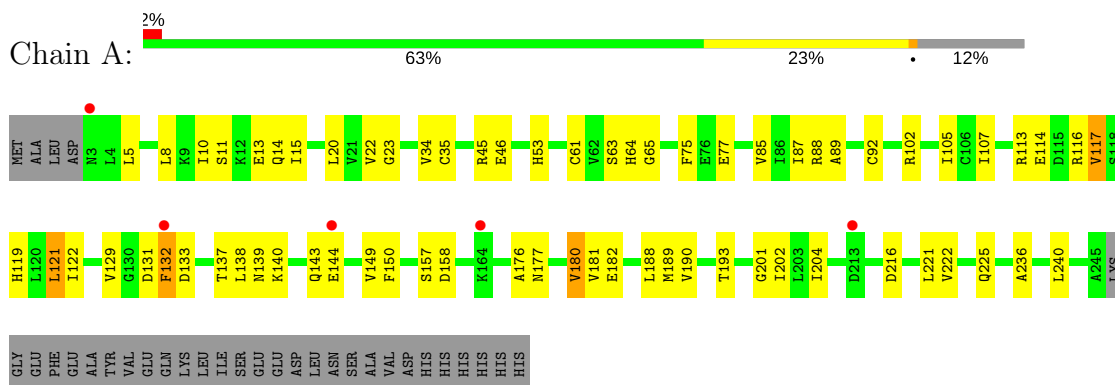
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 5   | A     | 32       | Total O<br>32 32 | 0       | 0       |
| 5   | B     | 28       | Total O<br>28 28 | 0       | 0       |
| 5   | C     | 34       | Total O<br>34 34 | 0       | 0       |
| 5   | D     | 51       | Total O<br>51 51 | 0       | 0       |
| 5   | E     | 54       | Total O<br>54 54 | 0       | 0       |
| 5   | F     | 49       | Total O<br>49 49 | 0       | 0       |

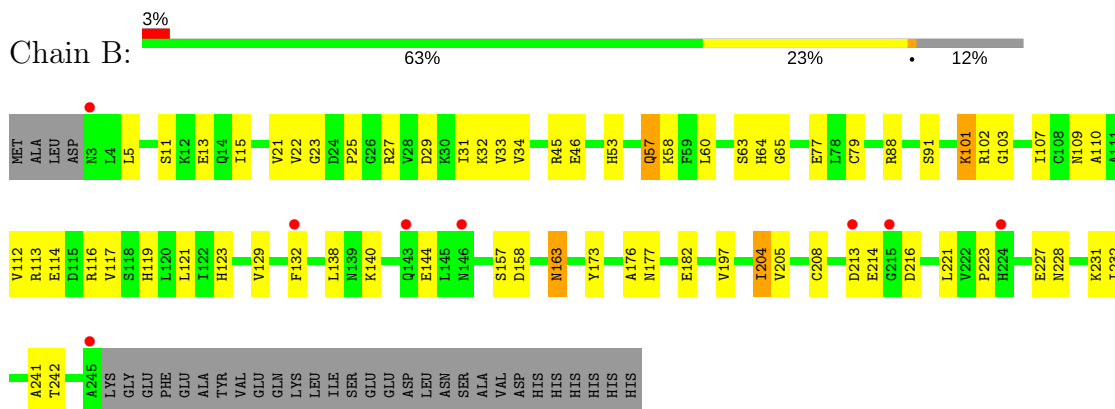
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

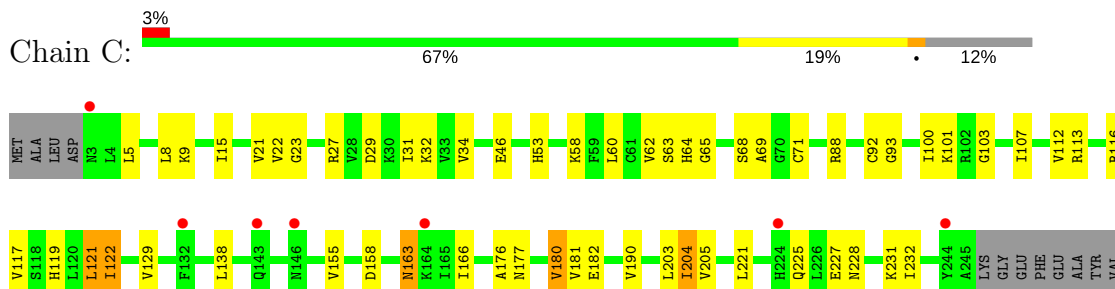
- Molecule 1: uridine phosphorylase, putative



- Molecule 1: uridine phosphorylase, putative



- Molecule 1: uridine phosphorylase, putative



GLU  
GLN  
LYS  
LEU  
LEU  
SER  
ILE  
GLU  
GLU  
ASP  
LEU  
ASN  
ASN  
SER  
ALA  
VAL  
ASP  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

- Molecule 1: uridine phosphorylase, putative



MET ALA ASP ASP N3 L4 L5 E13 Q14 I15 T16 P17 V21 V22 R27 V28 D29 K30 K31 K32 V33 V34 E46 E51 C52 H53 Q57 K58 F59 L60 G61 V62 S63 H64 G65 S68 C71 E77 S91 R102 V112 R113 E114 D115 R116 V117 S118 H119

L120 L121 D131 F132 D133 V134 T137 K140 K144 E144 S157 D158 M163 K164 Y173 A176 N177 E182 C200 I204 K211 W212 D213 D216 L221 L226 L230 A241 T242 K243 Y244 A245 LYS GLY PHE GLU ALA TYR VAL GLU GLN LYS LEU

ILE SER GLU ASP ASP LEU ASN SER ALA VAL ASP HIS HIS HIS HIS HIS HIS

- Molecule 1: uridine phosphorylase, putative



MET ALA ASP ASP N3 L4 L5 I10 E13 Q14 I15 L20 V21 V22 G23 D24 P25 G26 V28 I31 V34 R45 E46 Y54 Q57 C61 V62 S63 H64 G65 S68 C71 F75 E77 V85 K101 R102 N109 V112 R113 E114

V117 S118 H119 L120 L121 I122 F132 D133 V134 Y135 D136 K140 V155 S156 S157 D158 M159 P162 N163 Y173 A176 N177 E182 L188 G200 D213 E214 G215 D216 L221 L226 L234 L240 A245 LYS GLY PHE GLU ALA TYR VAL GLU GLN LYS

LEU ILE SER GLU ASP ASP LEU ASN SER ALA VAL ASP HIS HIS HIS HIS HIS HIS

- Molecule 1: uridine phosphorylase, putative



MET ALA ASP ASP N3 L4 L5 I10 S11 K12 I15 L20 V21 V22 R27 K32 V34 Y38 V39 D40 E46 V50 E51 K58 F59 L60 C61 V62 S63 H64 G65 E77 N81 R88 G93 I100 K101 R102 A110 A111 V112 R113 R116

V117 S118 H119 L120 L121 F132 K140 E144 L145 H146 D158 M163 K164 I165 Y173 A176 N177 V180 V181 E182 I202 V205 D216 V222 L223 H224 Q225 M229 A245 LYS GLY PHE GLU ALA TYR VAL GLU GLN LYS LEU ILE SER GLU GLU ASP

LEU ASN SER ALA VAL ASP HIS HIS HIS HIS HIS HIS HIS

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 86.55Å 92.28Å 239.64Å<br>90.00° 90.00° 90.00°               | Depositor        |
| Resolution (Å)  | 20.00 – 2.20<br>19.97 – 2.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 78.5 (20.00-2.20)<br>80.7 (19.97-2.20)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.06  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.17 (at 2.19Å)   | Xtriage          |
| Refinement program  | CNS 1.0   | Depositor        |
| R, $R_{free}$   | 0.207 , 0.248<br>0.212 , 0.252                              | Depositor<br>DCC |
| $R_{free}$ test set   | 3999 reflections (5.05%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 27.5  | Xtriage          |
| Anisotropy  | 0.439   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.38 , 50.6   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.94  | EDS              |
| Total number of atoms   | 11683   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 32.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A     | 0.33         | 0/1893  | 0.61        | 0/2561  |
| 1   | B     | 0.31         | 0/1893  | 0.58        | 0/2561  |
| 1   | C     | 0.34         | 0/1893  | 0.61        | 0/2561  |
| 1   | D     | 0.35         | 0/1893  | 0.60        | 0/2561  |
| 1   | E     | 0.36         | 0/1893  | 0.62        | 0/2561  |
| 1   | F     | 0.35         | 0/1893  | 0.61        | 0/2561  |
| All | All   | 0.34         | 0/11358 | 0.61        | 0/15366 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1861  | 0        | 1882     | 59      | 0            |
| 1   | B     | 1861  | 0        | 1882     | 52      | 0            |
| 1   | C     | 1861  | 0        | 1882     | 45      | 0            |
| 1   | D     | 1861  | 0        | 1882     | 44      | 0            |
| 1   | E     | 1861  | 0        | 1882     | 43      | 0            |
| 1   | F     | 1861  | 0        | 1882     | 40      | 0            |
| 2   | A     | 20    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | B     | 15    | 0        | 0        | 1       | 0            |
| 2   | C     | 10    | 0        | 0        | 0       | 0            |
| 2   | D     | 15    | 0        | 0        | 1       | 0            |
| 2   | E     | 15    | 0        | 0        | 0       | 0            |
| 2   | F     | 20    | 0        | 0        | 1       | 0            |
| 3   | A     | 19    | 0        | 13       | 1       | 0            |
| 3   | B     | 19    | 0        | 13       | 1       | 0            |
| 3   | C     | 19    | 0        | 13       | 1       | 0            |
| 3   | D     | 19    | 0        | 13       | 2       | 0            |
| 3   | E     | 19    | 0        | 13       | 1       | 0            |
| 3   | F     | 19    | 0        | 13       | 1       | 0            |
| 4   | A     | 12    | 0        | 24       | 1       | 0            |
| 4   | B     | 16    | 0        | 32       | 2       | 0            |
| 4   | C     | 4     | 0        | 8        | 0       | 0            |
| 4   | D     | 8     | 0        | 16       | 0       | 0            |
| 4   | E     | 8     | 0        | 16       | 1       | 0            |
| 4   | F     | 12    | 0        | 24       | 1       | 0            |
| 5   | A     | 32    | 0        | 0        | 2       | 0            |
| 5   | B     | 28    | 0        | 0        | 0       | 0            |
| 5   | C     | 34    | 0        | 0        | 0       | 0            |
| 5   | D     | 51    | 0        | 0        | 5       | 0            |
| 5   | E     | 54    | 0        | 0        | 3       | 0            |
| 5   | F     | 49    | 0        | 0        | 1       | 0            |
| All | All   | 11683 | 0        | 11490    | 262     | 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 11.

All (262) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:138:LEU:HD22 | 1:A:202:ILE:HD11 | 1.35                     | 1.08              |
| 1:E:117:VAL:HG23 | 5:E:628:HOH:O    | 1.78                     | 0.83              |
| 1:D:133:ASP:HB3  | 5:D:751:HOH:O    | 1.76                     | 0.82              |
| 1:D:31:ILE:O     | 1:D:34:VAL:HG12  | 1.83                     | 0.78              |
| 1:A:46:GLU:HB3   | 1:B:46:GLU:HB3   | 1.63                     | 0.78              |
| 1:E:121:LEU:HD12 | 1:F:163:ASN:HB3  | 1.66                     | 0.77              |
| 1:A:133:ASP:O    | 1:A:137:THR:HG23 | 1.85                     | 0.76              |
| 1:E:46:GLU:HB3   | 1:F:46:GLU:HB3   | 1.68                     | 0.75              |
| 1:C:117:VAL:HG22 | 1:D:158:ASP:HB3  | 1.69                     | 0.73              |
| 1:D:15:ILE:HA    | 1:D:60:LEU:HD11  | 1.71                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:163:ASN:HD22 | 1:B:163:ASN:H    | 1.38                     | 0.72              |
| 1:C:46:GLU:HB3   | 1:D:46:GLU:HB3   | 1.71                     | 0.71              |
| 1:F:102:ARG:HD2  | 1:F:216:ASP:OD1  | 1.92                     | 0.69              |
| 1:C:158:ASP:HB3  | 1:D:117:VAL:HG22 | 1.74                     | 0.69              |
| 1:A:138:LEU:CD2  | 1:A:202:ILE:HD11 | 2.20                     | 0.69              |
| 1:B:15:ILE:HA    | 1:B:60:LEU:HD11  | 1.75                     | 0.69              |
| 1:A:138:LEU:HD22 | 1:A:202:ILE:CD1  | 2.19                     | 0.68              |
| 1:E:163:ASN:C    | 1:E:163:ASN:HD22 | 1.96                     | 0.68              |
| 5:E:612:HOH:O    | 1:F:117:VAL:HG23 | 1.93                     | 0.68              |
| 1:F:5:LEU:HD13   | 1:F:77:GLU:HB3   | 1.76                     | 0.66              |
| 1:A:140:LYS:O    | 1:A:144:GLU:HG3  | 1.96                     | 0.65              |
| 1:B:31:ILE:O     | 1:B:34:VAL:HG22  | 1.96                     | 0.65              |
| 1:B:102:ARG:HD2  | 1:B:216:ASP:OD1  | 1.98                     | 0.64              |
| 1:C:204:ILE:HD12 | 1:C:221:LEU:HD22 | 1.80                     | 0.64              |
| 1:A:102:ARG:HD2  | 1:A:216:ASP:OD1  | 1.97                     | 0.64              |
| 1:A:64:HIS:HD2   | 1:A:65:GLY:O     | 1.81                     | 0.64              |
| 1:A:117:VAL:HG22 | 5:A:793:HOH:O    | 1.97                     | 0.64              |
| 1:D:64:HIS:HD2   | 1:D:65:GLY:O     | 1.82                     | 0.63              |
| 1:E:158:ASP:HB3  | 1:F:117:VAL:HG22 | 1.81                     | 0.63              |
| 1:D:102:ARG:HD2  | 1:D:216:ASP:OD1  | 1.97                     | 0.63              |
| 1:B:5:LEU:HD13   | 1:B:77:GLU:HB3   | 1.81                     | 0.62              |
| 1:F:51:GLU:OE2   | 1:F:58:LYS:HD3   | 1.98                     | 0.62              |
| 1:E:5:LEU:HD11   | 1:E:15:ILE:HD11  | 1.80                     | 0.62              |
| 1:A:132:PHE:CE1  | 1:F:132:PHE:HE1  | 2.18                     | 0.61              |
| 1:D:117:VAL:HG23 | 5:D:644:HOH:O    | 2.00                     | 0.61              |
| 1:B:228:ASN:O    | 1:B:232:ILE:HG13 | 2.01                     | 0.61              |
| 1:D:140:LYS:O    | 1:D:144:GLU:HG3  | 1.99                     | 0.61              |
| 1:C:180:VAL:HG13 | 1:C:181:VAL:N    | 2.16                     | 0.60              |
| 1:E:25:PRO:O     | 1:E:28:VAL:HG13  | 2.01                     | 0.60              |
| 1:E:31:ILE:O     | 1:E:34:VAL:HG22  | 2.01                     | 0.60              |
| 1:D:13:GLU:H     | 1:D:13:GLU:CD    | 2.03                     | 0.60              |
| 1:C:5:LEU:HD11   | 1:C:15:ILE:HD11  | 1.83                     | 0.60              |
| 1:A:107:ILE:HD13 | 1:A:138:LEU:HB3  | 1.84                     | 0.60              |
| 5:A:617:HOH:O    | 1:B:117:VAL:HG23 | 2.01                     | 0.60              |
| 1:B:140:LYS:O    | 1:B:144:GLU:HG3  | 2.02                     | 0.60              |
| 1:A:122:ILE:HD11 | 1:A:190:VAL:CG1  | 2.32                     | 0.59              |
| 1:E:64:HIS:HD2   | 1:E:65:GLY:O     | 1.85                     | 0.59              |
| 1:C:117:VAL:HG23 | 5:D:614:HOH:O    | 2.01                     | 0.59              |
| 1:C:64:HIS:HD2   | 1:C:65:GLY:O     | 1.86                     | 0.59              |
| 1:E:102:ARG:HD2  | 1:E:216:ASP:OD1  | 2.02                     | 0.59              |
| 1:E:117:VAL:HG22 | 1:F:158:ASP:HB3  | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:29:ASP:HA    | 1:D:32:LYS:HE2   | 1.84                     | 0.58              |
| 1:F:12:LYS:HG3   | 1:F:81:ASN:O     | 2.03                     | 0.58              |
| 3:D:304:IMH:H2'  | 3:D:304:IMH:N3   | 2.18                     | 0.58              |
| 1:A:122:ILE:HD11 | 1:A:190:VAL:HG11 | 1.86                     | 0.58              |
| 3:E:305:IMH:H2'  | 3:E:305:IMH:N3   | 2.19                     | 0.57              |
| 1:B:23:GLY:HA2   | 1:B:64:HIS:CD2   | 2.39                     | 0.57              |
| 1:A:5:LEU:HD12   | 1:A:8:LEU:HD12   | 1.87                     | 0.57              |
| 1:B:114:GLU:HB3  | 1:B:157:SER:HA   | 1.87                     | 0.57              |
| 1:F:5:LEU:HD11   | 1:F:15:ILE:HD11  | 1.87                     | 0.56              |
| 1:E:117:VAL:O    | 1:E:121:LEU:HD22 | 2.06                     | 0.56              |
| 1:C:116:ARG:HB2  | 1:D:116:ARG:HB2  | 1.87                     | 0.56              |
| 1:D:5:LEU:HD11   | 1:D:15:ILE:HD11  | 1.88                     | 0.56              |
| 1:A:117:VAL:O    | 1:A:121:LEU:HD22 | 2.04                     | 0.56              |
| 1:D:22:VAL:O     | 1:D:63:SER:HA    | 2.06                     | 0.56              |
| 1:C:113:ARG:O    | 1:C:119:HIS:HE1  | 1.89                     | 0.56              |
| 3:A:301:IMH:N3   | 3:A:301:IMH:H2'  | 2.21                     | 0.56              |
| 1:A:117:VAL:HG13 | 1:B:158:ASP:O    | 2.06                     | 0.55              |
| 3:C:303:IMH:H2'  | 3:C:303:IMH:N3   | 2.21                     | 0.55              |
| 1:D:132:PHE:HE1  | 1:E:132:PHE:HD1  | 1.54                     | 0.55              |
| 3:F:306:IMH:N3   | 3:F:306:IMH:H2'  | 2.20                     | 0.55              |
| 1:F:64:HIS:HD2   | 1:F:65:GLY:O     | 1.89                     | 0.55              |
| 1:A:22:VAL:O     | 1:A:63:SER:HA    | 2.07                     | 0.55              |
| 1:B:53:HIS:ND1   | 1:B:58:LYS:HG2   | 2.22                     | 0.55              |
| 1:F:93:GLY:O     | 1:F:180:VAL:HG22 | 2.06                     | 0.55              |
| 1:C:180:VAL:CG1  | 1:C:181:VAL:N    | 2.70                     | 0.55              |
| 1:E:163:ASN:C    | 1:E:163:ASN:ND2  | 2.60                     | 0.55              |
| 1:C:228:ASN:O    | 1:C:232:ILE:HG13 | 2.07                     | 0.55              |
| 1:D:5:LEU:HD13   | 1:D:77:GLU:HB3   | 1.89                     | 0.54              |
| 1:D:27:ARG:NH1   | 1:D:226:LEU:HD21 | 2.23                     | 0.54              |
| 1:E:221:LEU:HD13 | 1:E:226:LEU:HD13 | 1.89                     | 0.53              |
| 1:A:132:PHE:CD1  | 1:F:132:PHE:HE1  | 2.25                     | 0.53              |
| 3:B:302:IMH:N3   | 3:B:302:IMH:H2'  | 2.23                     | 0.53              |
| 1:F:40:ASP:HA    | 1:F:50:VAL:HG22  | 1.90                     | 0.53              |
| 1:A:189:MET:O    | 1:A:193:THR:HG23 | 2.09                     | 0.53              |
| 1:F:140:LYS:O    | 1:F:144:GLU:HG3  | 2.08                     | 0.53              |
| 1:F:27:ARG:NH2   | 2:F:415:SO4:O4   | 2.41                     | 0.53              |
| 1:C:34:VAL:HG12  | 1:C:34:VAL:O     | 2.09                     | 0.53              |
| 1:D:226:LEU:O    | 1:D:230:ILE:HG13 | 2.08                     | 0.53              |
| 1:E:113:ARG:O    | 1:E:119:HIS:HE1  | 1.92                     | 0.52              |
| 1:D:211:LYS:HE3  | 1:D:216:ASP:OD2  | 2.08                     | 0.52              |
| 1:A:149:VAL:HG12 | 1:A:150:PHE:O    | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:163:ASN:H    | 1:D:163:ASN:HD22 | 1.57                     | 0.52              |
| 1:C:176:ALA:O    | 1:C:177:ASN:HB2  | 2.10                     | 0.52              |
| 1:C:29:ASP:O     | 1:C:32:LYS:HG2   | 2.09                     | 0.52              |
| 1:F:15:ILE:HA    | 1:F:60:LEU:HD11  | 1.92                     | 0.52              |
| 1:A:5:LEU:HD13   | 1:A:77:GLU:HB3   | 1.92                     | 0.51              |
| 1:C:93:GLY:O     | 1:C:180:VAL:HG22 | 2.10                     | 0.51              |
| 1:C:227:GLU:HG2  | 1:C:231:LYS:HE3  | 1.91                     | 0.51              |
| 1:D:51:GLU:OE2   | 1:D:58:LYS:HE2   | 2.10                     | 0.51              |
| 1:A:92:CYS:HB2   | 1:A:180:VAL:HG13 | 1.93                     | 0.51              |
| 1:A:107:ILE:HG12 | 1:A:202:ILE:HG23 | 1.92                     | 0.51              |
| 1:E:119:HIS:HD2  | 5:E:806:HOH:O    | 1.93                     | 0.51              |
| 1:B:163:ASN:ND2  | 1:B:163:ASN:H    | 2.06                     | 0.51              |
| 1:D:53:HIS:HE1   | 1:D:58:LYS:HE3   | 1.75                     | 0.51              |
| 1:B:27:ARG:O     | 1:B:31:ILE:HG13  | 2.11                     | 0.51              |
| 1:D:29:ASP:O     | 1:D:32:LYS:HG2   | 2.12                     | 0.50              |
| 1:A:88:ARG:HG3   | 1:A:88:ARG:HH11  | 1.77                     | 0.50              |
| 1:E:20:LEU:O     | 1:E:61:CYS:HA    | 2.10                     | 0.50              |
| 1:F:180:VAL:HG13 | 1:F:181:VAL:N    | 2.26                     | 0.50              |
| 1:F:116:ARG:HE   | 4:F:511:IPA:H13  | 1.77                     | 0.50              |
| 1:A:13:GLU:CD    | 1:A:13:GLU:H     | 2.14                     | 0.50              |
| 1:C:122:ILE:HD11 | 1:C:190:VAL:CG1  | 2.42                     | 0.50              |
| 1:D:133:ASP:O    | 1:D:137:THR:HG23 | 2.11                     | 0.50              |
| 1:A:87:ILE:HD13  | 1:A:138:LEU:HD21 | 1.93                     | 0.50              |
| 1:C:53:HIS:HE1   | 1:C:58:LYS:HE2   | 1.76                     | 0.50              |
| 1:B:123:HIS:HA   | 4:B:508:IPA:H31  | 1.93                     | 0.49              |
| 1:D:176:ALA:O    | 1:D:177:ASN:HB2  | 2.12                     | 0.49              |
| 1:B:22:VAL:HG12  | 1:B:23:GLY:N     | 2.28                     | 0.49              |
| 1:C:112:VAL:HB   | 1:C:155:VAL:HA   | 1.93                     | 0.49              |
| 1:E:13:GLU:H     | 1:E:13:GLU:CD    | 2.15                     | 0.49              |
| 1:A:222:VAL:HB   | 1:A:225:GLN:HB2  | 1.94                     | 0.49              |
| 1:C:103:GLY:HA2  | 1:C:204:ILE:HD11 | 1.95                     | 0.49              |
| 1:A:5:LEU:HD11   | 1:A:15:ILE:HD11  | 1.94                     | 0.49              |
| 1:D:114:GLU:HB3  | 1:D:157:SER:HA   | 1.94                     | 0.49              |
| 1:E:176:ALA:O    | 1:E:177:ASN:HB2  | 2.11                     | 0.49              |
| 1:E:134:VAL:HG11 | 1:E:200:GLY:HA3  | 1.95                     | 0.49              |
| 1:A:88:ARG:O     | 1:A:201:GLY:HA2  | 2.13                     | 0.49              |
| 1:B:13:GLU:H     | 1:B:13:GLU:CD    | 2.17                     | 0.49              |
| 1:B:57:GLN:NE2   | 1:B:242:THR:HA   | 2.28                     | 0.49              |
| 1:C:100:ILE:HG22 | 1:C:205:VAL:HG21 | 1.94                     | 0.49              |
| 1:E:5:LEU:HG     | 1:E:10:ILE:O     | 2.13                     | 0.48              |
| 1:F:176:ALA:O    | 1:F:177:ASN:HB2  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:29:ASP:O     | 1:B:32:LYS:HG2   | 2.13                     | 0.48              |
| 1:C:68:SER:HA    | 1:C:71:CYS:SG    | 2.54                     | 0.48              |
| 1:A:23:GLY:HA2   | 1:A:64:HIS:CD2   | 2.49                     | 0.48              |
| 1:B:227:GLU:HG2  | 1:B:231:LYS:HE3  | 1.94                     | 0.48              |
| 1:A:149:VAL:HG12 | 1:A:150:PHE:N    | 2.28                     | 0.48              |
| 1:C:69:ALA:HA    | 1:C:117:VAL:HG21 | 1.96                     | 0.48              |
| 1:F:34:VAL:O     | 1:F:34:VAL:HG12  | 2.14                     | 0.48              |
| 1:F:20:LEU:O     | 1:F:61:CYS:HA    | 2.14                     | 0.48              |
| 1:A:113:ARG:O    | 1:A:119:HIS:HE1  | 1.96                     | 0.48              |
| 1:A:114:GLU:HB3  | 1:A:157:SER:HA   | 1.95                     | 0.48              |
| 1:C:27:ARG:O     | 1:C:31:ILE:HG13  | 2.13                     | 0.48              |
| 1:C:22:VAL:O     | 1:C:63:SER:HA    | 2.13                     | 0.48              |
| 1:D:131:ASP:OD1  | 1:D:133:ASP:HB2  | 2.13                     | 0.48              |
| 1:A:107:ILE:HG13 | 1:A:149:VAL:HG11 | 1.96                     | 0.47              |
| 1:B:204:ILE:HD12 | 1:B:221:LEU:HD22 | 1.96                     | 0.47              |
| 1:E:46:GLU:CB    | 1:F:46:GLU:HB3   | 2.41                     | 0.47              |
| 1:B:213:ASP:OD2  | 1:B:214:GLU:HG3  | 2.14                     | 0.47              |
| 1:B:110:ALA:HB2  | 1:C:129:VAL:HG11 | 1.95                     | 0.47              |
| 1:D:113:ARG:O    | 1:D:119:HIS:HE1  | 1.97                     | 0.47              |
| 1:F:100:ILE:HG22 | 1:F:205:VAL:HG21 | 1.97                     | 0.47              |
| 1:F:22:VAL:O     | 1:F:63:SER:HA    | 2.15                     | 0.47              |
| 1:A:45:ARG:HB3   | 1:A:46:GLU:OE2   | 2.14                     | 0.47              |
| 1:B:208:CYS:HB3  | 1:B:216:ASP:OD2  | 2.15                     | 0.47              |
| 1:F:5:LEU:HG     | 1:F:10:ILE:O     | 2.15                     | 0.47              |
| 1:B:113:ARG:O    | 1:B:119:HIS:HE1  | 1.98                     | 0.47              |
| 1:E:159:MET:SD   | 1:F:121:LEU:HD13 | 2.55                     | 0.47              |
| 1:E:159:MET:SD   | 1:E:162:PRO:HA   | 2.56                     | 0.46              |
| 1:A:11:SER:OG    | 1:A:14:GLN:HG3   | 2.16                     | 0.46              |
| 1:B:21:VAL:HG23  | 1:B:88:ARG:HA    | 1.97                     | 0.46              |
| 1:A:34:VAL:O     | 1:A:34:VAL:HG12  | 2.16                     | 0.46              |
| 1:B:64:HIS:HD2   | 1:B:65:GLY:O     | 1.99                     | 0.46              |
| 1:C:21:VAL:HG23  | 1:C:88:ARG:HA    | 1.96                     | 0.46              |
| 1:A:89:ALA:HA    | 1:A:202:ILE:O    | 2.15                     | 0.46              |
| 1:C:163:ASN:C    | 1:C:163:ASN:ND2  | 2.69                     | 0.46              |
| 1:F:163:ASN:HD21 | 1:F:165:ILE:HB   | 1.81                     | 0.46              |
| 1:C:163:ASN:C    | 1:C:163:ASN:HD22 | 2.19                     | 0.46              |
| 1:B:45:ARG:HE    | 4:B:501:IPA:H31  | 1.81                     | 0.46              |
| 1:C:92:CYS:HB2   | 1:C:180:VAL:HG13 | 1.97                     | 0.46              |
| 1:E:114:GLU:HB3  | 1:E:157:SER:HA   | 1.98                     | 0.46              |
| 1:A:35:CYS:HB3   | 1:A:53:HIS:O     | 2.15                     | 0.46              |
| 1:E:22:VAL:O     | 1:E:63:SER:HA    | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:180:VAL:CG1  | 1:A:181:VAL:N    | 2.80                     | 0.45              |
| 1:B:204:ILE:HD13 | 1:B:205:VAL:N    | 2.31                     | 0.45              |
| 1:F:113:ARG:O    | 1:F:119:HIS:HE1  | 2.00                     | 0.45              |
| 1:D:119:HIS:HD2  | 5:D:686:HOH:O    | 1.98                     | 0.45              |
| 1:C:46:GLU:CB    | 1:D:46:GLU:HB3   | 2.44                     | 0.45              |
| 1:F:27:ARG:HG2   | 5:F:843:HOH:O    | 2.15                     | 0.45              |
| 1:A:85:VAL:HG11  | 1:A:240:LEU:HD13 | 1.97                     | 0.45              |
| 1:A:139:ASN:O    | 1:A:143:GLN:HG3  | 2.17                     | 0.45              |
| 1:A:180:VAL:HG13 | 1:A:181:VAL:N    | 2.32                     | 0.45              |
| 1:B:11:SER:HB2   | 1:B:13:GLU:OE2   | 2.17                     | 0.45              |
| 1:D:91:SER:HA    | 1:D:204:ILE:O    | 2.16                     | 0.45              |
| 1:B:112:VAL:HG11 | 1:B:173:TYR:CZ   | 2.52                     | 0.45              |
| 1:C:204:ILE:HG23 | 1:C:221:LEU:HD22 | 1.98                     | 0.45              |
| 1:A:64:HIS:HE1   | 1:A:88:ARG:HH11  | 1.64                     | 0.45              |
| 1:C:225:GLN:OE1  | 1:C:225:GLN:HA   | 2.17                     | 0.45              |
| 1:C:92:CYS:HB3   | 1:C:203:LEU:HD13 | 2.00                     | 0.44              |
| 1:D:204:ILE:HG21 | 1:D:221:LEU:HD13 | 1.99                     | 0.44              |
| 1:E:68:SER:HA    | 1:E:71:CYS:SG    | 2.58                     | 0.44              |
| 1:D:132:PHE:HE1  | 1:E:132:PHE:CD1  | 2.35                     | 0.44              |
| 1:D:68:SER:HA    | 1:D:71:CYS:SG    | 2.58                     | 0.44              |
| 1:E:109:ASN:HB3  | 1:E:135:TYR:CD1  | 2.52                     | 0.44              |
| 1:A:158:ASP:HB3  | 1:B:117:VAL:HG22 | 2.00                     | 0.44              |
| 1:B:33:VAL:O     | 1:B:33:VAL:HG12  | 2.17                     | 0.44              |
| 3:D:304:IMH:H2   | 5:D:835:HOH:O    | 2.18                     | 0.44              |
| 1:F:112:VAL:HG11 | 1:F:173:TYR:CZ   | 2.52                     | 0.44              |
| 1:A:5:LEU:HG     | 1:A:10:ILE:O     | 2.18                     | 0.44              |
| 1:E:5:LEU:HD13   | 1:E:77:GLU:HB3   | 1.99                     | 0.44              |
| 1:A:116:ARG:HE   | 4:A:509:IPA:H13  | 1.84                     | 0.43              |
| 1:A:129:VAL:HG11 | 1:F:110:ALA:HB2  | 1.99                     | 0.43              |
| 1:A:121:LEU:HD12 | 1:B:163:ASN:HB3  | 2.01                     | 0.43              |
| 1:B:101:LYS:HB3  | 2:B:410:SO4:O4   | 2.17                     | 0.43              |
| 1:A:75:PHE:CE1   | 1:A:188:LEU:HB2  | 2.53                     | 0.43              |
| 1:A:20:LEU:O     | 1:A:61:CYS:HA    | 2.18                     | 0.43              |
| 1:F:32:LYS:HD2   | 1:F:38:TYR:CE1   | 2.54                     | 0.43              |
| 1:A:105:ILE:O    | 1:A:149:VAL:HG13 | 2.18                     | 0.43              |
| 1:C:122:ILE:HD11 | 1:C:190:VAL:HG11 | 2.00                     | 0.43              |
| 1:D:57:GLN:HG3   | 1:D:241:ALA:HB3  | 2.01                     | 0.43              |
| 1:E:158:ASP:O    | 1:F:117:VAL:HG22 | 2.19                     | 0.43              |
| 1:B:57:GLN:CG    | 1:B:241:ALA:HB3  | 2.49                     | 0.43              |
| 1:B:5:LEU:HD11   | 1:B:15:ILE:HD11  | 2.00                     | 0.43              |
| 1:C:46:GLU:HB3   | 1:D:46:GLU:CB    | 2.45                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:22:VAL:HG11  | 1:B:27:ARG:CG    | 2.49                     | 0.43              |
| 1:D:112:VAL:HG11 | 1:D:173:TYR:CZ   | 2.54                     | 0.43              |
| 1:A:204:ILE:HG21 | 1:A:221:LEU:HD13 | 2.00                     | 0.42              |
| 1:D:21:VAL:HA    | 1:D:62:VAL:O     | 2.18                     | 0.42              |
| 1:E:112:VAL:HG21 | 1:E:155:VAL:HG22 | 2.01                     | 0.42              |
| 1:E:54:TYR:CE2   | 1:E:234:LEU:HB3  | 2.53                     | 0.42              |
| 1:F:222:VAL:HB   | 1:F:225:GLN:HB2  | 2.01                     | 0.42              |
| 1:E:24:ASP:O     | 1:E:27:ARG:HB3   | 2.18                     | 0.42              |
| 1:E:75:PHE:CE1   | 1:E:188:LEU:HB2  | 2.54                     | 0.42              |
| 1:A:116:ARG:HB2  | 1:B:116:ARG:HB2  | 2.01                     | 0.42              |
| 1:A:176:ALA:O    | 1:A:177:ASN:HB2  | 2.19                     | 0.42              |
| 1:A:131:ASP:OD1  | 1:A:133:ASP:HB2  | 2.19                     | 0.42              |
| 1:E:46:GLU:HB3   | 1:F:46:GLU:CB    | 2.45                     | 0.42              |
| 1:C:23:GLY:HA2   | 1:C:64:HIS:CD2   | 2.55                     | 0.42              |
| 1:D:16:THR:HB    | 1:D:17:PRO:HD2   | 2.00                     | 0.42              |
| 1:E:85:VAL:HG11  | 1:E:240:LEU:HD13 | 2.01                     | 0.42              |
| 1:B:79:CYS:SG    | 1:B:197:VAL:HG21 | 2.60                     | 0.42              |
| 1:B:57:GLN:HG2   | 1:B:241:ALA:HB3  | 2.02                     | 0.42              |
| 1:D:102:ARG:HD3  | 2:D:417:SO4:O3   | 2.19                     | 0.42              |
| 1:D:57:GLN:CG    | 1:D:241:ALA:HB3  | 2.50                     | 0.42              |
| 1:A:46:GLU:HB3   | 1:B:46:GLU:CB    | 2.43                     | 0.42              |
| 1:B:109:ASN:O    | 1:B:129:VAL:HG23 | 2.20                     | 0.42              |
| 1:B:103:GLY:HA2  | 1:B:204:ILE:HD11 | 2.01                     | 0.42              |
| 1:B:22:VAL:O     | 1:B:63:SER:HA    | 2.20                     | 0.42              |
| 1:E:45:ARG:HE    | 4:E:506:IPA:H31  | 1.85                     | 0.42              |
| 1:B:22:VAL:HG11  | 1:B:27:ARG:HB3   | 2.02                     | 0.41              |
| 1:E:136:ASP:OD2  | 1:E:140:LYS:HE3  | 2.20                     | 0.41              |
| 1:C:163:ASN:HD21 | 1:C:166:ILE:H    | 1.67                     | 0.41              |
| 1:A:46:GLU:CB    | 1:B:46:GLU:HB3   | 2.43                     | 0.41              |
| 1:D:134:VAL:HG11 | 1:D:200:GLY:HA3  | 2.03                     | 0.41              |
| 1:A:138:LEU:HD23 | 1:A:236:ALA:CB   | 2.50                     | 0.41              |
| 1:B:107:ILE:HD13 | 1:B:138:LEU:HB3  | 2.03                     | 0.41              |
| 1:F:202:ILE:HG12 | 1:F:229:MET:HG3  | 2.03                     | 0.41              |
| 1:C:15:ILE:HA    | 1:C:60:LEU:HD11  | 2.03                     | 0.41              |
| 1:B:25:PRO:HA    | 1:B:63:SER:HB3   | 2.02                     | 0.41              |
| 1:C:117:VAL:O    | 1:C:121:LEU:HD22 | 2.21                     | 0.41              |
| 1:D:176:ALA:CB   | 1:E:122:ILE:HD12 | 2.51                     | 0.41              |
| 1:C:107:ILE:HD13 | 1:C:138:LEU:HB3  | 2.03                     | 0.41              |
| 1:F:225:GLN:HA   | 1:F:225:GLN:OE1  | 2.21                     | 0.41              |
| 1:B:176:ALA:O    | 1:B:177:ASN:HB2  | 2.21                     | 0.40              |
| 1:E:112:VAL:HG11 | 1:E:173:TYR:CZ   | 2.56                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:E:213:ASP:OD2  | 1:E:214:GLU:HG3 | 2.22                     | 0.40              |
| 1:B:91:SER:HA    | 1:B:204:ILE:O   | 2.22                     | 0.40              |
| 1:C:181:VAL:HG13 | 1:C:181:VAL:O   | 2.21                     | 0.40              |
| 1:C:21:VAL:HA    | 1:C:62:VAL:O    | 2.22                     | 0.40              |
| 1:C:8:LEU:O      | 1:C:9:LYS:HB2   | 2.21                     | 0.40              |
| 1:F:21:VAL:HG23  | 1:F:88:ARG:HA   | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 241/276 (87%)   | 228 (95%)  | 13 (5%) | 0        | 100         | 100 |
| 1   | B     | 241/276 (87%)   | 229 (95%)  | 11 (5%) | 1 (0%)   | 38          | 41  |
| 1   | C     | 241/276 (87%)   | 233 (97%)  | 8 (3%)  | 0        | 100         | 100 |
| 1   | D     | 241/276 (87%)   | 232 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 1   | E     | 241/276 (87%)   | 233 (97%)  | 8 (3%)  | 0        | 100         | 100 |
| 1   | F     | 241/276 (87%)   | 234 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| All | All   | 1446/1656 (87%) | 1389 (96%) | 56 (4%) | 1 (0%)   | 55          | 63  |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 223 | PRO  |

### 5.3.2 Protein sidechains [i](#)

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

resolution.

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 206/235 (88%)   | 201 (98%)  | 5 (2%)   | 54          | 67 |
| 1   | B     | 206/235 (88%)   | 199 (97%)  | 7 (3%)   | 42          | 53 |
| 1   | C     | 206/235 (88%)   | 199 (97%)  | 7 (3%)   | 42          | 53 |
| 1   | D     | 206/235 (88%)   | 201 (98%)  | 5 (2%)   | 54          | 67 |
| 1   | E     | 206/235 (88%)   | 198 (96%)  | 8 (4%)   | 37          | 46 |
| 1   | F     | 206/235 (88%)   | 202 (98%)  | 4 (2%)   | 62          | 76 |
| All | All   | 1236/1410 (88%) | 1200 (97%) | 36 (3%)  | 48          | 60 |

All (36) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 117 | VAL  |
| 1   | A     | 121 | LEU  |
| 1   | A     | 132 | PHE  |
| 1   | A     | 180 | VAL  |
| 1   | A     | 182 | GLU  |
| 1   | B     | 57  | GLN  |
| 1   | B     | 101 | LYS  |
| 1   | B     | 121 | LEU  |
| 1   | B     | 132 | PHE  |
| 1   | B     | 163 | ASN  |
| 1   | B     | 182 | GLU  |
| 1   | B     | 204 | ILE  |
| 1   | C     | 101 | LYS  |
| 1   | C     | 121 | LEU  |
| 1   | C     | 122 | ILE  |
| 1   | C     | 163 | ASN  |
| 1   | C     | 180 | VAL  |
| 1   | C     | 182 | GLU  |
| 1   | C     | 204 | ILE  |
| 1   | D     | 3   | ASN  |
| 1   | D     | 57  | GLN  |
| 1   | D     | 121 | LEU  |
| 1   | D     | 163 | ASN  |
| 1   | D     | 182 | GLU  |
| 1   | E     | 28  | VAL  |
| 1   | E     | 57  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 101 | LYS  |
| 1   | E     | 121 | LEU  |
| 1   | E     | 132 | PHE  |
| 1   | E     | 133 | ASP  |
| 1   | E     | 163 | ASN  |
| 1   | E     | 182 | GLU  |
| 1   | F     | 101 | LYS  |
| 1   | F     | 121 | LEU  |
| 1   | F     | 180 | VAL  |
| 1   | F     | 182 | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 44  | ASN  |
| 1   | A     | 57  | GLN  |
| 1   | A     | 64  | HIS  |
| 1   | A     | 119 | HIS  |
| 1   | A     | 139 | ASN  |
| 1   | B     | 57  | GLN  |
| 1   | B     | 64  | HIS  |
| 1   | B     | 119 | HIS  |
| 1   | C     | 44  | ASN  |
| 1   | C     | 53  | HIS  |
| 1   | C     | 64  | HIS  |
| 1   | C     | 119 | HIS  |
| 1   | C     | 163 | ASN  |
| 1   | C     | 224 | HIS  |
| 1   | C     | 228 | ASN  |
| 1   | D     | 44  | ASN  |
| 1   | D     | 53  | HIS  |
| 1   | D     | 57  | GLN  |
| 1   | D     | 64  | HIS  |
| 1   | D     | 119 | HIS  |
| 1   | D     | 163 | ASN  |
| 1   | D     | 219 | ASN  |
| 1   | E     | 44  | ASN  |
| 1   | E     | 57  | GLN  |
| 1   | E     | 64  | HIS  |
| 1   | E     | 119 | HIS  |
| 1   | E     | 151 | ASN  |
| 1   | E     | 163 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 44  | ASN  |
| 1   | F     | 53  | HIS  |
| 1   | F     | 64  | HIS  |
| 1   | F     | 119 | HIS  |
| 1   | F     | 151 | ASN  |
| 1   | F     | 163 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

40 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | IMH  | A     | 301 | -    | 19,21,21     | 2.24 | 7 (36%)     | 15,31,31    | 2.77 | 6 (40%)     |
| 2   | SO4  | A     | 401 | -    | 4,4,4        | 1.81 | 1 (25%)     | 6,6,6       | 0.88 | 0           |
| 2   | SO4  | A     | 411 | -    | 4,4,4        | 1.87 | 1 (25%)     | 6,6,6       | 0.86 | 0           |
| 2   | SO4  | A     | 412 | -    | 4,4,4        | 1.88 | 1 (25%)     | 6,6,6       | 0.89 | 0           |
| 2   | SO4  | A     | 413 | -    | 4,4,4        | 1.85 | 1 (25%)     | 6,6,6       | 0.81 | 0           |
| 4   | IPA  | A     | 502 | -    | 3,3,3        | 0.36 | 0           | 3,3,3       | 0.35 | 0           |
| 4   | IPA  | A     | 509 | -    | 3,3,3        | 0.35 | 0           | 3,3,3       | 0.37 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | IPA  | A     | 510 | -    | 3,3,3        | 0.36 | 0        | 3,3,3       | 0.37 | 0        |
| 3   | IMH  | B     | 302 | -    | 19,21,21     | 2.16 | 7 (36%)  | 15,31,31    | 2.77 | 6 (40%)  |
| 2   | SO4  | B     | 402 | -    | 4,4,4        | 1.84 | 1 (25%)  | 6,6,6       | 0.85 | 0        |
| 2   | SO4  | B     | 407 | -    | 4,4,4        | 1.82 | 1 (25%)  | 6,6,6       | 0.90 | 0        |
| 2   | SO4  | B     | 410 | -    | 4,4,4        | 1.87 | 1 (25%)  | 6,6,6       | 0.86 | 0        |
| 4   | IPA  | B     | 501 | -    | 3,3,3        | 0.40 | 0        | 3,3,3       | 0.42 | 0        |
| 4   | IPA  | B     | 507 | -    | 3,3,3        | 0.39 | 0        | 3,3,3       | 0.38 | 0        |
| 4   | IPA  | B     | 508 | -    | 3,3,3        | 0.39 | 0        | 3,3,3       | 0.37 | 0        |
| 4   | IPA  | B     | 515 | -    | 3,3,3        | 0.36 | 0        | 3,3,3       | 0.41 | 0        |
| 3   | IMH  | C     | 303 | -    | 19,21,21     | 2.06 | 7 (36%)  | 15,31,31    | 2.74 | 6 (40%)  |
| 2   | SO4  | C     | 403 | -    | 4,4,4        | 1.79 | 1 (25%)  | 6,6,6       | 0.85 | 0        |
| 2   | SO4  | C     | 418 | -    | 4,4,4        | 1.85 | 1 (25%)  | 6,6,6       | 0.87 | 0        |
| 4   | IPA  | C     | 504 | -    | 3,3,3        | 0.33 | 0        | 3,3,3       | 0.38 | 0        |
| 3   | IMH  | D     | 304 | -    | 19,21,21     | 2.12 | 7 (36%)  | 15,31,31    | 2.90 | 6 (40%)  |
| 2   | SO4  | D     | 404 | -    | 4,4,4        | 1.81 | 1 (25%)  | 6,6,6       | 0.86 | 0        |
| 2   | SO4  | D     | 408 | -    | 4,4,4        | 1.86 | 1 (25%)  | 6,6,6       | 0.90 | 0        |
| 2   | SO4  | D     | 417 | -    | 4,4,4        | 1.78 | 1 (25%)  | 6,6,6       | 0.87 | 0        |
| 4   | IPA  | D     | 503 | -    | 3,3,3        | 0.32 | 0        | 3,3,3       | 0.34 | 0        |
| 4   | IPA  | D     | 514 | -    | 3,3,3        | 0.25 | 0        | 3,3,3       | 0.30 | 0        |
| 3   | IMH  | E     | 305 | -    | 19,21,21     | 2.15 | 7 (36%)  | 15,31,31    | 2.91 | 7 (46%)  |
| 2   | SO4  | E     | 405 | -    | 4,4,4        | 1.86 | 1 (25%)  | 6,6,6       | 0.87 | 0        |
| 2   | SO4  | E     | 416 | -    | 4,4,4        | 1.86 | 1 (25%)  | 6,6,6       | 0.84 | 0        |
| 2   | SO4  | E     | 419 | -    | 4,4,4        | 1.87 | 1 (25%)  | 6,6,6       | 0.88 | 0        |
| 4   | IPA  | E     | 506 | -    | 3,3,3        | 0.36 | 0        | 3,3,3       | 0.41 | 0        |
| 4   | IPA  | E     | 513 | -    | 3,3,3        | 0.21 | 0        | 3,3,3       | 0.25 | 0        |
| 3   | IMH  | F     | 306 | -    | 19,21,21     | 2.23 | 7 (36%)  | 15,31,31    | 2.82 | 7 (46%)  |
| 2   | SO4  | F     | 406 | -    | 4,4,4        | 1.86 | 1 (25%)  | 6,6,6       | 0.85 | 0        |
| 2   | SO4  | F     | 409 | -    | 4,4,4        | 1.81 | 1 (25%)  | 6,6,6       | 0.83 | 0        |
| 2   | SO4  | F     | 414 | -    | 4,4,4        | 1.83 | 1 (25%)  | 6,6,6       | 0.87 | 0        |
| 2   | SO4  | F     | 415 | -    | 4,4,4        | 1.85 | 1 (25%)  | 6,6,6       | 0.86 | 0        |
| 4   | IPA  | F     | 505 | -    | 3,3,3        | 0.30 | 0        | 3,3,3       | 0.32 | 0        |
| 4   | IPA  | F     | 511 | -    | 3,3,3        | 0.42 | 0        | 3,3,3       | 0.34 | 0        |
| 4   | IPA  | F     | 512 | -    | 3,3,3        | 0.27 | 0        | 3,3,3       | 0.36 | 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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | IMH  | A     | 301 | -    | -       | 0/2/22/22 | 0/3/3/3 |
| 2   | SO4  | A     | 401 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | SO4  | A     | 411 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | SO4  | A     | 412 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | SO4  | A     | 413 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | A     | 502 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | A     | 509 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | A     | 510 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 3   | IMH  | B     | 302 | -    | -       | 0/2/22/22 | 0/3/3/3 |
| 2   | SO4  | B     | 402 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | SO4  | B     | 407 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | SO4  | B     | 410 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | B     | 501 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | B     | 507 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | B     | 508 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | B     | 515 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 3   | IMH  | C     | 303 | -    | -       | 0/2/22/22 | 0/3/3/3 |
| 2   | SO4  | C     | 403 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | SO4  | C     | 418 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | C     | 504 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 3   | IMH  | D     | 304 | -    | -       | 0/2/22/22 | 0/3/3/3 |
| 2   | SO4  | D     | 404 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | SO4  | D     | 408 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | SO4  | D     | 417 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | D     | 503 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | D     | 514 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 3   | IMH  | E     | 305 | -    | -       | 0/2/22/22 | 0/3/3/3 |
| 2   | SO4  | E     | 405 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | SO4  | E     | 416 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | SO4  | E     | 419 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | E     | 506 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | E     | 513 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 3   | IMH  | F     | 306 | -    | -       | 0/2/22/22 | 0/3/3/3 |
| 2   | SO4  | F     | 406 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | SO4  | F     | 409 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | SO4  | F     | 414 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 2   | SO4  | F     | 415 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | F     | 505 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | F     | 511 | -    | -       | 0/0/0/0   | 0/0/0/0 |
| 4   | IPA  | F     | 512 | -    | -       | 0/0/0/0   | 0/0/0/0 |

All (61) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | D     | 304 | IMH  | C3'-C4' | -4.73 | 1.49        | 1.53     |
| 3   | A     | 301 | IMH  | C1'-N4' | -4.33 | 1.42        | 1.47     |
| 3   | F     | 306 | IMH  | C3'-C4' | -4.12 | 1.50        | 1.53     |
| 3   | E     | 305 | IMH  | C3'-C4' | -4.04 | 1.50        | 1.53     |
| 3   | F     | 306 | IMH  | C1'-N4' | -4.01 | 1.42        | 1.47     |
| 3   | A     | 301 | IMH  | C3'-C4' | -3.89 | 1.50        | 1.53     |
| 3   | B     | 302 | IMH  | C1'-N4' | -3.67 | 1.43        | 1.47     |
| 3   | A     | 301 | IMH  | C4'-N4' | -3.58 | 1.42        | 1.48     |
| 3   | B     | 302 | IMH  | C3'-C4' | -3.47 | 1.50        | 1.53     |
| 3   | F     | 306 | IMH  | C4'-N4' | -3.45 | 1.43        | 1.48     |
| 3   | B     | 302 | IMH  | C4'-N4' | -3.32 | 1.43        | 1.48     |
| 3   | C     | 303 | IMH  | C4'-N4' | -3.31 | 1.43        | 1.48     |
| 3   | C     | 303 | IMH  | C3'-C4' | -3.19 | 1.50        | 1.53     |
| 3   | E     | 305 | IMH  | C4'-N4' | -3.17 | 1.43        | 1.48     |
| 3   | E     | 305 | IMH  | C1'-N4' | -3.17 | 1.43        | 1.47     |
| 3   | D     | 304 | IMH  | C4'-N4' | -3.07 | 1.43        | 1.48     |
| 3   | C     | 303 | IMH  | C1'-N4' | -3.05 | 1.43        | 1.47     |
| 3   | D     | 304 | IMH  | C1'-N4' | -2.97 | 1.43        | 1.47     |
| 3   | D     | 304 | IMH  | C8-N7   | -2.80 | 1.30        | 1.36     |
| 3   | B     | 302 | IMH  | C8-N7   | -2.73 | 1.31        | 1.36     |
| 3   | C     | 303 | IMH  | C8-N7   | -2.72 | 1.31        | 1.36     |
| 3   | F     | 306 | IMH  | C8-N7   | -2.72 | 1.31        | 1.36     |
| 3   | E     | 305 | IMH  | C8-N7   | -2.45 | 1.31        | 1.36     |
| 3   | A     | 301 | IMH  | C8-N7   | -2.43 | 1.31        | 1.36     |
| 3   | A     | 301 | IMH  | C4-N3   | 2.44  | 1.40        | 1.37     |
| 3   | B     | 302 | IMH  | C4-N3   | 2.50  | 1.40        | 1.37     |
| 3   | D     | 304 | IMH  | C4-N3   | 2.72  | 1.40        | 1.37     |
| 3   | E     | 305 | IMH  | C2-N3   | 2.90  | 1.37        | 1.32     |
| 3   | C     | 303 | IMH  | C4-N3   | 2.96  | 1.40        | 1.37     |
| 3   | F     | 306 | IMH  | C2-N3   | 2.98  | 1.37        | 1.32     |
| 3   | F     | 306 | IMH  | C4-N3   | 2.99  | 1.40        | 1.37     |
| 2   | A     | 401 | SO4  | O1-S    | 3.01  | 1.62        | 1.45     |
| 3   | D     | 304 | IMH  | C2-N3   | 3.02  | 1.37        | 1.32     |
| 2   | C     | 403 | SO4  | O1-S    | 3.02  | 1.62        | 1.45     |
| 2   | D     | 417 | SO4  | O1-S    | 3.03  | 1.62        | 1.45     |
| 2   | D     | 404 | SO4  | O1-S    | 3.04  | 1.62        | 1.45     |
| 3   | E     | 305 | IMH  | C4-N3   | 3.04  | 1.41        | 1.37     |
| 2   | F     | 409 | SO4  | O1-S    | 3.09  | 1.62        | 1.45     |
| 2   | B     | 402 | SO4  | O1-S    | 3.10  | 1.62        | 1.45     |
| 2   | E     | 405 | SO4  | O1-S    | 3.13  | 1.62        | 1.45     |
| 2   | F     | 414 | SO4  | O1-S    | 3.14  | 1.62        | 1.45     |
| 2   | F     | 415 | SO4  | O1-S    | 3.15  | 1.62        | 1.45     |
| 2   | F     | 406 | SO4  | O1-S    | 3.15  | 1.62        | 1.45     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | B     | 407 | SO4  | O1-S  | 3.16 | 1.62        | 1.45     |
| 2   | A     | 413 | SO4  | O1-S  | 3.18 | 1.62        | 1.45     |
| 2   | C     | 418 | SO4  | O1-S  | 3.19 | 1.62        | 1.45     |
| 2   | E     | 416 | SO4  | O1-S  | 3.19 | 1.63        | 1.45     |
| 2   | B     | 410 | SO4  | O1-S  | 3.21 | 1.63        | 1.45     |
| 2   | A     | 411 | SO4  | O1-S  | 3.21 | 1.63        | 1.45     |
| 2   | E     | 419 | SO4  | O1-S  | 3.21 | 1.63        | 1.45     |
| 2   | A     | 412 | SO4  | O1-S  | 3.22 | 1.63        | 1.45     |
| 3   | C     | 303 | IMH  | C2-N3 | 3.23 | 1.37        | 1.32     |
| 3   | A     | 301 | IMH  | C2-N3 | 3.26 | 1.37        | 1.32     |
| 2   | D     | 408 | SO4  | O1-S  | 3.27 | 1.63        | 1.45     |
| 3   | D     | 304 | IMH  | C2-N1 | 3.48 | 1.40        | 1.33     |
| 3   | C     | 303 | IMH  | C2-N1 | 3.56 | 1.40        | 1.33     |
| 3   | A     | 301 | IMH  | C2-N1 | 3.58 | 1.40        | 1.33     |
| 3   | B     | 302 | IMH  | C2-N3 | 3.62 | 1.38        | 1.32     |
| 3   | B     | 302 | IMH  | C2-N1 | 3.68 | 1.40        | 1.33     |
| 3   | F     | 306 | IMH  | C2-N1 | 3.93 | 1.41        | 1.33     |
| 3   | E     | 305 | IMH  | C2-N1 | 4.11 | 1.41        | 1.33     |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | C     | 303 | IMH  | N3-C2-N1    | -7.38 | 122.43      | 128.86   |
| 3   | A     | 301 | IMH  | N3-C2-N1    | -7.32 | 122.48      | 128.86   |
| 3   | E     | 305 | IMH  | N3-C2-N1    | -7.32 | 122.48      | 128.86   |
| 3   | F     | 306 | IMH  | N3-C2-N1    | -7.30 | 122.50      | 128.86   |
| 3   | B     | 302 | IMH  | N3-C2-N1    | -7.28 | 122.52      | 128.86   |
| 3   | D     | 304 | IMH  | N3-C2-N1    | -7.15 | 122.63      | 128.86   |
| 3   | D     | 304 | IMH  | C9-C1'-N4'  | -5.15 | 104.40      | 112.52   |
| 3   | E     | 305 | IMH  | C9-C1'-N4'  | -5.03 | 104.60      | 112.52   |
| 3   | F     | 306 | IMH  | C9-C1'-N4'  | -4.36 | 105.66      | 112.52   |
| 3   | B     | 302 | IMH  | C9-C1'-N4'  | -4.05 | 106.13      | 112.52   |
| 3   | A     | 301 | IMH  | C9-C1'-N4'  | -3.96 | 106.29      | 112.52   |
| 3   | C     | 303 | IMH  | C9-C1'-N4'  | -3.74 | 106.63      | 112.52   |
| 3   | D     | 304 | IMH  | O3'-C3'-C4' | -2.98 | 105.41      | 112.26   |
| 3   | E     | 305 | IMH  | O3'-C3'-C4' | -2.83 | 105.74      | 112.26   |
| 3   | A     | 301 | IMH  | O3'-C3'-C4' | -2.78 | 105.86      | 112.26   |
| 3   | F     | 306 | IMH  | O3'-C3'-C4' | -2.73 | 105.97      | 112.26   |
| 3   | B     | 302 | IMH  | O3'-C3'-C4' | -2.69 | 106.08      | 112.26   |
| 3   | C     | 303 | IMH  | O3'-C3'-C4' | -2.59 | 106.30      | 112.26   |
| 3   | C     | 303 | IMH  | C9-C4-C5    | -2.24 | 105.73      | 116.31   |
| 3   | F     | 306 | IMH  | C9-C4-C5    | -2.23 | 105.78      | 116.31   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | D     | 304 | IMH  | C9-C4-C5 | -2.23 | 105.82      | 116.31   |
| 3   | B     | 302 | IMH  | C9-C4-C5 | -2.21 | 105.90      | 116.31   |
| 3   | E     | 305 | IMH  | C9-C4-C5 | -2.21 | 105.90      | 116.31   |
| 3   | A     | 301 | IMH  | C9-C4-C5 | -2.19 | 105.98      | 116.31   |
| 3   | E     | 305 | IMH  | C2-N1-C6 | 2.01  | 124.52      | 117.26   |
| 3   | F     | 306 | IMH  | C2-N1-C6 | 2.03  | 124.60      | 117.26   |
| 3   | C     | 303 | IMH  | C9-C8-N7 | 3.26  | 115.01      | 108.79   |
| 3   | B     | 302 | IMH  | C9-C8-N7 | 3.32  | 115.13      | 108.79   |
| 3   | A     | 301 | IMH  | C9-C8-N7 | 3.34  | 115.16      | 108.79   |
| 3   | E     | 305 | IMH  | C9-C8-N7 | 3.36  | 115.21      | 108.79   |
| 3   | F     | 306 | IMH  | C9-C8-N7 | 3.37  | 115.23      | 108.79   |
| 3   | D     | 304 | IMH  | C9-C8-N7 | 3.44  | 115.37      | 108.79   |
| 3   | A     | 301 | IMH  | O6-C6-C5 | 3.79  | 127.00      | 119.71   |
| 3   | C     | 303 | IMH  | O6-C6-C5 | 3.83  | 127.06      | 119.71   |
| 3   | F     | 306 | IMH  | O6-C6-C5 | 3.87  | 127.14      | 119.71   |
| 3   | E     | 305 | IMH  | O6-C6-C5 | 3.88  | 127.16      | 119.71   |
| 3   | D     | 304 | IMH  | O6-C6-C5 | 3.88  | 127.16      | 119.71   |
| 3   | B     | 302 | IMH  | O6-C6-C5 | 3.92  | 127.25      | 119.71   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 15 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 301 | IMH  | 1       | 0            |
| 4   | A     | 509 | IPA  | 1       | 0            |
| 3   | B     | 302 | IMH  | 1       | 0            |
| 2   | B     | 410 | SO4  | 1       | 0            |
| 4   | B     | 501 | IPA  | 1       | 0            |
| 4   | B     | 508 | IPA  | 1       | 0            |
| 3   | C     | 303 | IMH  | 1       | 0            |
| 3   | D     | 304 | IMH  | 2       | 0            |
| 2   | D     | 417 | SO4  | 1       | 0            |
| 3   | E     | 305 | IMH  | 1       | 0            |
| 4   | E     | 506 | IPA  | 1       | 0            |
| 3   | F     | 306 | IMH  | 1       | 0            |
| 2   | F     | 415 | SO4  | 1       | 0            |
| 4   | F     | 511 | IPA  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 243/276 (88%)   | -0.21  | 5 (2%) 64 61  | 15, 32, 47, 60        | 0     |
| 1   | B     | 243/276 (88%)   | -0.10  | 8 (3%) 47 44  | 19, 37, 54, 59        | 0     |
| 1   | C     | 243/276 (88%)   | -0.09  | 7 (2%) 52 50  | 17, 33, 50, 61        | 0     |
| 1   | D     | 243/276 (88%)   | -0.36  | 5 (2%) 64 61  | 16, 29, 43, 56        | 0     |
| 1   | E     | 243/276 (88%)   | -0.38  | 5 (2%) 64 61  | 12, 26, 42, 53        | 0     |
| 1   | F     | 243/276 (88%)   | -0.34  | 4 (1%) 72 70  | 16, 27, 43, 54        | 0     |
| All | All   | 1458/1656 (88%) | -0.25  | 34 (2%) 61 58 | 12, 30, 49, 61        | 0     |

All (34) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 3   | ASN  | 4.5  |
| 1   | C     | 143 | GLN  | 4.5  |
| 1   | E     | 245 | ALA  | 4.0  |
| 1   | D     | 3   | ASN  | 3.6  |
| 1   | E     | 132 | PHE  | 3.4  |
| 1   | C     | 3   | ASN  | 3.4  |
| 1   | A     | 132 | PHE  | 3.2  |
| 1   | D     | 245 | ALA  | 2.9  |
| 1   | B     | 143 | GLN  | 2.9  |
| 1   | A     | 213 | ASP  | 2.8  |
| 1   | E     | 3   | ASN  | 2.8  |
| 1   | B     | 245 | ALA  | 2.7  |
| 1   | D     | 213 | ASP  | 2.7  |
| 1   | E     | 213 | ASP  | 2.6  |
| 1   | B     | 146 | ASN  | 2.6  |
| 1   | A     | 3   | ASN  | 2.6  |
| 1   | B     | 213 | ASP  | 2.5  |
| 1   | B     | 132 | PHE  | 2.4  |
| 1   | B     | 224 | HIS  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 132 | PHE  | 2.4  |
| 1   | C     | 224 | HIS  | 2.4  |
| 1   | B     | 215 | GLY  | 2.4  |
| 1   | C     | 146 | ASN  | 2.3  |
| 1   | A     | 144 | GLU  | 2.3  |
| 1   | C     | 244 | TYR  | 2.2  |
| 1   | A     | 164 | LYS  | 2.2  |
| 1   | E     | 214 | GLU  | 2.1  |
| 1   | F     | 33  | VAL  | 2.1  |
| 1   | F     | 146 | ASN  | 2.1  |
| 1   | D     | 164 | LYS  | 2.1  |
| 1   | C     | 164 | LYS  | 2.1  |
| 1   | F     | 224 | HIS  | 2.0  |
| 1   | F     | 3   | ASN  | 2.0  |
| 1   | D     | 243 | LYS  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 4   | IPA  | B     | 501 | 4/4   | 0.81 | 0.21 | 5.68 | 26,31,32,33                | 0     |
| 4   | IPA  | F     | 505 | 4/4   | 0.79 | 0.23 | 5.07 | 31,34,34,34                | 0     |
| 4   | IPA  | E     | 506 | 4/4   | 0.91 | 0.20 | 4.67 | 16,18,18,20                | 0     |
| 4   | IPA  | A     | 510 | 4/4   | 0.83 | 0.18 | 4.39 | 33,33,35,36                | 0     |
| 2   | SO4  | F     | 415 | 5/5   | 0.94 | 0.27 | 4.13 | 64,65,66,67                | 0     |
| 4   | IPA  | E     | 513 | 4/4   | 0.86 | 0.18 | 3.29 | 12,16,17,20                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 4   | IPA  | B     | 508 | 4/4   | 0.88 | 0.17 | 3.11  | 27,29,31,32                 | 0     |
| 4   | IPA  | C     | 504 | 4/4   | 0.83 | 0.14 | 2.72  | 21,22,23,25                 | 0     |
| 4   | IPA  | D     | 514 | 4/4   | 0.82 | 0.17 | 2.26  | 16,19,19,20                 | 0     |
| 4   | IPA  | D     | 503 | 4/4   | 0.92 | 0.19 | 1.97  | 24,26,28,29                 | 0     |
| 2   | SO4  | D     | 408 | 5/5   | 0.99 | 0.11 | 1.68  | 27,29,30,30                 | 0     |
| 4   | IPA  | F     | 512 | 4/4   | 0.81 | 0.14 | 1.65  | 22,23,24,25                 | 0     |
| 2   | SO4  | F     | 409 | 5/5   | 0.99 | 0.11 | 1.45  | 24,25,26,26                 | 0     |
| 4   | IPA  | A     | 502 | 4/4   | 0.88 | 0.16 | 1.04  | 32,33,33,35                 | 0     |
| 3   | IMH  | D     | 304 | 19/19 | 0.95 | 0.12 | 0.78  | 17,21,28,28                 | 0     |
| 3   | IMH  | C     | 303 | 19/19 | 0.93 | 0.11 | 0.39  | 29,35,37,38                 | 0     |
| 4   | IPA  | B     | 515 | 4/4   | 0.91 | 0.12 | 0.38  | 22,23,24,25                 | 0     |
| 3   | IMH  | A     | 301 | 19/19 | 0.96 | 0.11 | 0.09  | 27,28,31,31                 | 0     |
| 3   | IMH  | E     | 305 | 19/19 | 0.94 | 0.10 | -0.08 | 25,27,29,31                 | 0     |
| 2   | SO4  | B     | 407 | 5/5   | 0.99 | 0.08 | -0.08 | 28,28,31,32                 | 0     |
| 2   | SO4  | A     | 413 | 5/5   | 0.99 | 0.08 | -0.23 | 24,25,27,28                 | 0     |
| 3   | IMH  | F     | 306 | 19/19 | 0.97 | 0.09 | -0.52 | 20,23,27,30                 | 0     |
| 3   | IMH  | B     | 302 | 19/19 | 0.96 | 0.10 | -0.60 | 31,35,38,39                 | 0     |
| 2   | SO4  | D     | 404 | 5/5   | 0.98 | 0.09 | -0.91 | 37,38,40,41                 | 0     |
| 2   | SO4  | C     | 418 | 5/5   | 0.99 | 0.08 | -1.15 | 30,30,32,33                 | 0     |
| 2   | SO4  | A     | 401 | 5/5   | 0.99 | 0.08 | -1.19 | 37,39,39,41                 | 0     |
| 2   | SO4  | A     | 412 | 5/5   | 0.98 | 0.08 | -1.47 | 49,50,51,51                 | 0     |
| 2   | SO4  | D     | 417 | 5/5   | 0.99 | 0.06 | -1.47 | 30,30,31,33                 | 0     |
| 2   | SO4  | B     | 402 | 5/5   | 0.99 | 0.07 | -1.69 | 42,42,43,44                 | 0     |
| 2   | SO4  | C     | 403 | 5/5   | 0.99 | 0.07 | -1.70 | 31,32,33,35                 | 0     |
| 2   | SO4  | F     | 406 | 5/5   | 0.99 | 0.06 | -1.83 | 28,29,30,31                 | 0     |
| 2   | SO4  | E     | 405 | 5/5   | 0.99 | 0.05 | -2.03 | 27,29,31,31                 | 0     |
| 2   | SO4  | E     | 419 | 5/5   | 0.98 | 0.11 | -     | 54,54,56,57                 | 0     |
| 4   | IPA  | A     | 509 | 4/4   | 0.86 | 0.14 | -     | 26,26,26,30                 | 0     |
| 2   | SO4  | B     | 410 | 5/5   | 0.94 | 0.15 | -     | 62,62,63,63                 | 0     |
| 4   | IPA  | B     | 507 | 4/4   | 0.89 | 0.12 | -     | 24,26,28,29                 | 0     |
| 2   | SO4  | A     | 411 | 5/5   | 0.94 | 0.29 | -     | 64,65,65,67                 | 0     |
| 4   | IPA  | F     | 511 | 4/4   | 0.83 | 0.16 | -     | 19,21,23,28                 | 0     |
| 2   | SO4  | F     | 414 | 5/5   | 0.99 | 0.08 | -     | 33,33,36,36                 | 0     |
| 2   | SO4  | E     | 416 | 5/5   | 0.99 | 0.15 | -     | 29,29,30,31                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.