



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 1NW4 / pdb\_00001nw4  
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.; Furneaux, R.H.; Kim, K.; Almo, S.C.; Schramm, V.L.  
Deposited on : 2003-02-05  
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

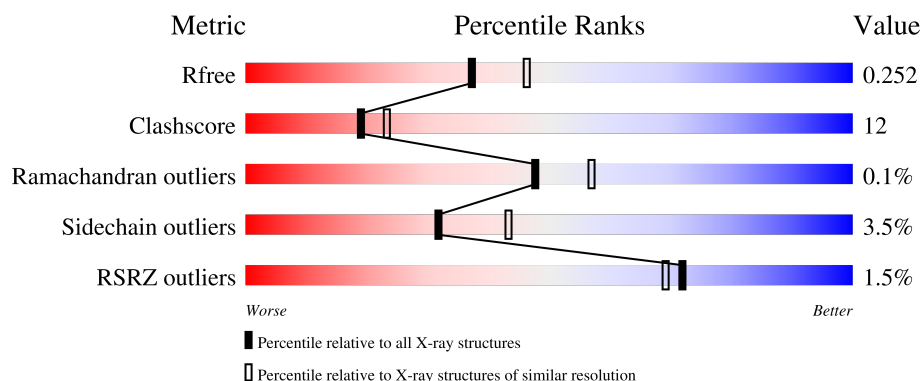
# 1 Overall quality at a glance

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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 6164 (2.20-2.20)                                      |
| Clashscore            | 190562                      | 6851 (2.20-2.20)                                      |
| Ramachandran outliers | 187476                      | 6768 (2.20-2.20)                                      |
| Sidechain outliers    | 187428                      | 6769 (2.20-2.20)                                      |
| RSRZ outliers         | 180081                      | 6166 (2.20-2.20)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                                                                                                                                                                                                                                          |
|-----|-------|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1   | A     | 276    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 25%, green 61%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>61%</span> <span>25%</span> <span>•</span> <span>12%</span> </div> </div>  |
| 1   | B     | 276    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 25%, green 61%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>61%</span> <span>25%</span> <span>•</span> <span>12%</span> </div> </div> |
| 1   | C     | 276    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 21%, green 65%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>65%</span> <span>21%</span> <span>•</span> <span>12%</span> </div> </div> |
| 1   | D     | 276    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 21%, green 64%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>64%</span> <span>21%</span> <span>•</span> <span>12%</span> </div> </div>  |

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| Mol | Chain | Length | Quality of chain                                                                                               |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------------|
| 1   | E     | 276    | <div><div><div>%</div><div><div></div></div><div>64%</div><div>22%</div><div>•</div><div>12%</div></div></div> |
| 1   | F     | 276    | <div><div><div>%</div><div><div></div></div><div>67%</div><div>20%</div><div>•</div><div>12%</div></div></div> |

## 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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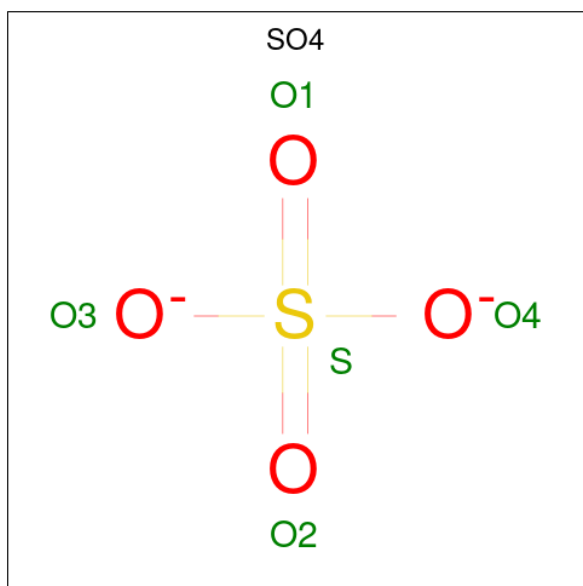
| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| E     | 263     | LEU      | -      | cloning artifact | UNP Q8I3X4 |
| E     | 264     | ASN      | -      | cloning artifact | UNP Q8I3X4 |
| E     | 265     | 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 (CCD ID: SO4) (formula: O<sub>4</sub>S).



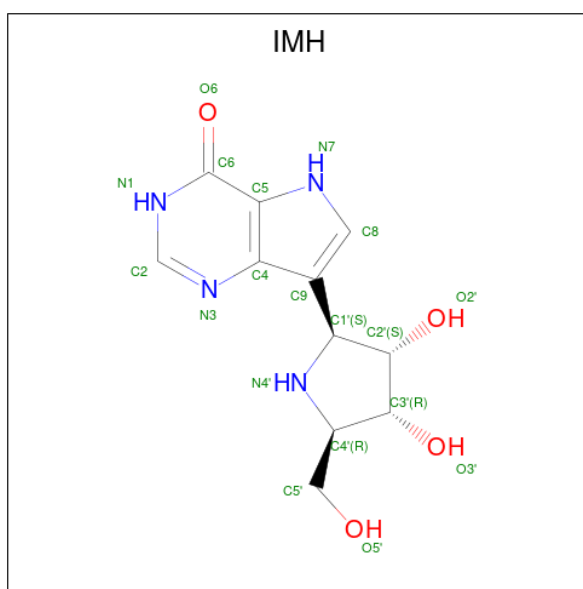
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0    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

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| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 2   | D     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 2   | E     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 2   | E     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 2   | E     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 2   | F     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 2   | F     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 2   | F     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 2   | F     | 1        | Total O S<br>5 4 1 | 0       | 0       |

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



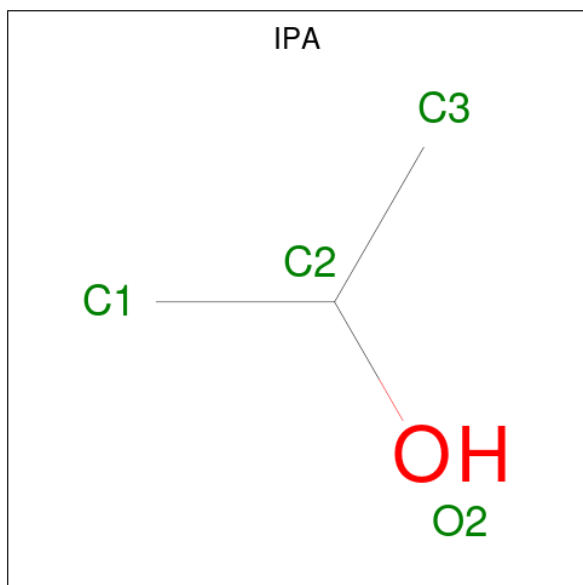
| Mol | Chain | Residues | Atoms                    | ZeroOcc | AltConf |
|-----|-------|----------|--------------------------|---------|---------|
| 3   | A     | 1        | Total C N O<br>19 11 4 4 | 0       | 0       |
| 3   | B     | 1        | Total C N O<br>19 11 4 4 | 0       | 0       |
| 3 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

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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 (CCD ID: IPA) (formula:  $C_3H_8O$ ).



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

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

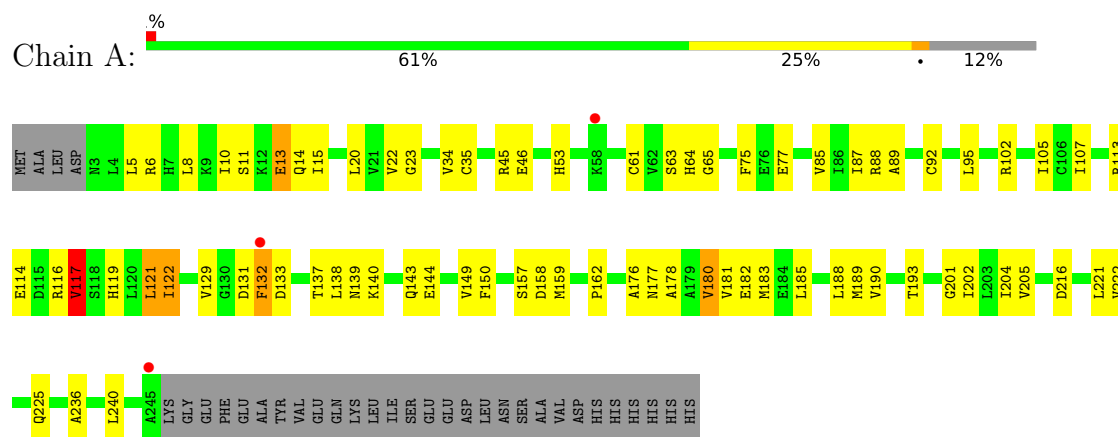
- Molecule 5 is water.

| 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       |

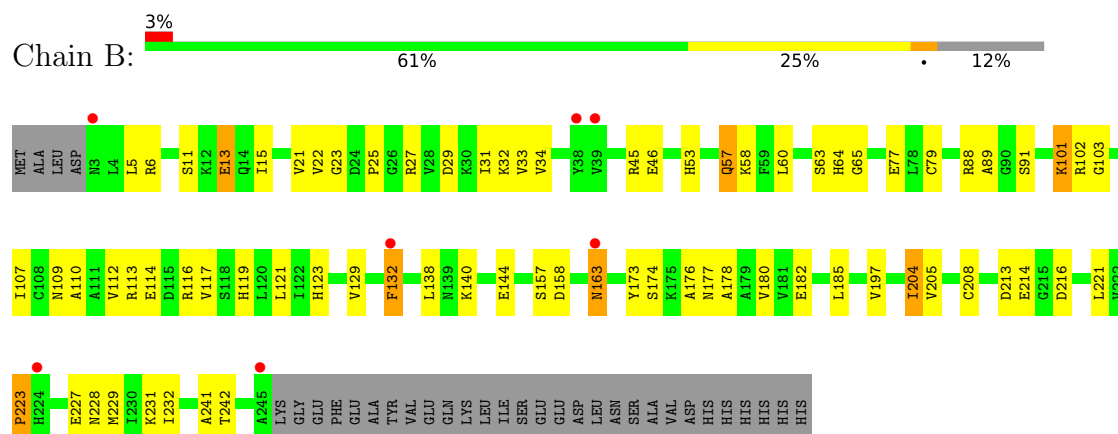
### 3 Residue-property plots

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

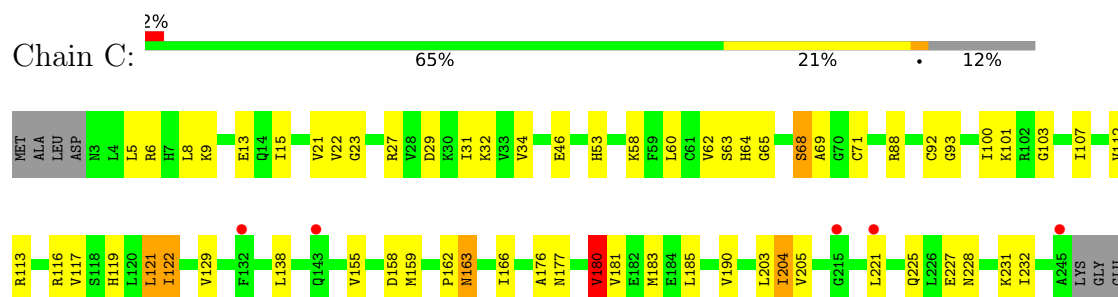
- Molecule 1: uridine phosphorylase, putative



- Molecule 1: uridine phosphorylase, putative



- Molecule 1: uridine phosphorylase, putative



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

- Molecule 1: uridine phosphorylase, putative



MET  
ALA  
LEU  
ASP  
N3  
L4  
L5  
E13  
Q14  
I15  
T16  
P17  
V21  
V22  
G23  
D24  
R27  
V28  
D29  
K30  
I31  
K32  
V33  
V34  
R45  
E46  
E51  
C52  
H53  
Q57  
K58  
F59  
L60  
C61  
V62  
S63  
H64  
G65  
S68  
C71  
E77  
G82  
A89  
G90  
S91  
R102  
V112

R113  
E114  
D115  
R116  
V117  
S118  
L119  
H120  
L121  
D131  
F132  
D133  
V134  
T137  
K140  
E144  
S157  
D158  
R159  
N163  
Y173  
A176  
N177  
A178  
E182  
G200  
I204  
V205  
K211  
D216  
L221  
H224  
Q225  
L226  
M229  
I230  
A241  
A245  
LYS  
GLY  
PHE  
GLU

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

- Molecule 1: uridine phosphorylase, putative



MET  
ALA  
LEU  
ASP  
N3  
L4  
L5  
R6  
I10  
E13  
Q14  
I15  
L20  
V21  
G23  
D24  
P25  
G26  
R27  
V28  
I31  
V34  
R45  
E46  
Y54  
Q57  
C61  
V62  
S63  
H64  
G65  
S68  
C71  
F75  
E76  
E77  
G82  
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  
M163  
Y173  
S174  
K175  
A176  
N177  
E182  
M183  
E184  
L185  
L188  
G200  
D213  
E214  
G215  
D216  
L221  
V222  
L226  
L234  
L240  
A245  
LYS  
GLY  
GLU

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

- Molecule 1: uridine phosphorylase, putative



MET  
ALA  
LEU  
ASP  
N3  
L4  
L5  
I10  
S11  
K12  
E13  
Q14  
I15  
L20  
V21  
V22  
R27  
K32  
V33  
V34  
Y38  
V39  
D40  
R45  
E46  
V50  
E51  
K58  
F59  
L60  
C61  
V62  
S63  
H64  
G65  
E77  
N81  
G82  
R83  
A89  
G93  
I100  
K101  
R102  
A110  
A111

V112  
R113  
R116  
V117  
S118  
H119  
L120  
L121  
F132  
K140  
E144  
L145  
N146  
D158  
M163  
K164  
I165  
Y173  
A176  
M177  
A178  
A179  
V180  
V181  
E182  
M183  
I202  
V205  
D216  
V222  
Q225  
M229  
A245  
LYS  
GLY  
PHE  
GLU  
GLU  
ALA  
TYR  
VAL  
GLU  
LYS  
LEU

ILE  
SER  
GLU  
ASP  
LEU  
ASN  
SER  
ALA  
VAL  
ASP  
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>20.00 – 2.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 78.5 (20.00-2.20)<br>80.6 (20.00-2.20)                      | 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                                                     | 4001 reflections (5.05%)                                    | wwPDB-VP         |
| 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> ) | 0.39 , 48.0                                                 | 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: IPA, SO4, IMH

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     | 0.40         | 0/1893      | 0.94        | 7/2561 (0.3%)   |
| 1   | B     | 0.37         | 0/1893      | 0.90        | 5/2561 (0.2%)   |
| 1   | C     | 0.40         | 0/1893      | 0.92        | 5/2561 (0.2%)   |
| 1   | D     | 0.41         | 0/1893      | 0.95        | 7/2561 (0.3%)   |
| 1   | E     | 0.42         | 0/1893      | 0.94        | 8/2561 (0.3%)   |
| 1   | F     | 0.41         | 0/1893      | 0.94        | 4/2561 (0.2%)   |
| All | All   | 0.40         | 0/11358     | 0.93        | 36/15366 (0.2%) |

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 82  | GLY  | N-CA-C | 7.73  | 121.85      | 113.58   |
| 1   | F     | 183 | MET  | N-CA-C | 7.56  | 123.60      | 112.94   |
| 1   | A     | 178 | ALA  | N-CA-C | -7.30 | 99.48       | 110.28   |
| 1   | D     | 82  | GLY  | N-CA-C | 7.12  | 121.20      | 113.58   |
| 1   | C     | 68  | SER  | N-CA-C | 6.20  | 118.11      | 111.36   |

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     | 60      | 0            |
| 1   | B     | 1861  | 0        | 1882     | 54      | 0            |
| 1   | C     | 1861  | 0        | 1882     | 46      | 0            |
| 1   | D     | 1861  | 0        | 1882     | 47      | 0            |
| 1   | E     | 1861  | 0        | 1882     | 44      | 0            |
| 1   | F     | 1861  | 0        | 1882     | 41      | 0            |
| 2   | A     | 20    | 0        | 0        | 0       | 0            |
| 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    | 271     | 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 12.

The worst 5 of 271 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              |

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| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:46:GLU:HB3 | 1:B:46:GLU:HB3 | 1.63                     | 0.78              |

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%)   | 30          | 34  |
| 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%)   | 48          | 57  |

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%)   | 199 (97%)  | 7 (3%)   | 32          | 44 |
| 1   | B     | 206/235 (88%)   | 197 (96%)  | 9 (4%)   | 25          | 34 |
| 1   | C     | 206/235 (88%)   | 199 (97%)  | 7 (3%)   | 32          | 44 |
| 1   | D     | 206/235 (88%)   | 199 (97%)  | 7 (3%)   | 32          | 44 |
| 1   | E     | 206/235 (88%)   | 197 (96%)  | 9 (4%)   | 25          | 34 |
| 1   | F     | 206/235 (88%)   | 202 (98%)  | 4 (2%)   | 50          | 66 |
| All | All   | 1236/1410 (88%) | 1193 (96%) | 43 (4%)  | 32          | 43 |

5 of 43 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 163 | ASN  |
| 1   | E     | 132 | PHE  |
| 1   | D     | 182 | GLU  |
| 1   | E     | 57  | GLN  |
| 1   | E     | 163 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 151 | ASN  |
| 1   | F     | 163 | ASN  |
| 1   | E     | 163 | ASN  |
| 1   | F     | 64  | HIS  |
| 1   | F     | 220 | 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 oligosaccharides 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$ |
| 2   | SO4  | A     | 412 | -    | 4,4,4        | 1.50 | 1 (25%)     | 6,6,6       | 0.78 | 0           |
| 2   | SO4  | B     | 407 | -    | 4,4,4        | 1.81 | 1 (25%)     | 6,6,6       | 0.87 | 0           |
| 2   | SO4  | A     | 411 | -    | 4,4,4        | 1.48 | 1 (25%)     | 6,6,6       | 0.76 | 0           |
| 2   | SO4  | D     | 408 | -    | 4,4,4        | 1.34 | 0           | 6,6,6       | 0.88 | 0           |
| 3   | IMH  | F     | 306 | -    | 21,21,21     | 1.87 | 7 (33%)     | 22,31,31    | 1.84 | 5 (22%)     |
| 2   | SO4  | C     | 403 | -    | 4,4,4        | 1.44 | 1 (25%)     | 6,6,6       | 0.73 | 0           |
| 4   | IPA  | A     | 510 | -    | 3,3,3        | 0.40 | 0           | 3,3,3       | 0.38 | 0           |
| 4   | IPA  | F     | 505 | -    | 3,3,3        | 0.33 | 0           | 3,3,3       | 0.33 | 0           |
| 4   | IPA  | B     | 507 | -    | 3,3,3        | 0.43 | 0           | 3,3,3       | 0.39 | 0           |
| 2   | SO4  | F     | 406 | -    | 4,4,4        | 1.86 | 2 (50%)     | 6,6,6       | 0.81 | 0           |
| 2   | SO4  | F     | 409 | -    | 4,4,4        | 1.34 | 1 (25%)     | 6,6,6       | 0.83 | 0           |
| 2   | SO4  | E     | 405 | -    | 4,4,4        | 1.39 | 1 (25%)     | 6,6,6       | 0.85 | 0           |
| 2   | SO4  | B     | 402 | -    | 4,4,4        | 1.92 | 2 (50%)     | 6,6,6       | 0.84 | 0           |
| 2   | SO4  | F     | 415 | -    | 4,4,4        | 1.92 | 2 (50%)     | 6,6,6       | 0.86 | 0           |
| 4   | IPA  | A     | 509 | -    | 3,3,3        | 0.39 | 0           | 3,3,3       | 0.38 | 0           |
| 2   | SO4  | C     | 418 | -    | 4,4,4        | 1.46 | 1 (25%)     | 6,6,6       | 0.76 | 0           |
| 4   | IPA  | C     | 504 | -    | 3,3,3        | 0.36 | 0           | 3,3,3       | 0.39 | 0           |
| 4   | IPA  | D     | 514 | -    | 3,3,3        | 0.29 | 0           | 3,3,3       | 0.31 | 0           |
| 4   | IPA  | A     | 502 | -    | 3,3,3        | 0.41 | 0           | 3,3,3       | 0.36 | 0           |
| 4   | IPA  | E     | 506 | -    | 3,3,3        | 0.40 | 0           | 3,3,3       | 0.43 | 0           |
| 4   | IPA  | F     | 511 | -    | 3,3,3        | 0.45 | 0           | 3,3,3       | 0.35 | 0           |
| 2   | SO4  | D     | 404 | -    | 4,4,4        | 1.36 | 1 (25%)     | 6,6,6       | 0.86 | 0           |
| 3   | IMH  | C     | 303 | -    | 21,21,21     | 1.75 | 5 (23%)     | 22,31,31    | 1.79 | 5 (22%)     |
| 4   | IPA  | B     | 501 | -    | 3,3,3        | 0.44 | 0           | 3,3,3       | 0.44 | 0           |
| 4   | IPA  | B     | 515 | -    | 3,3,3        | 0.41 | 0           | 3,3,3       | 0.43 | 0           |
| 3   | IMH  | D     | 304 | -    | 21,21,21     | 1.79 | 5 (23%)     | 22,31,31    | 1.88 | 5 (22%)     |
| 3   | IMH  | E     | 305 | -    | 21,21,21     | 1.90 | 6 (28%)     | 22,31,31    | 1.89 | 5 (22%)     |
| 4   | IPA  | D     | 503 | -    | 3,3,3        | 0.36 | 0           | 3,3,3       | 0.35 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | SO4  | F     | 414 | -    | 4,4,4        | 1.82 | 2 (50%)  | 6,6,6       | 0.78 | 0        |
| 3   | IMH  | A     | 301 | -    | 21,21,21     | 1.93 | 7 (33%)  | 22,31,31    | 1.84 | 5 (22%)  |
| 2   | SO4  | A     | 413 | -    | 4,4,4        | 1.37 | 1 (25%)  | 6,6,6       | 0.80 | 0        |
| 4   | IPA  | F     | 512 | -    | 3,3,3        | 0.29 | 0        | 3,3,3       | 0.37 | 0        |
| 4   | IPA  | E     | 513 | -    | 3,3,3        | 0.20 | 0        | 3,3,3       | 0.26 | 0        |
| 2   | SO4  | A     | 401 | -    | 4,4,4        | 1.81 | 2 (50%)  | 6,6,6       | 0.84 | 0        |
| 4   | IPA  | B     | 508 | -    | 3,3,3        | 0.44 | 0        | 3,3,3       | 0.38 | 0        |
| 3   | IMH  | B     | 302 | -    | 21,21,21     | 1.87 | 6 (28%)  | 22,31,31    | 1.80 | 5 (22%)  |
| 2   | SO4  | E     | 419 | -    | 4,4,4        | 1.95 | 2 (50%)  | 6,6,6       | 0.85 | 0        |
| 2   | SO4  | D     | 417 | -    | 4,4,4        | 1.77 | 1 (25%)  | 6,6,6       | 0.78 | 0        |
| 2   | SO4  | B     | 410 | -    | 4,4,4        | 1.49 | 1 (25%)  | 6,6,6       | 0.76 | 0        |
| 2   | SO4  | E     | 416 | -    | 4,4,4        | 1.84 | 2 (50%)  | 6,6,6       | 0.74 | 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  | F     | 306 | -    | -       | 4/6/22/22 | 0/3/3/3 |
| 3   | IMH  | B     | 302 | -    | -       | 4/6/22/22 | 0/3/3/3 |
| 3   | IMH  | C     | 303 | -    | -       | 4/6/22/22 | 0/3/3/3 |
| 3   | IMH  | D     | 304 | -    | -       | 4/6/22/22 | 0/3/3/3 |
| 3   | IMH  | E     | 305 | -    | -       | 4/6/22/22 | 0/3/3/3 |
| 3   | IMH  | A     | 301 | -    | -       | 4/6/22/22 | 0/3/3/3 |

The worst 5 of 61 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | B     | 302 | IMH  | C2-N3   | 4.38  | 1.38        | 1.30     |
| 3   | A     | 301 | IMH  | C2-N3   | 4.03  | 1.37        | 1.30     |
| 3   | C     | 303 | IMH  | C2-N3   | 4.00  | 1.37        | 1.30     |
| 3   | D     | 304 | IMH  | C2-N3   | 3.79  | 1.37        | 1.30     |
| 3   | D     | 304 | IMH  | C3'-C4' | -3.79 | 1.49        | 1.53     |

The worst 5 of 30 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | D     | 304 | IMH  | C9-C8-N7 | 4.64 | 115.37      | 108.70   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | F     | 306 | IMH  | C9-C8-N7 | 4.54 | 115.23      | 108.70   |
| 3   | E     | 305 | IMH  | C9-C8-N7 | 4.53 | 115.21      | 108.70   |
| 3   | A     | 301 | IMH  | C9-C8-N7 | 4.49 | 115.16      | 108.70   |
| 3   | B     | 302 | IMH  | C9-C8-N7 | 4.47 | 115.13      | 108.70   |

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 3   | A     | 301 | IMH  | C2'-C1'-C9-C8 |
| 3   | A     | 301 | IMH  | C2'-C1'-C9-C4 |
| 3   | B     | 302 | IMH  | C2'-C1'-C9-C8 |
| 3   | B     | 302 | IMH  | C2'-C1'-C9-C4 |
| 3   | C     | 303 | IMH  | C2'-C1'-C9-C8 |

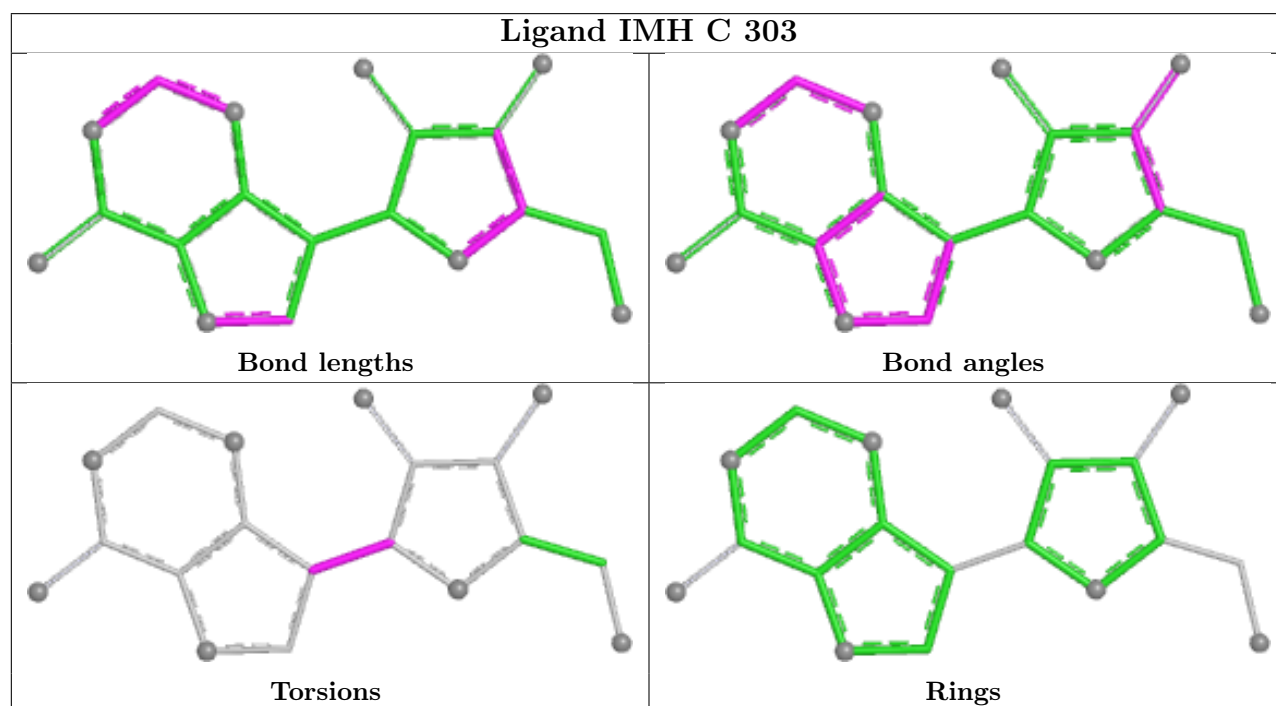
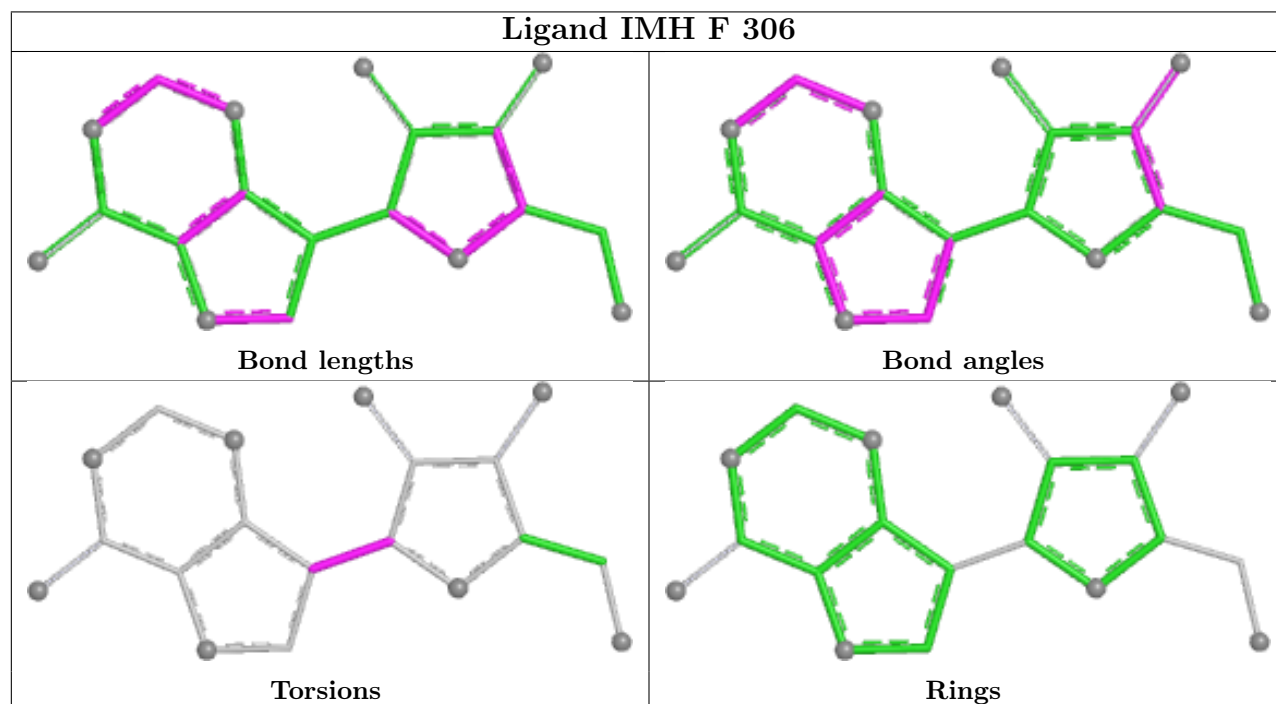
There are no ring outliers.

14 monomers are involved in 15 short contacts:

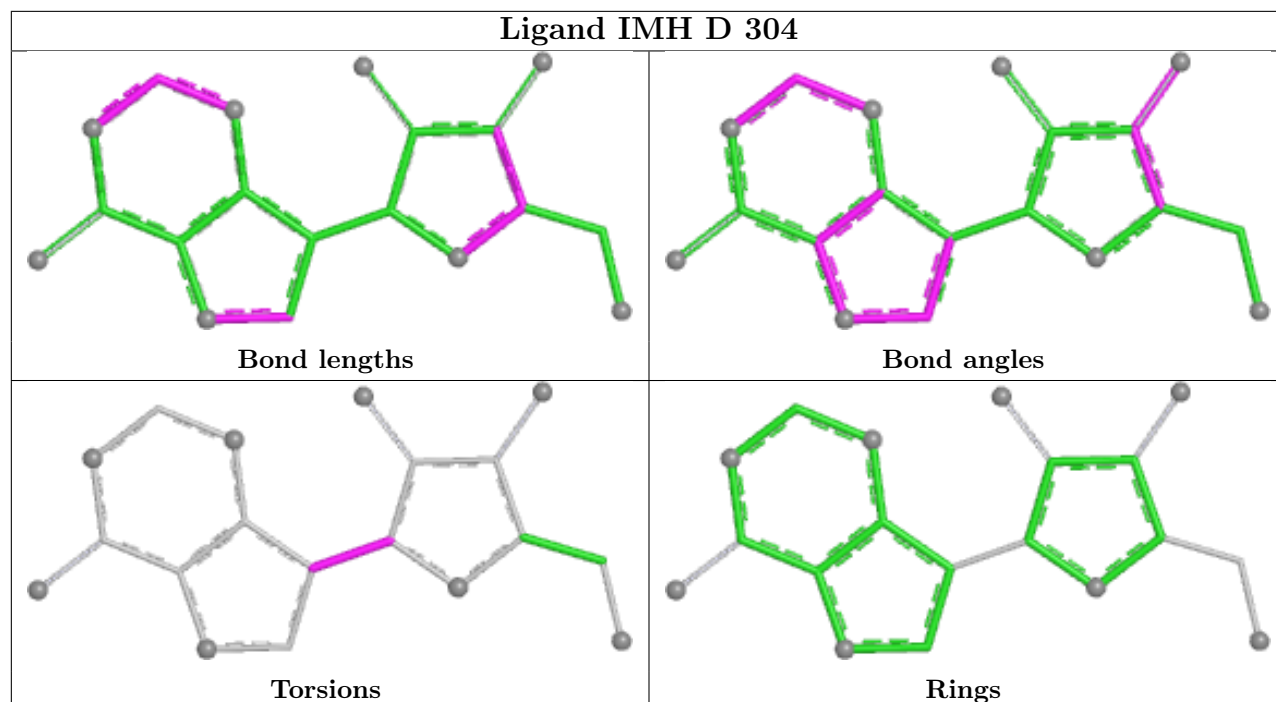
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | F     | 306 | IMH  | 1       | 0            |
| 2   | F     | 415 | SO4  | 1       | 0            |
| 4   | A     | 509 | IPA  | 1       | 0            |
| 4   | E     | 506 | IPA  | 1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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

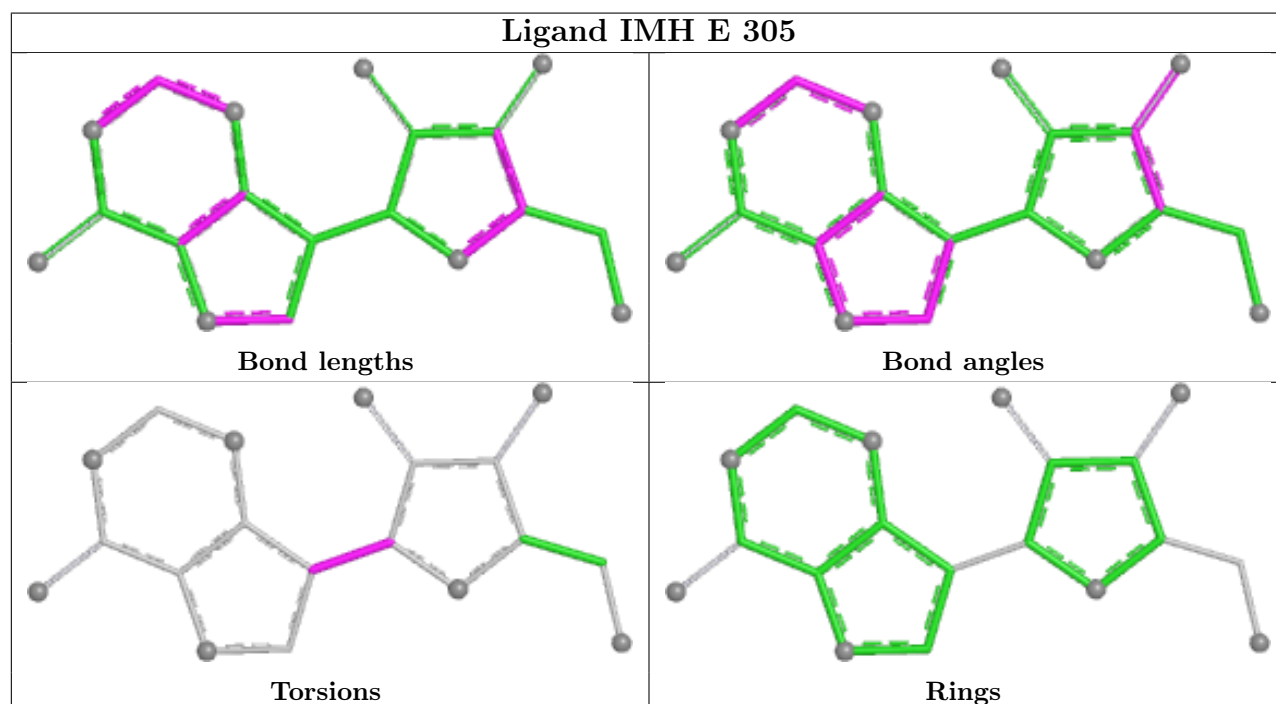
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

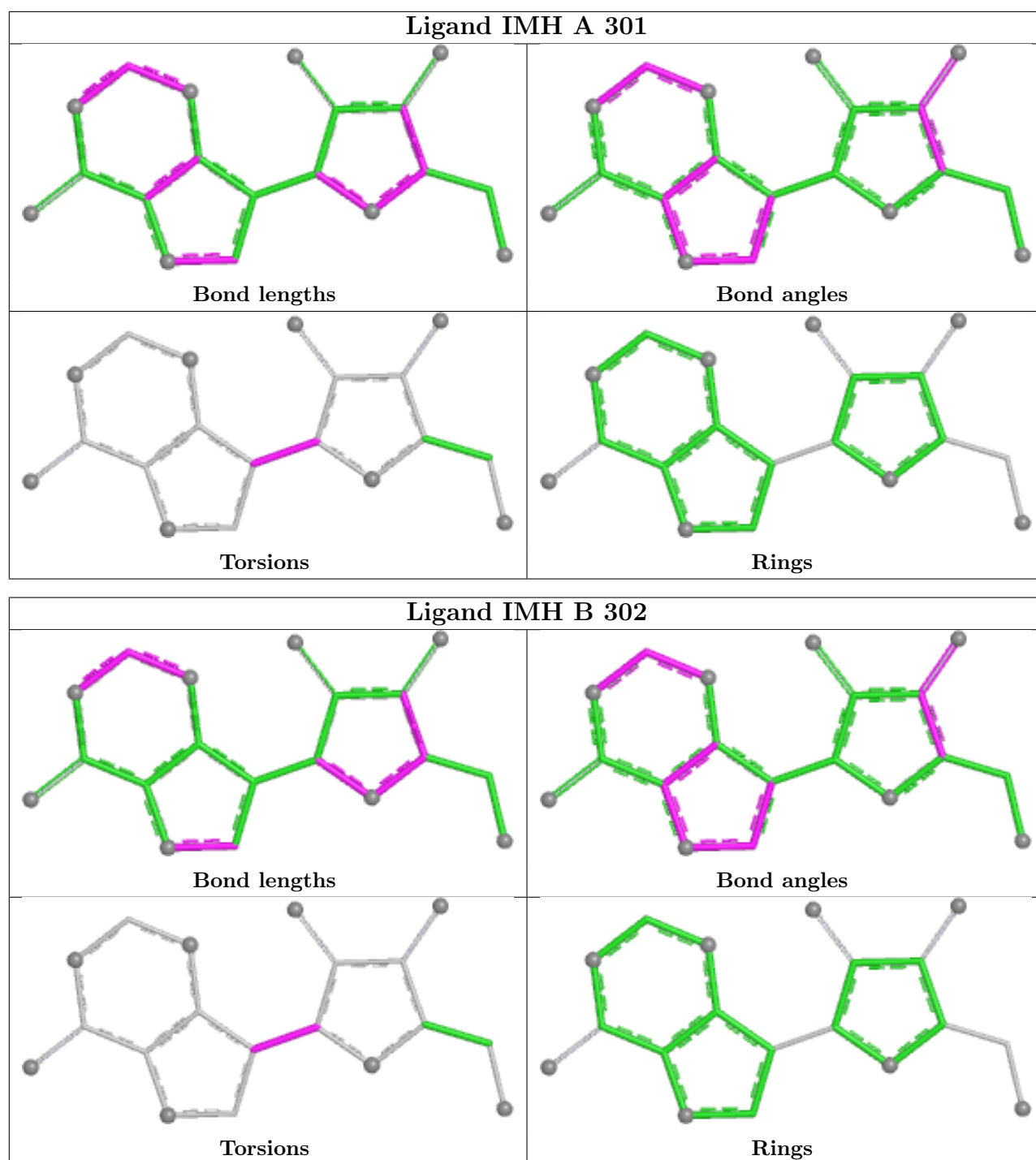


## Ligand IMH D 304



## Ligand IMH E 305





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)   | -0.03  | 3 (1%) 76 74  | 15, 32, 47, 60        | 0     |
| 1   | B     | 243/276 (88%)   | 0.19   | 7 (2%) 53 50  | 19, 37, 54, 59        | 0     |
| 1   | C     | 243/276 (88%)   | 0.20   | 5 (2%) 63 60  | 17, 33, 50, 61        | 0     |
| 1   | D     | 243/276 (88%)   | -0.22  | 3 (1%) 76 74  | 16, 29, 43, 56        | 0     |
| 1   | E     | 243/276 (88%)   | -0.33  | 2 (0%) 82 80  | 12, 26, 42, 53        | 0     |
| 1   | F     | 243/276 (88%)   | -0.26  | 2 (0%) 82 80  | 16, 27, 43, 54        | 0     |
| All | All   | 1458/1656 (88%) | -0.07  | 22 (1%) 72 69 | 12, 30, 49, 61        | 0     |

The worst 5 of 22 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 132 | PHE  | 5.6  |
| 1   | E     | 132 | PHE  | 4.3  |
| 1   | B     | 132 | PHE  | 3.9  |
| 1   | B     | 245 | ALA  | 3.7  |
| 1   | F     | 245 | ALA  | 3.2  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

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

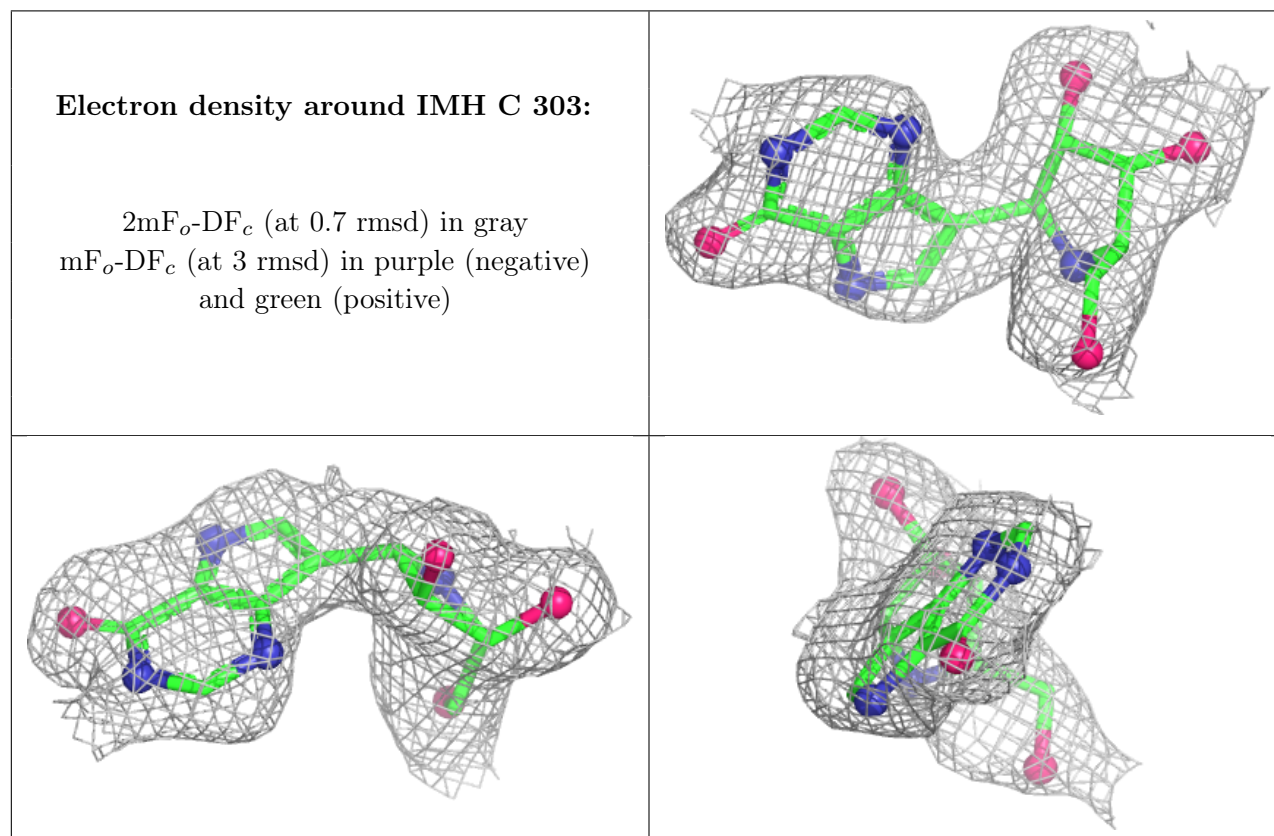
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | IPA  | F     | 505 | 4/4   | 0.49 | 0.20 | 31,34,34,34                | 0     |
| 4   | IPA  | F     | 511 | 4/4   | 0.60 | 0.20 | 19,21,23,28                | 0     |
| 4   | IPA  | D     | 514 | 4/4   | 0.67 | 0.15 | 16,19,19,20                | 0     |
| 4   | IPA  | B     | 501 | 4/4   | 0.68 | 0.19 | 26,31,32,33                | 0     |
| 4   | IPA  | A     | 510 | 4/4   | 0.70 | 0.19 | 33,33,35,36                | 0     |
| 4   | IPA  | A     | 502 | 4/4   | 0.70 | 0.19 | 32,33,33,35                | 0     |
| 4   | IPA  | B     | 515 | 4/4   | 0.70 | 0.14 | 22,23,24,25                | 0     |
| 4   | IPA  | E     | 513 | 4/4   | 0.73 | 0.15 | 12,16,17,20                | 0     |
| 4   | IPA  | F     | 512 | 4/4   | 0.74 | 0.15 | 22,23,24,25                | 0     |
| 4   | IPA  | C     | 504 | 4/4   | 0.76 | 0.14 | 21,22,23,25                | 0     |
| 4   | IPA  | E     | 506 | 4/4   | 0.76 | 0.18 | 16,18,18,20                | 0     |
| 4   | IPA  | D     | 503 | 4/4   | 0.77 | 0.18 | 24,26,28,29                | 0     |
| 4   | IPA  | B     | 508 | 4/4   | 0.79 | 0.14 | 27,29,31,32                | 0     |
| 4   | IPA  | A     | 509 | 4/4   | 0.80 | 0.17 | 26,26,26,30                | 0     |
| 4   | IPA  | B     | 507 | 4/4   | 0.81 | 0.18 | 24,26,28,29                | 0     |
| 2   | SO4  | F     | 415 | 5/5   | 0.88 | 0.19 | 64,65,66,67                | 0     |
| 2   | SO4  | B     | 410 | 5/5   | 0.89 | 0.11 | 62,62,63,63                | 0     |
| 3   | IMH  | C     | 303 | 19/19 | 0.91 | 0.09 | 29,35,37,38                | 0     |
| 2   | SO4  | A     | 411 | 5/5   | 0.91 | 0.15 | 64,65,65,67                | 0     |
| 3   | IMH  | E     | 305 | 19/19 | 0.92 | 0.07 | 25,27,29,31                | 0     |
| 3   | IMH  | D     | 304 | 19/19 | 0.93 | 0.07 | 17,21,28,28                | 0     |
| 3   | IMH  | A     | 301 | 19/19 | 0.94 | 0.07 | 27,28,31,31                | 0     |
| 2   | SO4  | E     | 419 | 5/5   | 0.95 | 0.07 | 54,54,56,57                | 0     |
| 3   | IMH  | B     | 302 | 19/19 | 0.95 | 0.07 | 31,35,38,39                | 0     |
| 3   | IMH  | F     | 306 | 19/19 | 0.96 | 0.06 | 20,23,27,30                | 0     |
| 2   | SO4  | A     | 412 | 5/5   | 0.96 | 0.09 | 49,50,51,51                | 0     |
| 2   | SO4  | D     | 404 | 5/5   | 0.97 | 0.07 | 37,38,40,41                | 0     |
| 2   | SO4  | D     | 417 | 5/5   | 0.97 | 0.06 | 30,30,31,33                | 0     |
| 2   | SO4  | B     | 407 | 5/5   | 0.97 | 0.07 | 28,28,31,32                | 0     |
| 2   | SO4  | B     | 402 | 5/5   | 0.97 | 0.06 | 42,42,43,44                | 0     |
| 2   | SO4  | C     | 403 | 5/5   | 0.97 | 0.06 | 31,32,33,35                | 0     |
| 2   | SO4  | F     | 406 | 5/5   | 0.98 | 0.04 | 28,29,30,31                | 0     |
| 2   | SO4  | F     | 414 | 5/5   | 0.98 | 0.06 | 33,33,36,36                | 0     |
| 2   | SO4  | A     | 401 | 5/5   | 0.98 | 0.07 | 37,39,39,41                | 0     |
| 2   | SO4  | A     | 413 | 5/5   | 0.98 | 0.06 | 24,25,27,28                | 0     |
| 2   | SO4  | E     | 416 | 5/5   | 0.98 | 0.08 | 29,29,30,31                | 0     |
| 2   | SO4  | C     | 418 | 5/5   | 0.98 | 0.06 | 30,30,32,33                | 0     |

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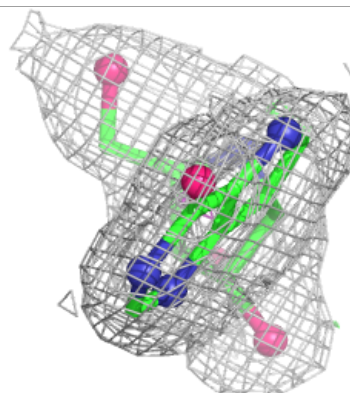
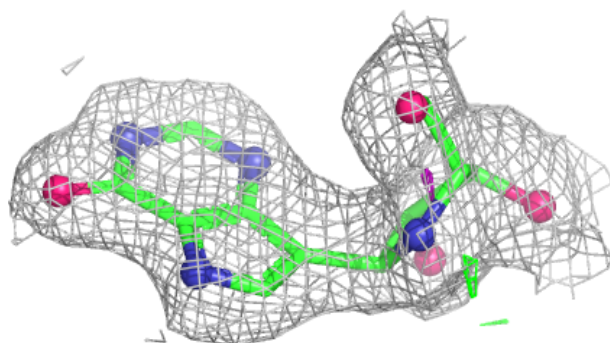
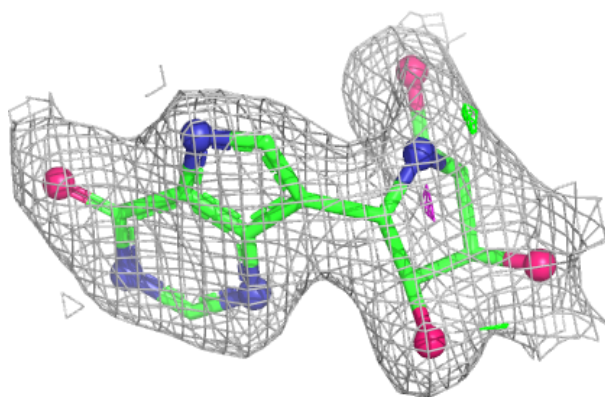
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | SO4  | F     | 409 | 5/5   | 0.99 | 0.07 | 24,25,26,26                 | 0     |
| 2   | SO4  | E     | 405 | 5/5   | 0.99 | 0.04 | 27,29,31,31                 | 0     |
| 2   | SO4  | D     | 408 | 5/5   | 0.99 | 0.08 | 27,29,30,30                 | 0     |

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

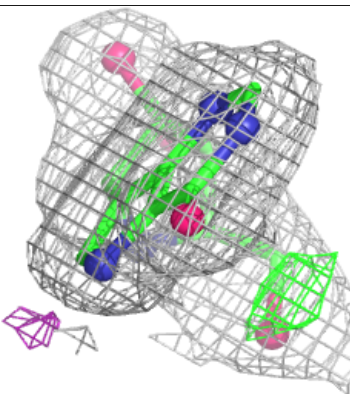
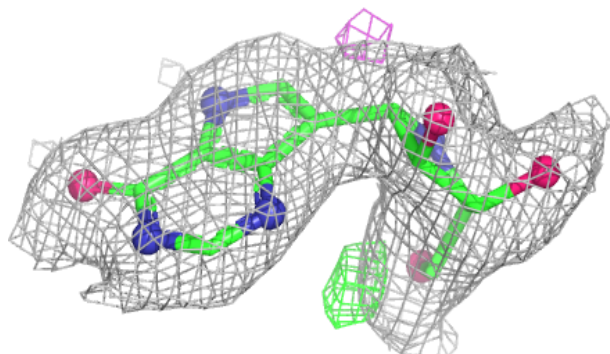
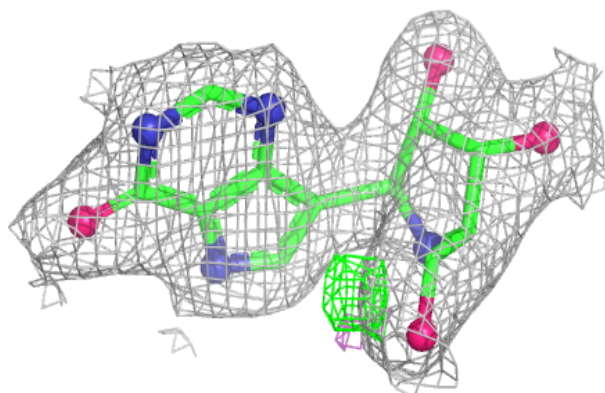


**Electron density around IMH E 305:**

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

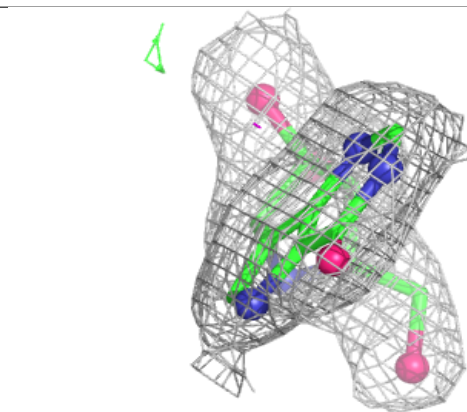
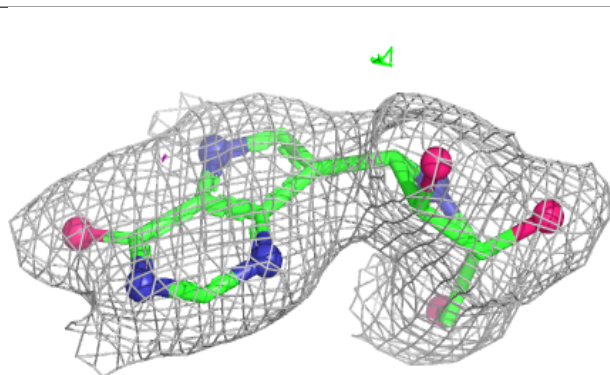
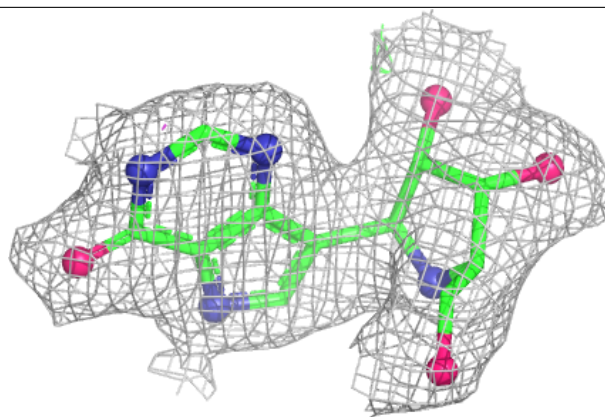
**Electron density around IMH D 304:**

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

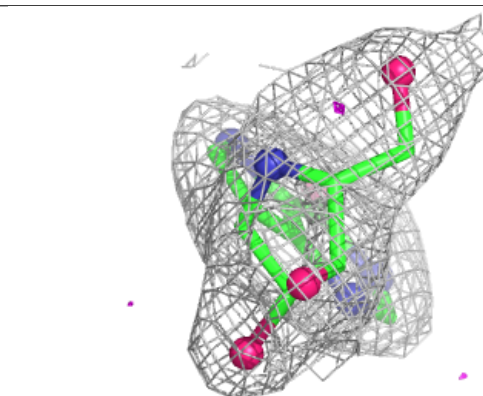
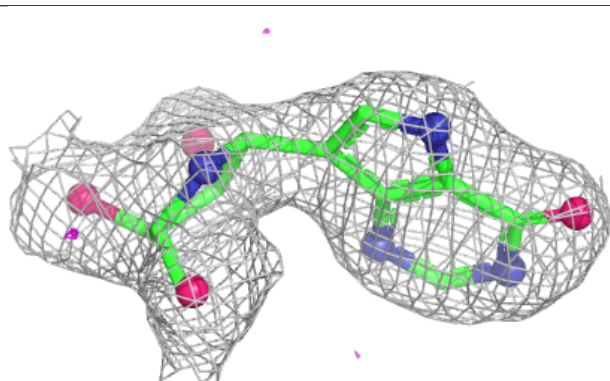
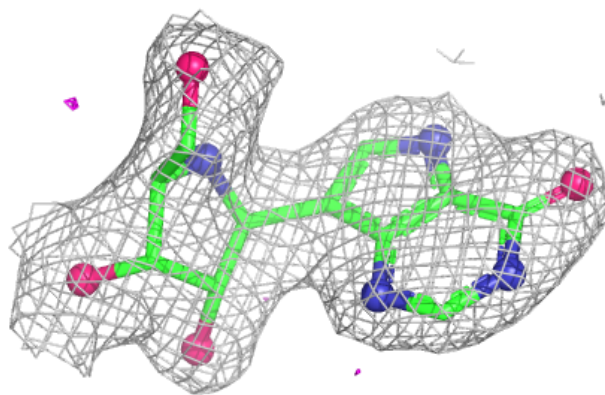


**Electron density around IMH A 301:**

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

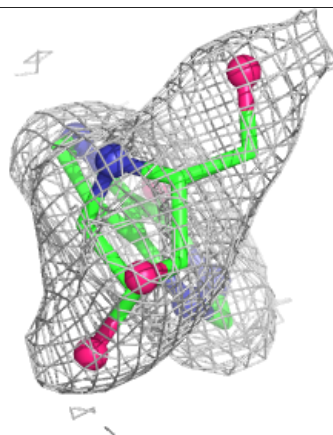
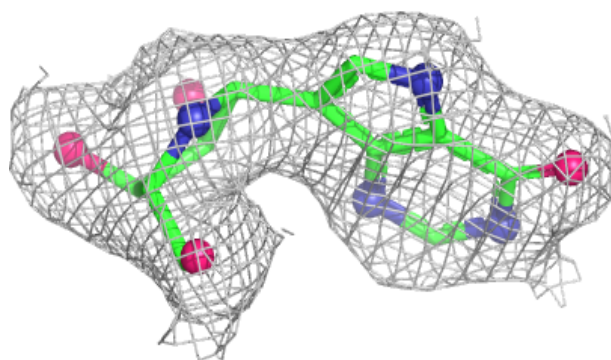
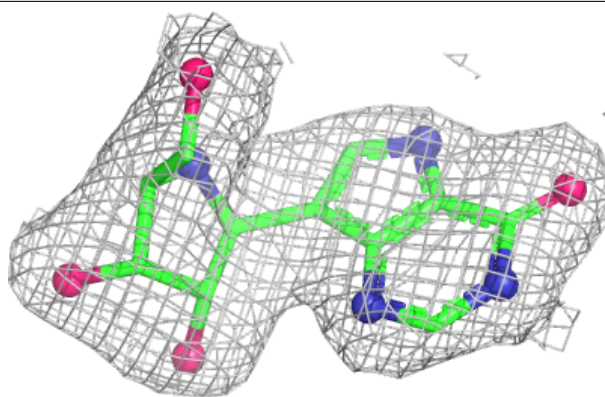
**Electron density around IMH B 302:**

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



**Electron density around IMH F 306:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.