



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 27, 2022 – 02:14 PM EDT

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.; 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

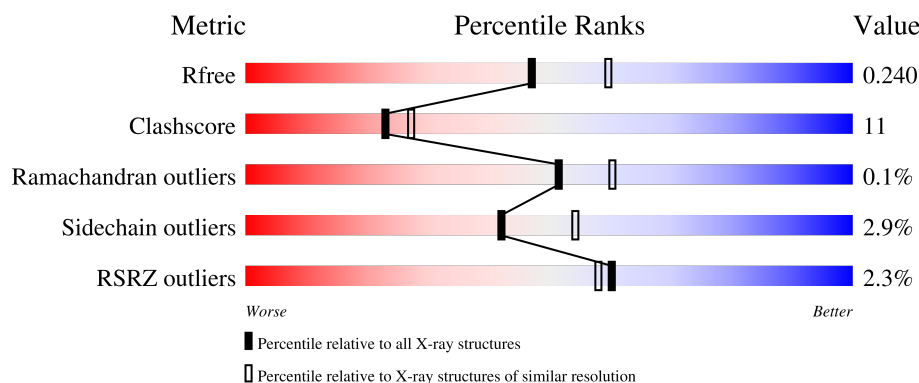
# 1 Overall quality at a glance

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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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	
1	B	276	
1	C	276	
1	D	276	

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Mol	Chain	Length	Quality of chain
1	E	276	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>66%</div><div>20%</div><div>•</div><div>12%</div></div></div>
1	F	276	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>69%</div><div>18%</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

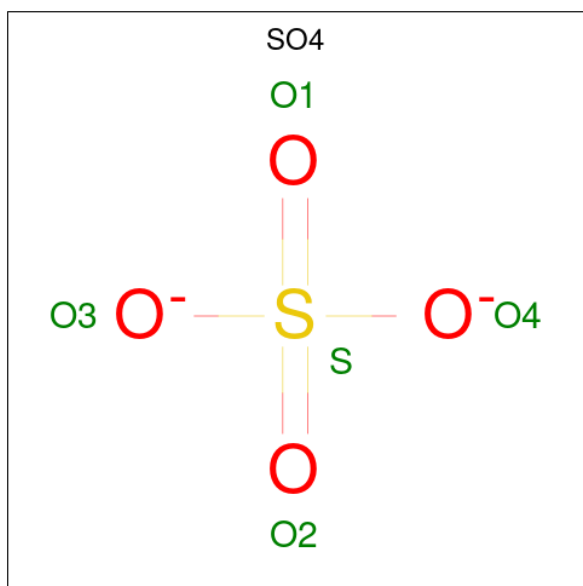
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Chain	Residue	Modelled	Actual	Comment	Reference
F	274	HIS	-	expression tag	UNP Q8I3X4

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



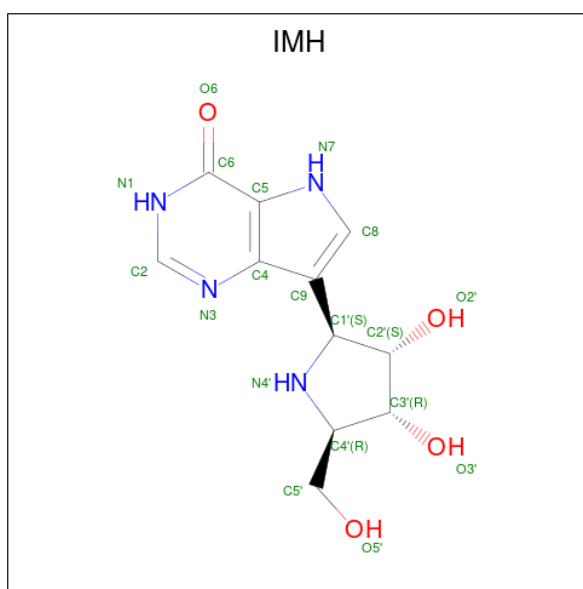
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

- 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>).



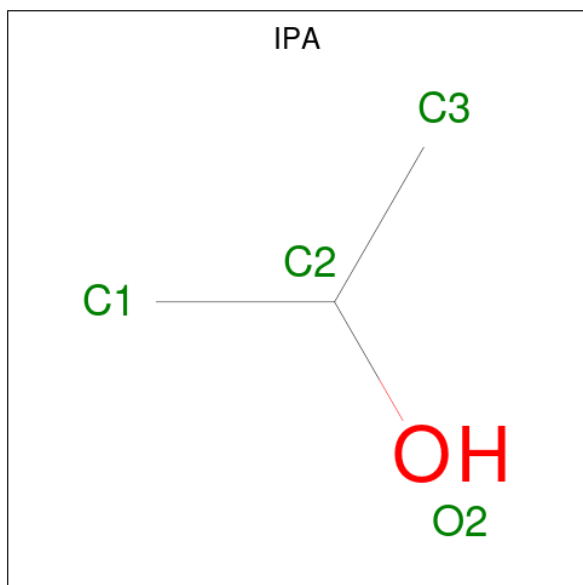
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 19 11 4 4	0	0
3	B	1	Total C N O 19 11 4 4	0	0
3	C	1	Total C N O 19 11 4 4	0	0

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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 (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



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 4 3 1	0	0
4	D	1	Total C O 4 3 1	0	0
4	E	1	Total C O 4 3 1	0	0
4	E	1	Total C O 4 3 1	0	0
4	F	1	Total C O 4 3 1	0	0
4	F	1	Total C O 4 3 1	0	0
4	F	1	Total C O 4 3 1	0	0

- Molecule 5 is water.

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



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

- Molecule 1: uridine phosphorylase, putative

Chain D: 

MET ALA ASP N3 L4 L5 E13 Q14 I15 T16 P17 V21 V22 R27 V28 D29 I31 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 S157 D158 N163 K164 Y173 A176 N177 E182 G200 I204 K211 K212 D213 D216 L221 L226 L230 A241 T242 K243 Y244 A245 LYS GLY GLU 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

- Molecule 1: uridine phosphorylase, putative

Chain E: 

MET ALA ASP N3 L4 L5 I10 D133 E13 Q14 I15 L20 V21 V22 G23 D24 P25 G26 V28 I31 V34 R45 E46 Y54 Q57 C61 V62 S63 H64 G65 S68 C71 F76 E77 V85 K101 R102 N109 V112 E114

V117 S118 L120 L121 I122 F132 V134 D136 K140 V155 S156 D158 M159 P162 R163 Y173 A176 N177 E182 L188 G200 D213 E214 G215 D216 L221 L226 L234 L240 A245 LYS GLY PHE GLU TYR VAL GLU GLN LYS

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

- Molecule 1: uridine phosphorylase, putative

Chain F: 

MET ALA ASP N3 L4 L5 I10 S11 K12 I15 L20 V21 V22 R27 K32 V33 V38 V39 D40 E46 V50 E51 K58 F59 L60 C61 V62 S63 H64 G65 E77 N81 R88 G93 I100 K101 R102 A110 V112 R113 R116

V117 S118 H119 L121 L122 F132 K140 E144 N145 N146 D158 N163 K164 I165 Y173 A176 N177 V180 V181 E182 I202 V205 D216 P222 P223 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

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.55Å 92.28Å 239.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	78.5 (20.00-2.20) 80.7 (19.97-2.20)	Depositor 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 0.201 , 0.240	Depositor 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> )	0.38 , 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, IPA, 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	0.33	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

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.

The worst 5 of 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

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	241/276 (87%)	228 (95%)	13 (5%)	0	100	100
1	B	241/276 (87%)	229 (95%)	11 (5%)	1 (0%)	34	37
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%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	223	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/235 (88%)	201 (98%)	5 (2%)	49	62
1	B	206/235 (88%)	199 (97%)	7 (3%)	37	47
1	C	206/235 (88%)	199 (97%)	7 (3%)	37	47
1	D	206/235 (88%)	201 (98%)	5 (2%)	49	62
1	E	206/235 (88%)	198 (96%)	8 (4%)	32	41
1	F	206/235 (88%)	202 (98%)	4 (2%)	57	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1236/1410 (88%)	1200 (97%)	36 (3%)	42 54

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	132	PHE
1	F	182	GLU
1	E	133	ASP
1	F	101	LYS
1	C	101	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	44	ASN
1	F	53	HIS
1	F	151	ASN
1	C	163	ASN
1	C	119	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	B	302	-	18,21,21	2.17	6 (33%)	13,31,31	1.40	2 (15%)
3	IMH	C	303	-	18,21,21	2.05	6 (33%)	13,31,31	1.37	2 (15%)
4	IPA	A	502	-	3,3,3	0.40	0	3,3,3	0.36	0
4	IPA	B	515	-	3,3,3	0.39	0	3,3,3	0.42	0
4	IPA	E	506	-	3,3,3	0.38	0	3,3,3	0.42	0
4	IPA	B	508	-	3,3,3	0.42	0	3,3,3	0.37	0
2	SO4	D	404	-	4,4,4	1.37	1 (25%)	6,6,6	0.85	0
2	SO4	E	419	-	4,4,4	2.10	2 (50%)	6,6,6	0.84	0
2	SO4	A	401	-	4,4,4	1.83	2 (50%)	6,6,6	0.91	0
4	IPA	A	509	-	3,3,3	0.38	0	3,3,3	0.37	0
2	SO4	F	406	-	4,4,4	1.88	2 (50%)	6,6,6	0.88	0
2	SO4	D	408	-	4,4,4	1.34	0	6,6,6	0.88	0
2	SO4	A	412	-	4,4,4	1.67	1 (25%)	6,6,6	0.90	0
2	SO4	F	414	-	4,4,4	1.85	1 (25%)	6,6,6	0.81	0
2	SO4	B	402	-	4,4,4	2.08	2 (50%)	6,6,6	0.83	0
3	IMH	A	301	-	18,21,21	2.23	6 (33%)	13,31,31	1.41	2 (15%)
4	IPA	C	504	-	3,3,3	0.35	0	3,3,3	0.38	0
2	SO4	C	403	-	4,4,4	1.62	1 (25%)	6,6,6	0.74	0
2	SO4	B	410	-	4,4,4	1.66	1 (25%)	6,6,6	0.86	0
4	IPA	D	514	-	3,3,3	0.28	0	3,3,3	0.31	0
3	IMH	F	306	-	18,21,21	2.21	6 (33%)	13,31,31	1.42	2 (15%)
3	IMH	E	305	-	18,21,21	2.10	6 (33%)	13,31,31	1.45	2 (15%)
4	IPA	F	511	-	3,3,3	0.44	0	3,3,3	0.34	0
2	SO4	A	411	-	4,4,4	1.65	1 (25%)	6,6,6	0.87	0
4	IPA	F	505	-	3,3,3	0.32	0	3,3,3	0.32	0
4	IPA	B	501	-	3,3,3	0.43	0	3,3,3	0.42	0
2	SO4	F	409	-	4,4,4	1.33	1 (25%)	6,6,6	0.82	0
2	SO4	E	416	-	4,4,4	1.87	2 (50%)	6,6,6	0.77	0
3	IMH	D	304	-	18,21,21	2.09	6 (33%)	13,31,31	1.47	2 (15%)
2	SO4	C	418	-	4,4,4	1.63	1 (25%)	6,6,6	0.86	0
2	SO4	D	417	-	4,4,4	1.79	1 (25%)	6,6,6	0.81	0
2	SO4	E	405	-	4,4,4	1.39	1 (25%)	6,6,6	0.85	0
4	IPA	A	510	-	3,3,3	0.39	0	3,3,3	0.37	0
4	IPA	F	512	-	3,3,3	0.28	0	3,3,3	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	IPA	D	503	-	3,3,3	0.35	0	3,3,3	0.34	0
2	SO4	F	415	-	4,4,4	2.08	2 (50%)	6,6,6	0.85	0
2	SO4	B	407	-	4,4,4	1.83	1 (25%)	6,6,6	0.94	0
4	IPA	B	507	-	3,3,3	0.42	0	3,3,3	0.39	0
2	SO4	A	413	-	4,4,4	1.36	1 (25%)	6,6,6	0.80	0
4	IPA	E	513	-	3,3,3	0.21	0	3,3,3	0.25	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	B	302	-	-	0/2/22/22	0/3/3/3
3	IMH	D	304	-	-	0/2/22/22	0/3/3/3
3	IMH	C	303	-	-	0/2/22/22	0/3/3/3
3	IMH	F	306	-	-	0/2/22/22	0/3/3/3
3	IMH	E	305	-	-	0/2/22/22	0/3/3/3
3	IMH	A	301	-	-	0/2/22/22	0/3/3/3

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	IMH	C2-N3	4.63	1.38	1.29
3	A	301	IMH	C1'-N4'	-4.36	1.42	1.47
3	A	301	IMH	C2-N3	4.30	1.37	1.29
3	C	303	IMH	C2-N3	4.27	1.37	1.29
3	D	304	IMH	C2-N3	4.07	1.37	1.29

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	304	IMH	C9-C8-N7	3.44	115.37	108.79
3	F	306	IMH	C9-C8-N7	3.37	115.23	108.79
3	E	305	IMH	C9-C8-N7	3.36	115.21	108.79
3	A	301	IMH	C9-C8-N7	3.34	115.16	108.79
3	B	302	IMH	C9-C8-N7	3.32	115.13	108.79

There are no chirality outliers.

There are no torsion outliers.

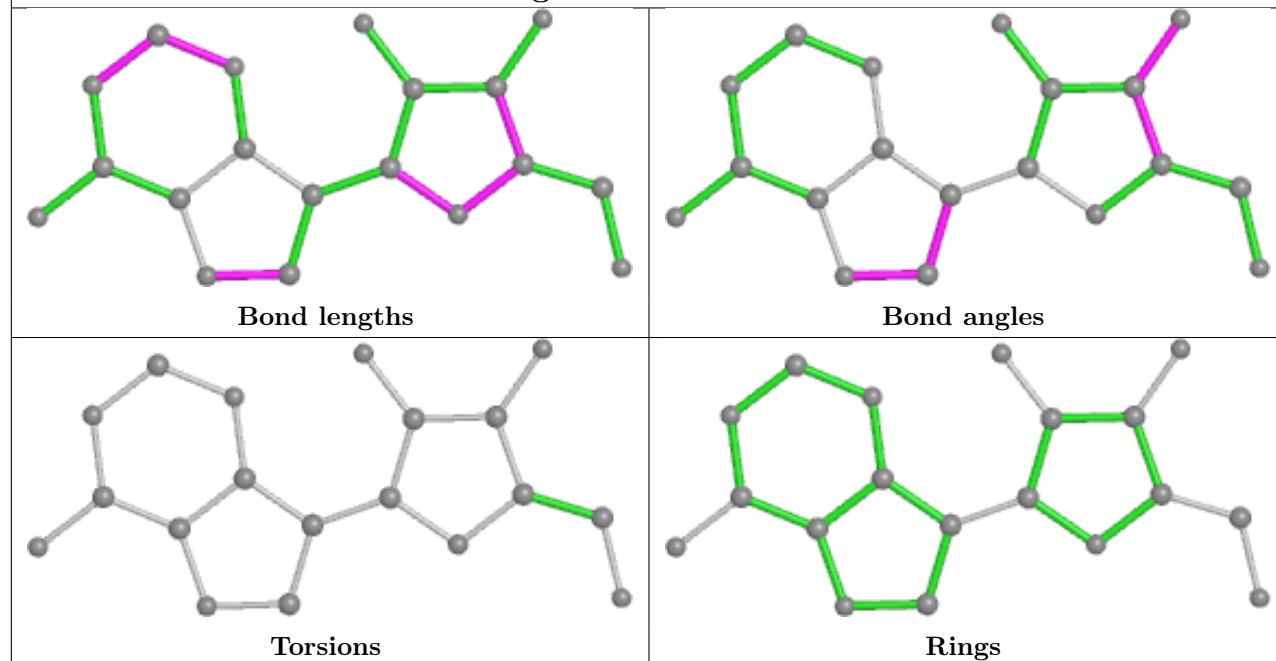
There are no ring outliers.

14 monomers are involved in 15 short contacts:

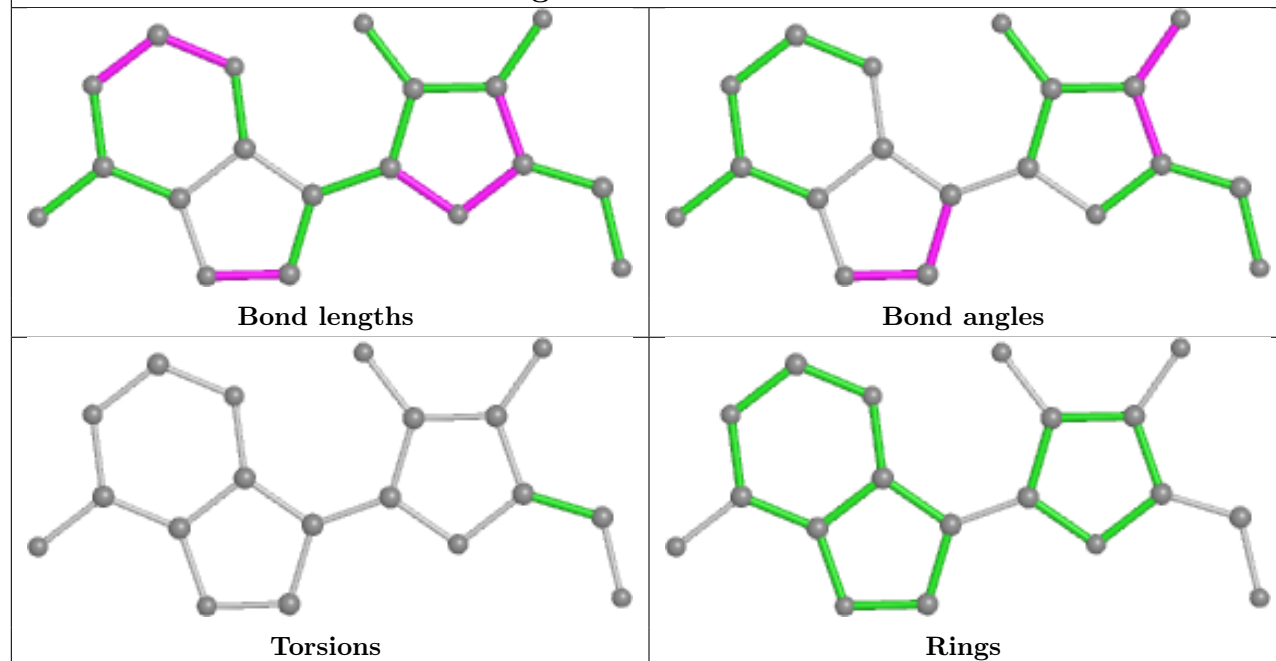
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	IMH	1	0
3	C	303	IMH	1	0
4	E	506	IPA	1	0
4	B	508	IPA	1	0
4	A	509	IPA	1	0
3	A	301	IMH	1	0
2	B	410	SO4	1	0
3	F	306	IMH	1	0
3	E	305	IMH	1	0
4	F	511	IPA	1	0
4	B	501	IPA	1	0
3	D	304	IMH	2	0
2	D	417	SO4	1	0
2	F	415	SO4	1	0

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.

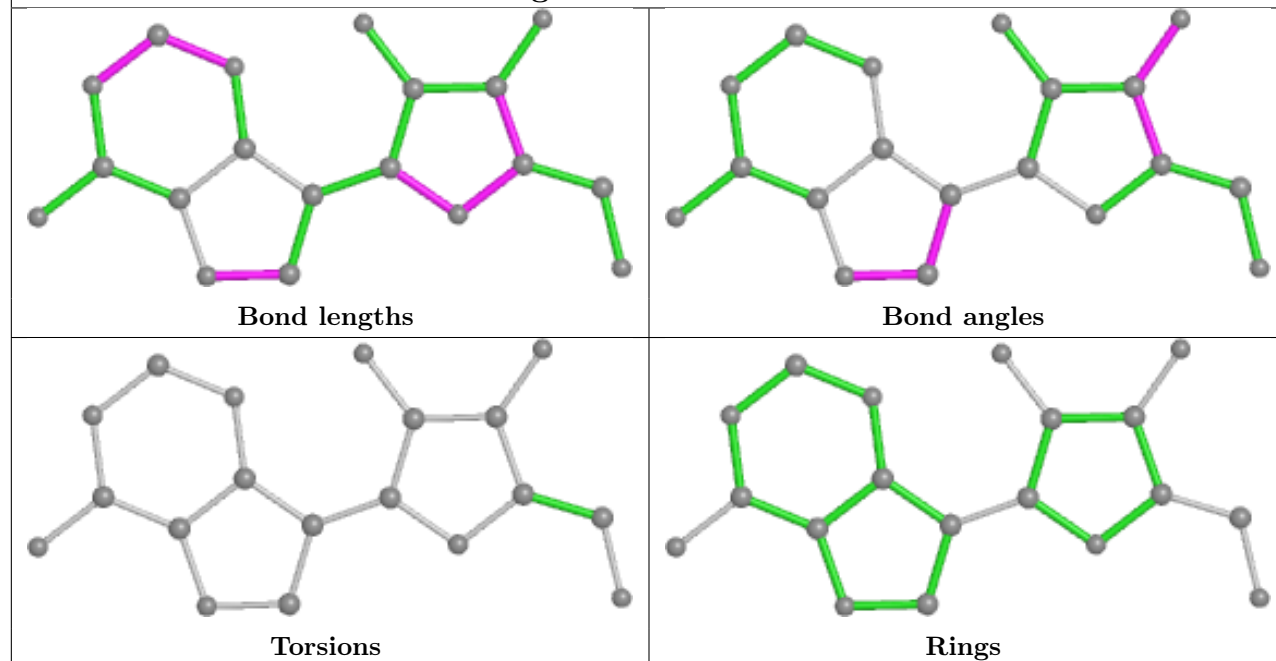
## Ligand IMH B 302



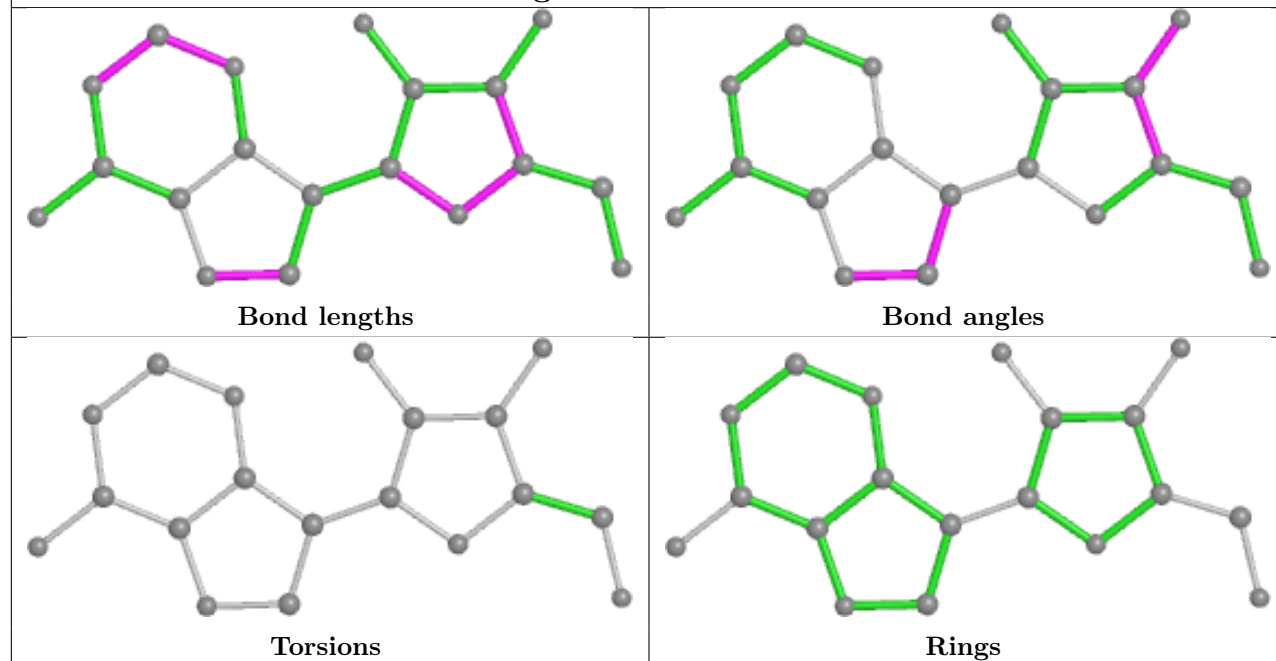
## Ligand IMH C 303



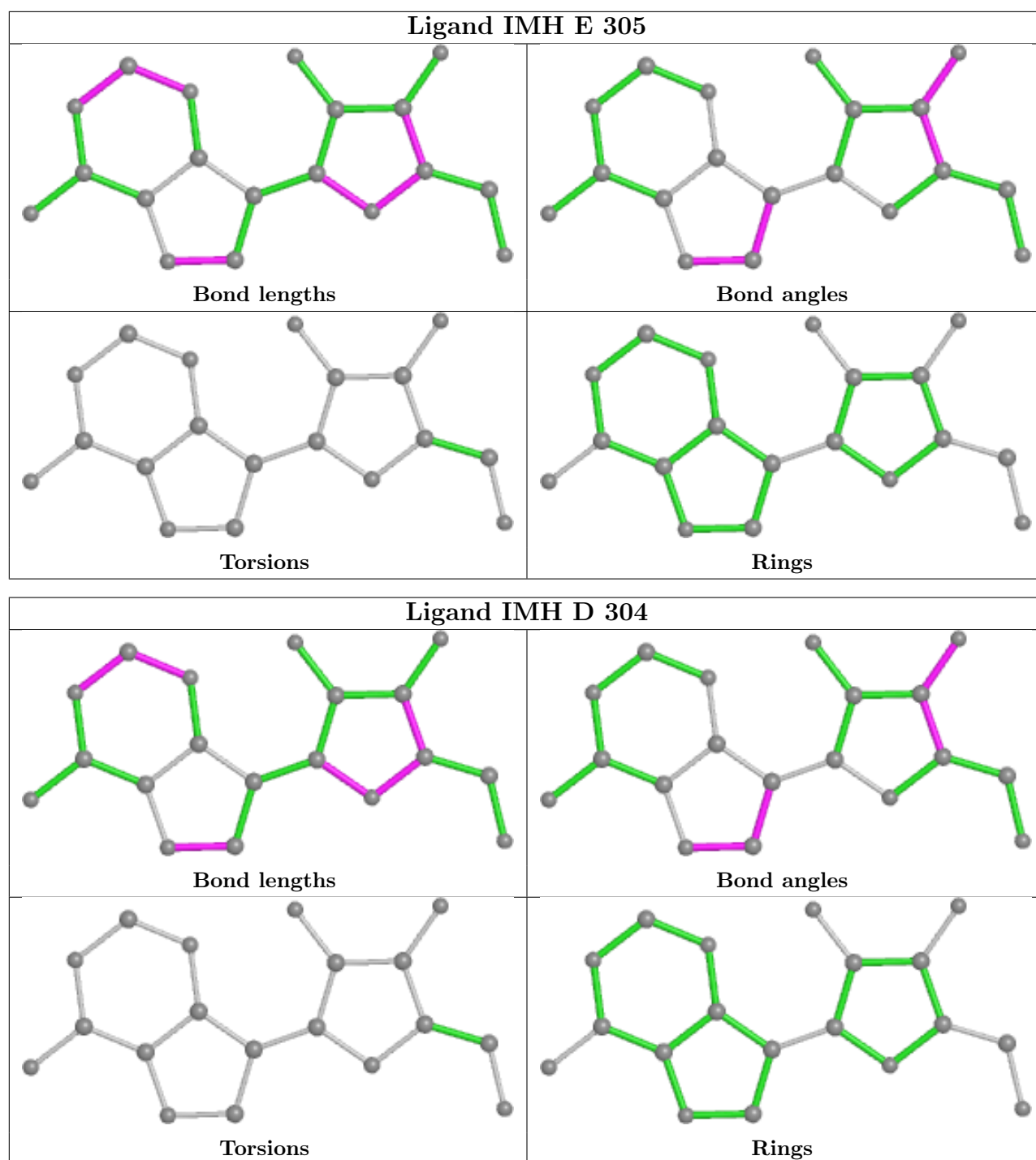
## Ligand IMH A 301



## Ligand IMH F 306







## 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%)	-0.22	5 (2%) 63 61	15, 32, 47, 60	0
1	B	243/276 (88%)	-0.10	8 (3%) 46 44	19, 37, 54, 59	0
1	C	243/276 (88%)	-0.09	7 (2%) 51 49	17, 33, 50, 61	0
1	D	243/276 (88%)	-0.36	5 (2%) 63 61	16, 29, 43, 56	0
1	E	243/276 (88%)	-0.39	5 (2%) 63 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%) 60 58	12, 30, 49, 61	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ASN	4.6
1	C	143	GLN	4.4
1	E	245	ALA	4.1
1	D	3	ASN	3.6
1	C	3	ASN	3.4

### 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 monosaccharides 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	0.80	0.23	31,34,34,34	0
4	IPA	B	501	4/4	0.81	0.21	26,31,32,33	0
4	IPA	F	512	4/4	0.81	0.14	22,23,24,25	0
4	IPA	C	504	4/4	0.83	0.14	21,22,23,25	0
4	IPA	F	511	4/4	0.83	0.16	19,21,23,28	0
4	IPA	D	514	4/4	0.83	0.16	16,19,19,20	0
4	IPA	A	510	4/4	0.84	0.18	33,33,35,36	0
4	IPA	E	513	4/4	0.86	0.18	12,16,17,20	0
4	IPA	A	509	4/4	0.87	0.14	26,26,26,30	0
4	IPA	B	508	4/4	0.88	0.17	27,29,31,32	0
4	IPA	B	507	4/4	0.89	0.12	24,26,28,29	0
4	IPA	A	502	4/4	0.89	0.16	32,33,33,35	0
4	IPA	B	515	4/4	0.91	0.12	22,23,24,25	0
4	IPA	E	506	4/4	0.91	0.20	16,18,18,20	0
4	IPA	D	503	4/4	0.92	0.19	24,26,28,29	0
2	SO4	A	411	5/5	0.94	0.29	64,65,65,67	0
2	SO4	B	410	5/5	0.94	0.16	62,62,63,63	0
2	SO4	F	415	5/5	0.94	0.27	64,65,66,67	0
3	IMH	C	303	19/19	0.94	0.11	29,35,37,38	0
3	IMH	E	305	19/19	0.94	0.10	25,27,29,31	0
3	IMH	D	304	19/19	0.95	0.12	17,21,28,28	0
3	IMH	A	301	19/19	0.96	0.11	27,28,31,31	0
3	IMH	B	302	19/19	0.96	0.10	31,35,38,39	0
3	IMH	F	306	19/19	0.97	0.08	20,23,27,30	0
2	SO4	D	404	5/5	0.98	0.09	37,38,40,41	0
2	SO4	E	419	5/5	0.98	0.11	54,54,56,57	0
2	SO4	A	412	5/5	0.98	0.07	49,50,51,51	0
2	SO4	B	402	5/5	0.99	0.07	42,42,43,44	0
2	SO4	F	406	5/5	0.99	0.06	28,29,30,31	0
2	SO4	F	409	5/5	0.99	0.11	24,25,26,26	0
2	SO4	F	414	5/5	0.99	0.08	33,33,36,36	0
2	SO4	B	407	5/5	0.99	0.08	28,28,31,32	0
2	SO4	A	401	5/5	0.99	0.09	37,39,39,41	0
2	SO4	C	403	5/5	0.99	0.08	31,32,33,35	0
2	SO4	C	418	5/5	0.99	0.08	30,30,32,33	0
2	SO4	A	413	5/5	0.99	0.08	24,25,27,28	0
2	SO4	D	408	5/5	0.99	0.11	27,29,30,30	0

*Continued on next page...*

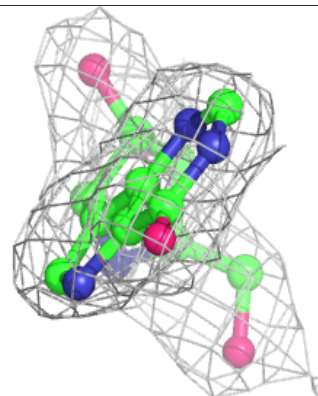
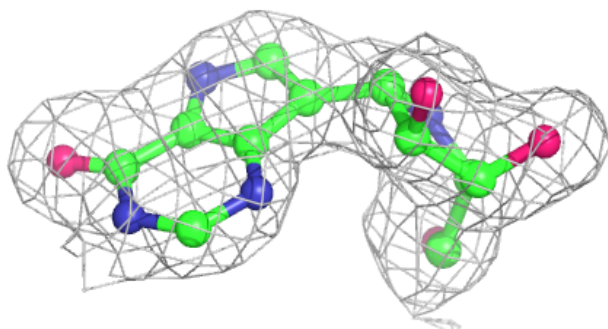
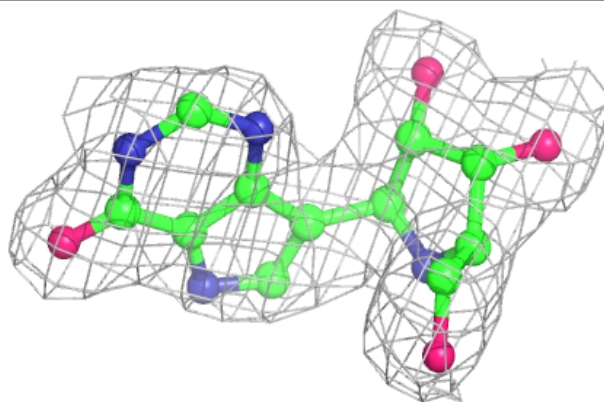
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	417	5/5	0.99	0.06	30,30,31,33	0
2	SO4	E	405	5/5	0.99	0.05	27,29,31,31	0
2	SO4	E	416	5/5	0.99	0.14	29,29,30,31	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.

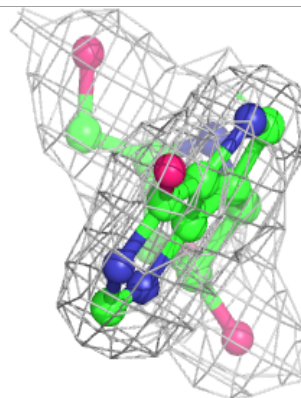
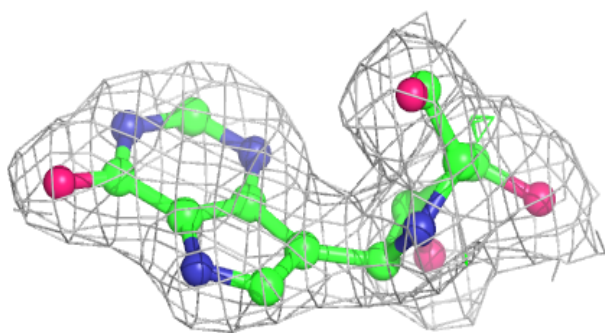
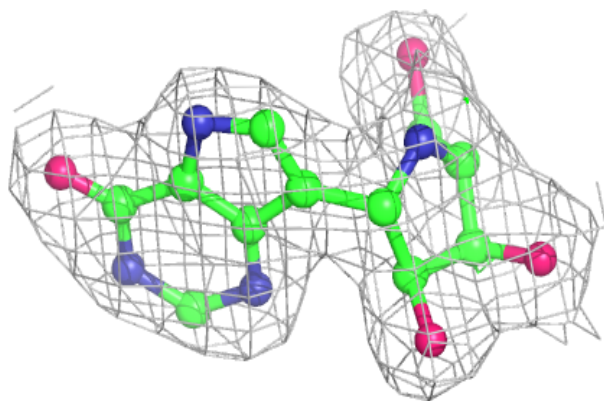
**Electron density around IMH C 303:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

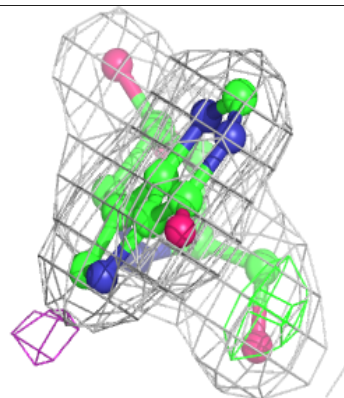
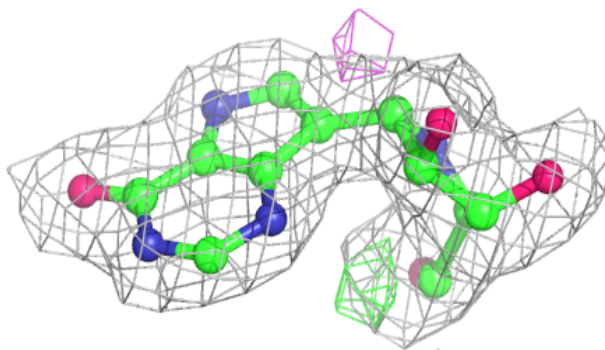
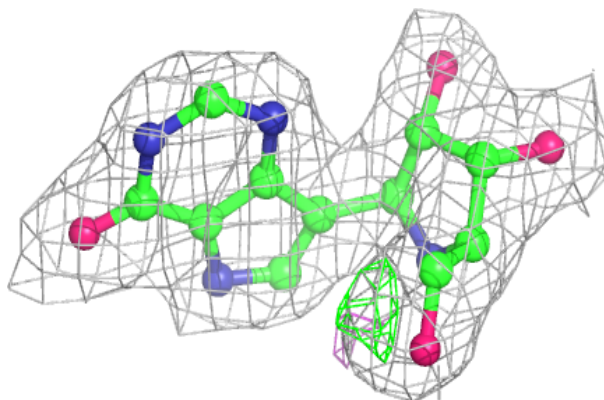


**Electron density around IMH E 305:**

$2mF_o-DF_c$  (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:**

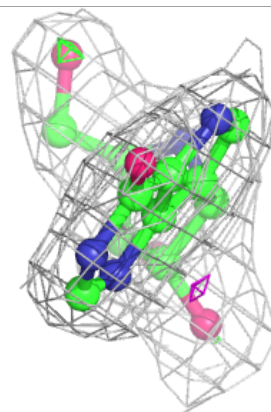
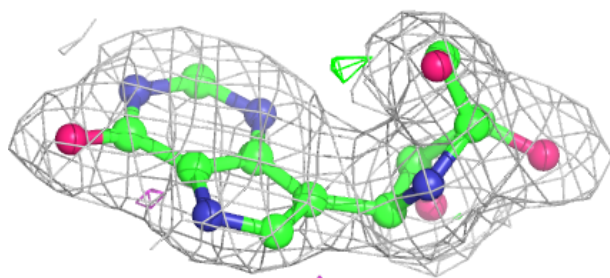
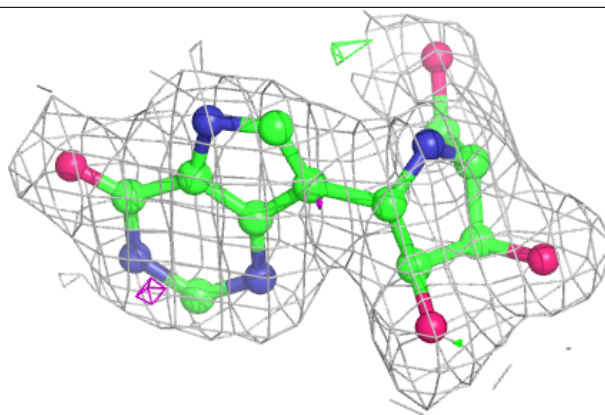
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



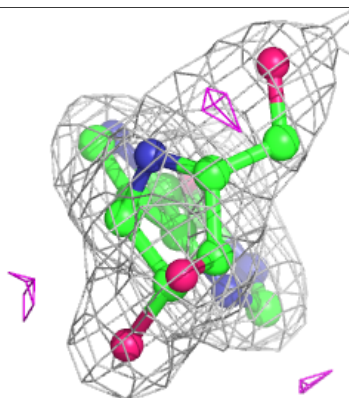
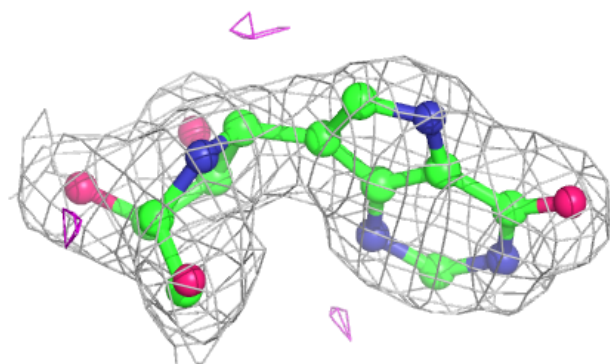
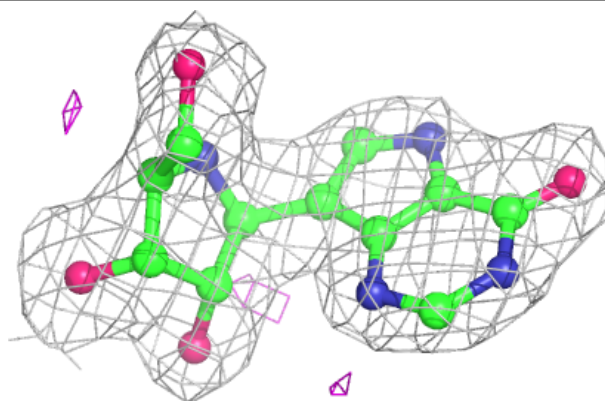


**Electron density around IMH A 301:**

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

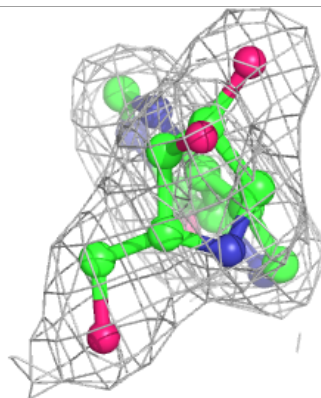
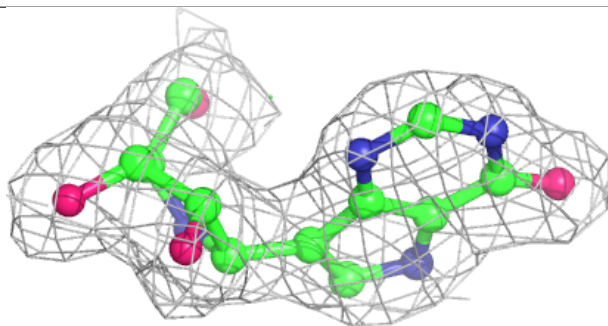
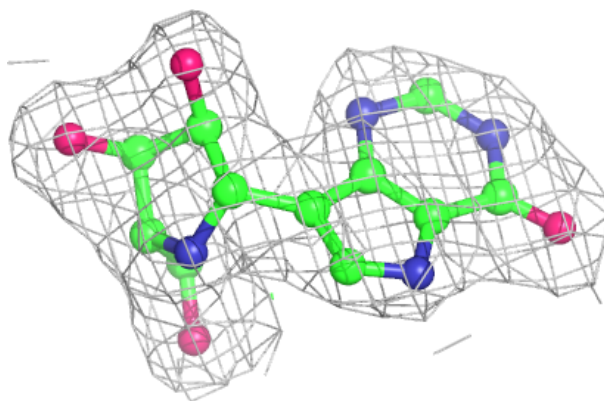
**Electron density around IMH B 302:**

$2mF_o-DF_c$  (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.