



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:24 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

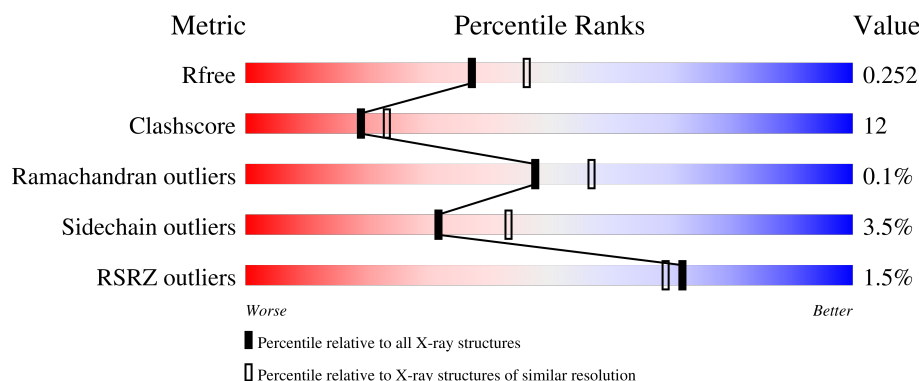
1 Overall quality at a glance

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 (#Entries)	Similar resolution (#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 ≥ 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	0.1% 61% 25% • 12%
1	B	276	3% 61% 25% • 12%
1	C	276	2% 65% 21% • 12%
1	D	276	0.1% 64% 21% • 12%

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Mol	Chain	Length	Quality of chain
1	E	276	% 64% 22% • 12%
1	F	276	% 67% 20% • 12%

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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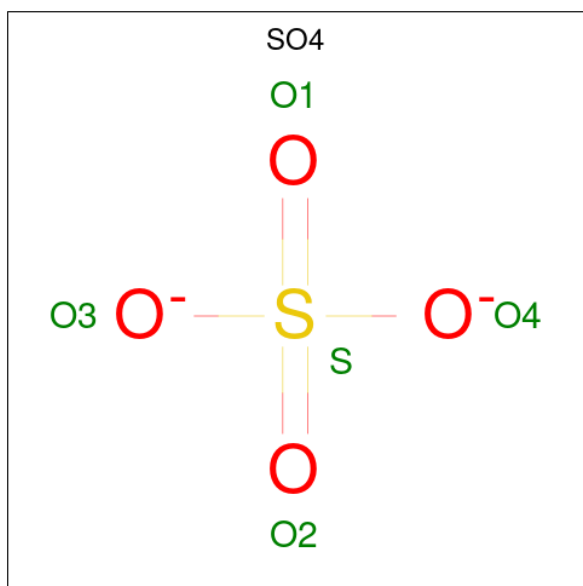
Chain	Residue	Modelled	Actual	Comment	Reference
E	263	LEU	-	cloning artifact	UNP Q8I3X4
E	264	ASN	-	cloning artifact	UNP Q8I3X4
E	265	SER	-	cloning artifact	UNP Q8I3X4
E	266	ALA	-	cloning artifact	UNP Q8I3X4
E	267	VAL	-	cloning artifact	UNP Q8I3X4
E	268	ASP	-	cloning artifact	UNP Q8I3X4
E	269	HIS	-	expression 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: O₄S).



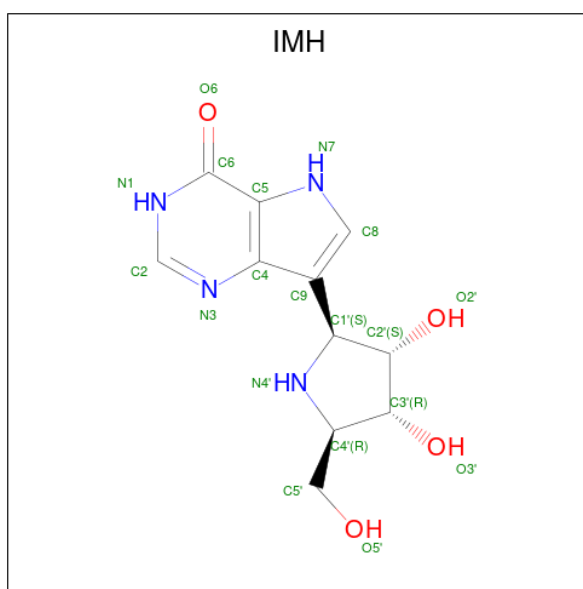
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	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 (CCD ID: IMH) (formula: C₁₁H₁₄N₄O₄).



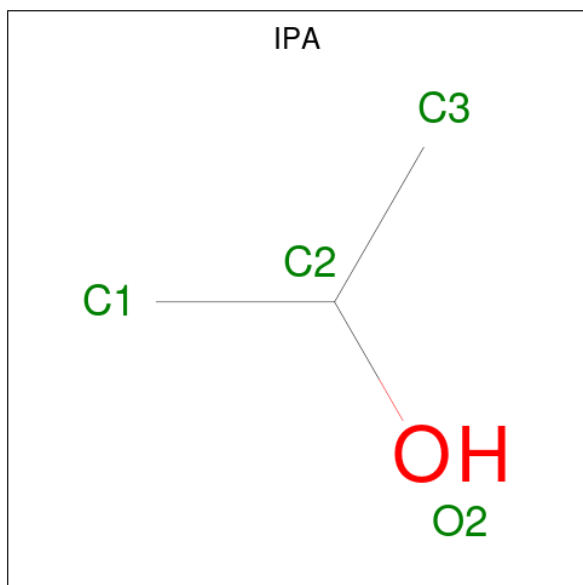
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 19 11 4 4	0	0
3	B	1	Total C N O 19 11 4 4	0	0
3	C	1	Total C N O 19 11 4 4	0	0

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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 (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 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

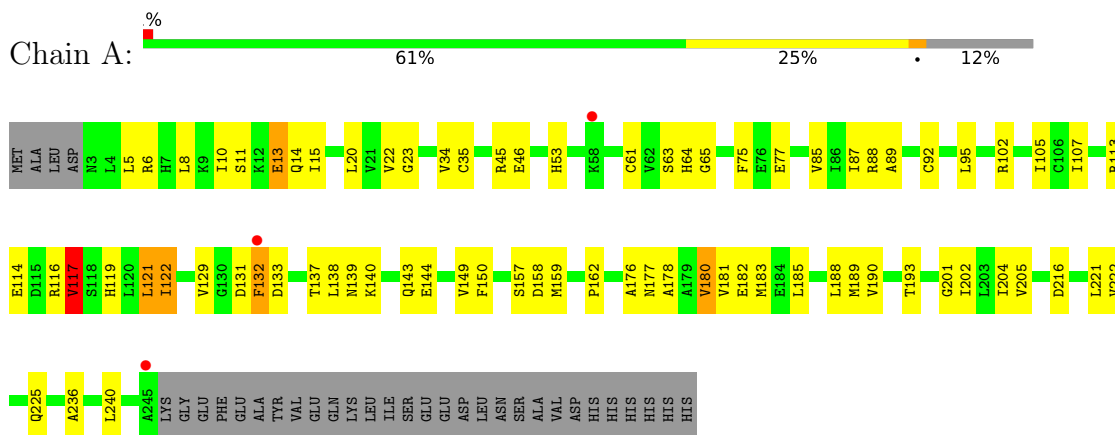
- Molecule 5 is water.

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

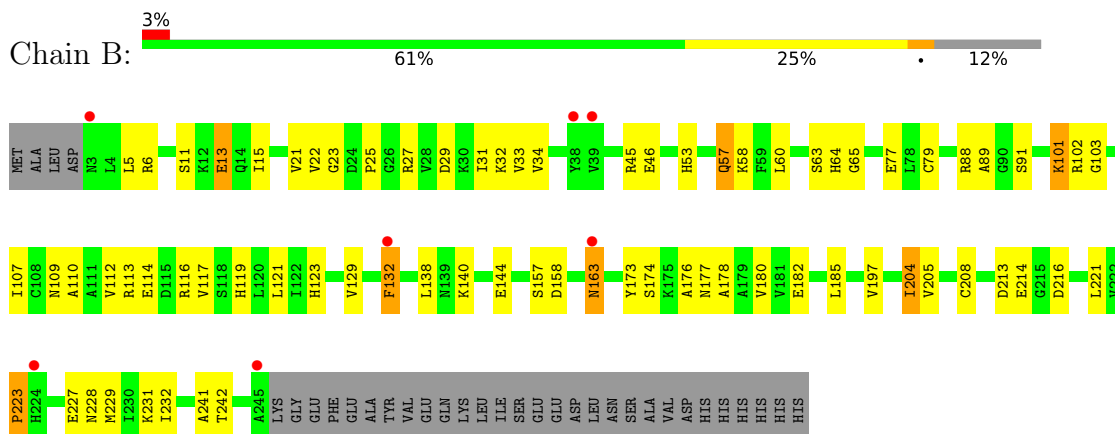
3 Residue-property plots

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.

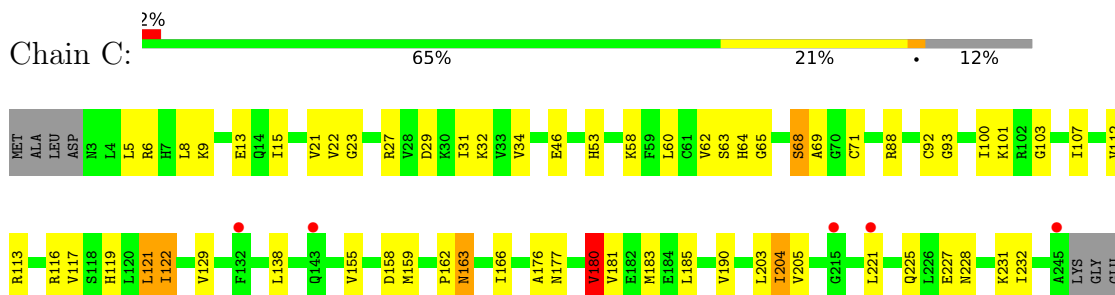
- Molecule 1: uridine phosphorylase, putative



- Molecule 1: uridine phosphorylase, putative



- Molecule 1: uridine phosphorylase, putative



PHE
GLU
ALA
TYR
VAL
GLU
GLN
LYS
LEU
SER
ILE
SER
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
K159
N163
Y173
A176
N177
A178
E182
G200
I204
V205
K211
D216
L221
H224
Q225
L226
M229
I230
A241
A245
LYS
GLY
PHE
GLU

ALA
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GLU
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- Molecule 1: uridine phosphorylase, putative



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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
L122
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
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- Molecule 1: uridine phosphorylase, putative



MET
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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
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.55Å 92.28Å 239.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	78.5 (20.00-2.20) 80.6 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.248 0.212 , 0.252	Depositor DCC
R_{free} test set	4001 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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.

All (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
1	E	183	MET	N-CA-C	6.15	122.19	113.02
1	B	6	ARG	N-CA-C	6.06	118.38	111.11
1	B	180	VAL	N-CA-C	5.85	115.95	108.82
1	C	183	MET	N-CA-C	5.84	121.72	113.02
1	E	82	GLY	N-CA-C	5.84	121.72	114.37
1	C	180	VAL	N-CA-C	5.71	116.92	108.65
1	F	178	ALA	N-CA-C	-5.60	101.99	110.28
1	A	185	LEU	N-CA-C	5.59	117.82	111.11
1	D	117	VAL	N-CA-C	5.59	116.23	110.36
1	E	174	SER	N-CA-C	-5.52	105.35	111.36
1	D	45	ARG	CB-CA-C	-5.52	110.20	116.54
1	A	117	VAL	CB-CA-C	-5.46	104.89	112.04
1	E	6	ARG	N-CA-C	5.43	117.63	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	185	LEU	N-CA-C	5.43	117.20	111.28
1	A	95	LEU	N-CA-C	-5.38	106.08	113.30
1	D	178	ALA	N-CA-C	-5.34	102.38	110.28
1	A	6	ARG	N-CA-C	5.30	117.75	111.33
1	C	185	LEU	N-CA-C	5.29	117.48	111.02
1	A	183	MET	N-CA-C	5.29	120.91	113.02
1	D	24	ASP	N-CA-C	5.20	116.47	109.24
1	F	45	ARG	CB-CA-C	-5.19	110.57	116.54
1	A	205	VAL	N-CA-C	5.17	115.72	108.89
1	E	5	LEU	N-CA-C	-5.16	102.65	110.28
1	D	205	VAL	N-CA-C	5.15	115.69	108.89
1	B	185	LEU	N-CA-C	5.14	117.28	111.11
1	B	174	SER	N-CA-C	-5.14	105.68	111.28
1	D	68	SER	N-CA-C	5.07	116.50	111.07
1	B	178	ALA	N-CA-C	-5.04	102.24	110.20
1	E	222	VAL	CA-C-N	5.03	126.13	119.84
1	E	222	VAL	C-N-CA	5.03	126.13	119.84
1	C	6	ARG	N-CA-C	5.03	119.67	111.37

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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:A:46:GLU:HB3	1:B:46:GLU:HB3	1.63	0.78
1:E:121:LEU:HD12	1:F:163:ASN:HB3	1.66	0.77
1:A:133:ASP:O	1:A:137:THR:HG23	1.85	0.76
1:E:46:GLU:HB3	1:F:46:GLU:HB3	1.68	0.75
1:C:117:VAL:HG22	1:D:158:ASP:HB3	1.69	0.73
1:E:163:ASN:C	1:E:163:ASN:HD22	1.96	0.73
1:D:15:ILE:HA	1:D:60:LEU:HD11	1.71	0.72
1:B:163:ASN:HD22	1:B:163:ASN:H	1.38	0.72
1:C:46:GLU:HB3	1:D:46:GLU:HB3	1.71	0.71
1:F:102:ARG:HD2	1:F:216:ASP:OD1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ASP:HB3	1:D:117:VAL:HG22	1.74	0.69
1:A:138:LEU:CD2	1:A:202:ILE:HD11	2.20	0.69
1:B:15:ILE:HA	1:B:60:LEU:HD11	1.75	0.69
1:A:138:LEU:HD22	1:A:202:ILE:CD1	2.19	0.68
5:E:612:HOH:O	1:F:117:VAL:HG23	1.93	0.68
1:F:5:LEU:HD13	1:F:77:GLU:HB3	1.76	0.66
1:D:13:GLU:H	1:D:13:GLU:CD	2.03	0.65
1:A:140:LYS:O	1:A:144:GLU:HG3	1.96	0.65
1:B:31:ILE:O	1:B:34:VAL:HG22	1.96	0.65
1:B:102:ARG:HD2	1:B:216:ASP:OD1	1.98	0.64
1:C:204:ILE:HD12	1:C:221:LEU:HD22	1.80	0.64
1:A:102:ARG:HD2	1:A:216:ASP:OD1	1.97	0.64
1:A:64:HIS:HD2	1:A:65:GLY:O	1.81	0.64
1:A:117:VAL:HG22	5:A:793:HOH:O	1.97	0.64
1:D:64:HIS:HD2	1:D:65:GLY:O	1.82	0.63
1:E:158:ASP:HB3	1:F:117:VAL:HG22	1.81	0.63
1:D:102:ARG:HD2	1:D:216:ASP:OD1	1.97	0.63
1:B:5:LEU:HD13	1:B:77:GLU:HB3	1.81	0.62
1:F:51:GLU:OE2	1:F:58:LYS:HD3	1.98	0.62
1:E:5:LEU:HD11	1:E:15:ILE:HD11	1.80	0.62
1:A:132:PHE:CE1	1:F:132:PHE:HE1	2.18	0.61
1:D:117:VAL:HG23	5:D:644:HOH:O	2.00	0.61
1:B:228:ASN:O	1:B:232:ILE:HG13	2.01	0.61
1:D:140:LYS:O	1:D:144:GLU:HG3	1.99	0.61
1:C:180:VAL:HG13	1:C:181:VAL:N	2.16	0.60
1:E:25:PRO:O	1:E:28:VAL:HG13	2.01	0.60
1:E:31:ILE:O	1:E:34:VAL:HG22	2.01	0.60
1:C:5:LEU:HD11	1:C:15:ILE:HD11	1.83	0.60
1:A:107:ILE:HD13	1:A:138:LEU:HB3	1.84	0.60
5:A:617:HOH:O	1:B:117:VAL:HG23	2.01	0.60
1:B:140:LYS:O	1:B:144:GLU:HG3	2.02	0.60
1:A:122:ILE:HD11	1:A:190:VAL:CG1	2.32	0.59
1:E:163:ASN:C	1:E:163:ASN:ND2	2.60	0.59
1:E:64:HIS:HD2	1:E:65:GLY:O	1.85	0.59
1:C:64:HIS:HD2	1:C:65:GLY:O	1.86	0.59
1:C:117:VAL:HG23	5:D:614:HOH:O	2.01	0.59
1:E:102:ARG:HD2	1:E:216:ASP:OD1	2.02	0.59
1:E:117:VAL:HG22	1:F:158:ASP:HB3	1.85	0.59
1:C:159:MET:HE3	1:C:162:PRO:HB3	1.83	0.59
1:D:29:ASP:HA	1:D:32:LYS:HE2	1.84	0.58
1:F:12:LYS:HG3	1:F:81:ASN:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:304:IMH:N3	3:D:304:IMH:H2'	2.18	0.58
1:A:122:ILE:HD11	1:A:190:VAL:HG11	1.86	0.58
3:E:305:IMH:N3	3:E:305:IMH:H2'	2.19	0.57
1:B:23:GLY:HA2	1:B:64:HIS:CD2	2.39	0.57
1:A:5:LEU:HD12	1:A:8:LEU:HD12	1.87	0.57
1:B:114:GLU:HB3	1:B:157:SER:HA	1.87	0.57
1:F:5:LEU:HD11	1:F:15:ILE:HD11	1.87	0.56
1:C:116:ARG:HB2	1:D:116:ARG:HB2	1.87	0.56
1:E:117:VAL:O	1:E:121:LEU:HD22	2.06	0.56
1:D:5:LEU:HD11	1:D:15:ILE:HD11	1.88	0.56
1:A:117:VAL:O	1:A:121:LEU:HD22	2.04	0.56
1:D:22:VAL:O	1:D:63:SER:HA	2.06	0.56
1:A:13:GLU:H	1:A:13:GLU:CD	2.14	0.56
1:C:113:ARG:O	1:C:119:HIS:HE1	1.89	0.56
3:A:301:IMH:N3	3:A:301:IMH:H2'	2.21	0.56
1:A:117:VAL:HG13	1:B:158:ASP:O	2.06	0.55
3:C:303:IMH:N3	3:C:303:IMH:H2'	2.21	0.55
1:D:132:PHE:HE1	1:E:132:PHE:HD1	1.54	0.55
3:F:306:IMH:H2'	3:F:306:IMH:N3	2.20	0.55
1:F:64:HIS:HD2	1:F:65:GLY:O	1.89	0.55
1:A:22:VAL:O	1:A:63:SER:HA	2.07	0.55
1:B:53:HIS:ND1	1:B:58:LYS:HG2	2.22	0.55
1:F:93:GLY:O	1:F:180:VAL:HG22	2.06	0.55
1:C:180:VAL:CG1	1:C:181:VAL:N	2.70	0.55
1:C:228:ASN:O	1:C:232:ILE:HG13	2.07	0.55
1:D:5:LEU:HD13	1:D:77:GLU:HB3	1.89	0.54
1:E:13:GLU:CD	1:E:13:GLU:H	2.15	0.54
1:D:27:ARG:NH1	1:D:226:LEU:HD21	2.23	0.54
1:F:89:ALA:HB1	1:F:229:MET:HE3	1.89	0.54
1:B:13:GLU:CD	1:B:13:GLU:H	2.17	0.53
1:E:221:LEU:HD13	1:E:226:LEU:HD13	1.89	0.53
1:A:132:PHE:CD1	1:F:132:PHE:HE1	2.25	0.53
3:B:302:IMH:N3	3:B:302:IMH:H2'	2.23	0.53
1:F:40:ASP:HA	1:F:50:VAL:HG22	1.90	0.53
1:A:189:MET:O	1:A:193:THR:HG23	2.09	0.53
1:F:140:LYS:O	1:F:144:GLU:HG3	2.08	0.53
1:F:27:ARG:NH2	2:F:415:SO4:O4	2.41	0.53
1:D:226:LEU:O	1:D:230:ILE:HG13	2.08	0.53
1:E:113:ARG:O	1:E:119:HIS:HE1	1.92	0.52
1:D:211:LYS:HE3	1:D:216:ASP:OD2	2.08	0.52
1:A:149:VAL:HG12	1:A:150:PHE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ASN:HD22	1:D:163:ASN:H	1.57	0.52
1:C:29:ASP:O	1:C:32:LYS:HG2	2.09	0.52
1:C:176:ALA:O	1:C:177:ASN:HB2	2.10	0.52
1:F:15:ILE:HA	1:F:60:LEU:HD11	1.92	0.52
1:A:5:LEU:HD13	1:A:77:GLU:HB3	1.92	0.51
1:C:93:GLY:O	1:C:180:VAL:HG22	2.10	0.51
1:C:227:GLU:HG2	1:C:231:LYS:HE3	1.91	0.51
1:D:51:GLU:OE2	1:D:58:LYS:HE2	2.10	0.51
1:A:92:CYS:HB2	1:A:180:VAL:HG13	1.93	0.51
1:D:89:ALA:HB1	1:D:229:MET:HE3	1.92	0.51
1:A:107:ILE:HG12	1:A:202:ILE:HG23	1.92	0.51
1:C:34:VAL:HG12	1:C:34:VAL:O	2.09	0.51
1:E:119:HIS:HD2	5:E:806:HOH:O	1.93	0.51
1:E:159:MET:HE3	1:E:162:PRO:HB3	1.91	0.51
1:B:163:ASN:H	1:B:163:ASN:ND2	2.06	0.51
1:D:53:HIS:HE1	1:D:58:LYS:HE3	1.75	0.51
1:B:27:ARG:O	1:B:31:ILE:HG13	2.11	0.51
1:C:163:ASN:C	1:C:163:ASN:ND2	2.69	0.51
1:C:163:ASN:C	1:C:163:ASN:HD22	2.19	0.50
1:D:29:ASP:O	1:D:32:LYS:HG2	2.12	0.50
1:A:88:ARG:HG3	1:A:88:ARG:HH11	1.77	0.50
1:E:20:LEU:O	1:E:61:CYS:HA	2.10	0.50
1:F:180:VAL:HG13	1:F:181:VAL:N	2.26	0.50
1:F:116:ARG:HE	4:F:511:IPA:H13	1.77	0.50
1:C:122:ILE:HD11	1:C:190:VAL:CG1	2.42	0.50
1:D:133:ASP:O	1:D:137:THR:HG23	2.11	0.50
1:A:87:ILE:HD13	1:A:138:LEU:HD21	1.93	0.50
1:C:53:HIS:HE1	1:C:58:LYS:HE2	1.76	0.50
1:B:123:HIS:HA	4:B:508:IPA:H31	1.93	0.49
1:D:176:ALA:O	1:D:177:ASN:HB2	2.12	0.49
1:B:22:VAL:HG12	1:B:23:GLY:N	2.28	0.49
1:C:112:VAL:HB	1:C:155:VAL:HA	1.93	0.49
1:A:222:VAL:HB	1:A:225:GLN:HB2	1.94	0.49
1:C:103:GLY:HA2	1:C:204:ILE:HD11	1.95	0.49
1:A:5:LEU:HD11	1:A:15:ILE:HD11	1.94	0.49
1:D:114:GLU:HB3	1:D:157:SER:HA	1.94	0.49
1:E:176:ALA:O	1:E:177:ASN:HB2	2.11	0.49
1:E:134:VAL:HG11	1:E:200:GLY:HA3	1.95	0.49
1:A:88:ARG:O	1:A:201:GLY:HA2	2.13	0.49
1:B:57:GLN:NE2	1:B:242:THR:HA	2.28	0.49
1:C:100:ILE:HG22	1:C:205:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:LEU:HG	1:E:10:ILE:O	2.13	0.48
1:F:176:ALA:O	1:F:177:ASN:HB2	2.13	0.48
1:B:29:ASP:O	1:B:32:LYS:HG2	2.13	0.48
1:C:68:SER:HA	1:C:71:CYS:SG	2.54	0.48
1:A:23:GLY:HA2	1:A:64:HIS:CD2	2.49	0.48
1:B:227:GLU:HG2	1:B:231:LYS:HE3	1.94	0.48
1:A:149:VAL:HG12	1:A:150:PHE:N	2.28	0.48
1:C:69:ALA:HA	1:C:117:VAL:HG21	1.96	0.48
1:F:20:LEU:O	1:F:61:CYS:HA	2.14	0.48
1:A:113:ARG:O	1:A:119:HIS:HE1	1.96	0.48
1:A:114:GLU:HB3	1:A:157:SER:HA	1.95	0.48
1:C:27:ARG:O	1:C:31:ILE:HG13	2.13	0.48
1:C:22:VAL:O	1:C:63:SER:HA	2.13	0.48
1:D:131:ASP:OD1	1:D:133:ASP:HB2	2.13	0.48
1:F:34:VAL:HG12	1:F:34:VAL:O	2.14	0.48
1:A:107:ILE:HG13	1:A:149:VAL:HG11	1.96	0.47
1:B:204:ILE:HD12	1:B:221:LEU:HD22	1.96	0.47
1:E:46:GLU:CB	1:F:46:GLU:HB3	2.41	0.47
1:B:213:ASP:OD2	1:B:214:GLU:HG3	2.14	0.47
1:B:89:ALA:HB1	1:B:229:MET:HE3	1.96	0.47
1:B:110:ALA:HB2	1:C:129:VAL:HG11	1.95	0.47
1:D:113:ARG:O	1:D:119:HIS:HE1	1.97	0.47
1:F:22:VAL:O	1:F:63:SER:HA	2.15	0.47
1:F:100:ILE:HG22	1:F:205:VAL:HG21	1.97	0.47
1:A:45:ARG:HB3	1:A:46:GLU:OE2	2.14	0.47
1:B:208:CYS:HB3	1:B:216:ASP:OD2	2.15	0.47
1:F:5:LEU:HG	1:F:10:ILE:O	2.15	0.47
1:B:113:ARG:O	1:B:119:HIS:HE1	1.98	0.47
1:E:159:MET:SD	1:F:121:LEU:HD13	2.55	0.47
1:E:159:MET:SD	1:E:162:PRO:HA	2.56	0.46
1:A:11:SER:OG	1:A:14:GLN:HG3	2.16	0.46
1:B:21:VAL:HG23	1:B:88:ARG:HA	1.97	0.46
1:A:34:VAL:O	1:A:34:VAL:HG12	2.16	0.46
1:B:64:HIS:HD2	1:B:65:GLY:O	1.99	0.46
1:C:21:VAL:HG23	1:C:88:ARG:HA	1.96	0.46
1:A:89:ALA:HA	1:A:202:ILE:O	2.15	0.46
1:F:163:ASN:HD21	1:F:165:ILE:HB	1.81	0.46
1:B:45:ARG:HE	4:B:501:IPA:H31	1.81	0.46
1:C:92:CYS:HB2	1:C:180:VAL:HG13	1.97	0.46
1:E:114:GLU:HB3	1:E:157:SER:HA	1.98	0.46
1:A:35:CYS:HB3	1:A:53:HIS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:VAL:O	1:E:63:SER:HA	2.16	0.46
1:A:180:VAL:CG1	1:A:181:VAL:N	2.80	0.45
1:B:204:ILE:HD13	1:B:205:VAL:N	2.31	0.45
1:F:113:ARG:O	1:F:119:HIS:HE1	2.00	0.45
1:C:46:GLU:CB	1:D:46:GLU:HB3	2.44	0.45
1:D:119:HIS:HD2	5:D:686:HOH:O	1.98	0.45
1:F:27:ARG:HG2	5:F:843:HOH:O	2.15	0.45
1:A:85:VAL:HG11	1:A:240:LEU:HD13	1.97	0.45
1:A:139:ASN:O	1:A:143:GLN:HG3	2.17	0.45
1:A:180:VAL:HG13	1:A:181:VAL:N	2.32	0.45
1:B:11:SER:HB2	1:B:13:GLU:OE2	2.17	0.45
1:D:91:SER:HA	1:D:204:ILE:O	2.16	0.45
1:B:112:VAL:HG11	1:B:173:TYR:CZ	2.52	0.45
1:C:204:ILE:HG23	1:C:221:LEU:HD22	1.98	0.45
1:A:64:HIS:HE1	1:A:88:ARG:HH11	1.64	0.45
1:C:225:GLN:HA	1:C:225:GLN:OE1	2.17	0.45
1:C:92:CYS:HB3	1:C:203:LEU:HD13	2.00	0.44
1:D:204:ILE:HG21	1:D:221:LEU:HD13	1.99	0.44
1:E:68:SER:HA	1:E:71:CYS:SG	2.58	0.44
1:D:132:PHE:HE1	1:E:132:PHE:CD1	2.35	0.44
1:D:68:SER:HA	1:D:71:CYS:SG	2.58	0.44
1:E:109:ASN:HB3	1:E:135:TYR:CD1	2.52	0.44
1:A:158:ASP:HB3	1:B:117:VAL:HG22	2.00	0.44
1:B:33:VAL:O	1:B:33:VAL:HG12	2.17	0.44
3:D:304:IMH:H2	5:D:835:HOH:O	2.18	0.44
1:F:112:VAL:HG11	1:F:173:TYR:CZ	2.52	0.44
1:A:5:LEU:HG	1:A:10:ILE:O	2.18	0.44
1:E:5:LEU:HD13	1:E:77:GLU:HB3	1.99	0.44
1:A:116:ARG:HE	4:A:509:IPA:H13	1.84	0.43
1:A:129:VAL:HG11	1:F:110:ALA:HB2	1.99	0.43
1:A:121:LEU:HD12	1:B:163:ASN:HB3	2.01	0.43
1:B:101:LYS:HB3	2:B:410:SO4:O4	2.17	0.43
1:A:20:LEU:O	1:A:61:CYS:HA	2.18	0.43
1:A:75:PHE:CE1	1:A:188:LEU:HB2	2.53	0.43
1:F:32:LYS:HD2	1:F:38:TYR:CE1	2.54	0.43
1:A:105:ILE:O	1:A:149:VAL:HG13	2.18	0.43
1:C:122:ILE:HD11	1:C:190:VAL:HG11	2.00	0.43
1:D:57:GLN:HG3	1:D:241:ALA:HB3	2.01	0.43
1:E:158:ASP:O	1:F:117:VAL:HG22	2.19	0.43
1:B:5:LEU:HD11	1:B:15:ILE:HD11	2.00	0.43
1:B:57:GLN:CG	1:B:241:ALA:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLU:HB3	1:D:46:GLU:CB	2.45	0.43
1:B:22:VAL:HG11	1:B:27:ARG:CG	2.49	0.43
1:D:112:VAL:HG11	1:D:173:TYR:CZ	2.54	0.43
1:A:204:ILE:HG21	1:A:221:LEU:HD13	2.00	0.42
1:B:132:PHE:CD1	1:B:132:PHE:C	2.95	0.42
1:D:21:VAL:HA	1:D:62:VAL:O	2.18	0.42
1:E:112:VAL:HG21	1:E:155:VAL:HG22	2.01	0.42
1:E:54:TYR:CE2	1:E:234:LEU:HB3	2.53	0.42
1:F:222:VAL:HB	1:F:225:GLN:HB2	2.01	0.42
1:E:24:ASP:O	1:E:27:ARG:HB3	2.18	0.42
1:E:75:PHE:CE1	1:E:188:LEU:HB2	2.54	0.42
1:A:116:ARG:HB2	1:B:116:ARG:HB2	2.01	0.42
1:A:176:ALA:O	1:A:177:ASN:HB2	2.19	0.42
1:A:131:ASP:OD1	1:A:133:ASP:HB2	2.19	0.42
1:E:46:GLU:HB3	1:F:46:GLU:CB	2.45	0.42
1:C:23:GLY:HA2	1:C:64:HIS:CD2	2.55	0.42
1:D:16:THR:HB	1:D:17:PRO:HD2	2.00	0.42
1:E:85:VAL:HG11	1:E:240:LEU:HD13	2.01	0.42
1:B:57:GLN:HG2	1:B:241:ALA:HB3	2.02	0.42
1:B:79:CYS:SG	1:B:197:VAL:HG21	2.60	0.42
1:D:57:GLN:CG	1:D:241:ALA:HB3	2.50	0.42
1:D:102:ARG:HD3	2:D:417:SO4:O3	2.19	0.42
1:A:46:GLU:HB3	1:B:46:GLU:CB	2.43	0.42
1:B:103:GLY:HA2	1:B:204:ILE:HD11	2.01	0.42
1:B:109:ASN:O	1:B:129:VAL:HG23	2.20	0.42
1:B:22:VAL:O	1:B:63:SER:HA	2.20	0.42
1:E:45:ARG:HE	4:E:506:IPA:H31	1.85	0.42
1:B:22:VAL:HG11	1:B:27:ARG:HB3	2.02	0.41
1:D:115:ASP:OD1	1:D:115:ASP:C	2.63	0.41
1:E:136:ASP:OD2	1:E:140:LYS:HE3	2.20	0.41
1:C:163:ASN:HD21	1:C:166:ILE:H	1.67	0.41
1:A:46:GLU:CB	1:B:46:GLU:HB3	2.43	0.41
1:D:134:VAL:HG11	1:D:200:GLY:HA3	2.03	0.41
1:A:138:LEU:HD23	1:A:236:ALA:CB	2.50	0.41
1:B:107:ILE:HD13	1:B:138:LEU:HB3	2.03	0.41
1:F:202:ILE:HG12	1:F:229:MET:HG3	2.03	0.41
1:A:159:MET:HE3	1:A:162:PRO:HB3	2.01	0.41
1:B:25:PRO:HA	1:B:63:SER:HB3	2.02	0.41
1:C:15:ILE:HA	1:C:60:LEU:HD11	2.03	0.41
1:C:117:VAL:O	1:C:121:LEU:HD22	2.21	0.41
1:D:176:ALA:CB	1:E:122:ILE:HD12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ILE:HD13	1:C:138:LEU:HB3	2.03	0.41
1:F:225:GLN:OE1	1:F:225:GLN:HA	2.21	0.41
1:D:163:ASN:ND2	1:D:163:ASN:C	2.79	0.40
1:B:176:ALA:O	1:B:177:ASN:HB2	2.21	0.40
1:E:112:VAL:HG11	1:E:173:TYR:CZ	2.56	0.40
1:E:213:ASP:OD2	1:E:214:GLU:HG3	2.22	0.40
1:B:91:SER:HA	1:B:204:ILE:O	2.22	0.40
1:C:8:LEU:O	1:C:9:LYS:HB2	2.21	0.40
1:C:21:VAL:HA	1:C:62:VAL:O	2.22	0.40
1:C:181:VAL:O	1:C:181:VAL:HG13	2.21	0.40
1:F:21:VAL:HG23	1:F:88:ARG:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

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

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	117	VAL
1	A	121	LEU
1	A	122	ILE
1	A	132	PHE
1	A	180	VAL
1	A	182	GLU
1	B	13	GLU
1	B	57	GLN
1	B	101	LYS
1	B	121	LEU
1	B	132	PHE
1	B	163	ASN
1	B	182	GLU
1	B	204	ILE
1	B	223	PRO
1	C	13	GLU
1	C	101	LYS
1	C	121	LEU
1	C	122	ILE
1	C	163	ASN
1	C	180	VAL

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Mol	Chain	Res	Type
1	C	204	ILE
1	D	3	ASN
1	D	13	GLU
1	D	57	GLN
1	D	102	ARG
1	D	121	LEU
1	D	163	ASN
1	D	182	GLU
1	E	13	GLU
1	E	28	VAL
1	E	57	GLN
1	E	101	LYS
1	E	121	LEU
1	E	132	PHE
1	E	133	ASP
1	E	163	ASN
1	E	182	GLU
1	F	13	GLU
1	F	121	LEU
1	F	180	VAL
1	F	182	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	57	GLN
1	A	64	HIS
1	A	119	HIS
1	A	177	ASN
1	B	57	GLN
1	B	64	HIS
1	B	119	HIS
1	B	151	ASN
1	B	219	ASN
1	C	44	ASN
1	C	53	HIS
1	C	57	GLN
1	C	64	HIS
1	C	119	HIS
1	C	151	ASN
1	C	163	ASN

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Mol	Chain	Res	Type
1	C	224	HIS
1	D	44	ASN
1	D	53	HIS
1	D	57	GLN
1	D	64	HIS
1	D	119	HIS
1	D	163	ASN
1	E	44	ASN
1	E	57	GLN
1	E	64	HIS
1	E	119	HIS
1	E	151	ASN
1	E	163	ASN
1	F	44	ASN
1	F	53	HIS
1	F	64	HIS
1	F	81	ASN
1	F	119	HIS
1	F	163	ASN
1	F	177	ASN
1	F	220	ASN

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 oligosaccharides 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
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

All (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
3	F	306	IMH	C2-N3	3.76	1.37	1.30
3	E	305	IMH	C2-N3	3.68	1.37	1.30
3	A	301	IMH	C4'-N4'	-3.49	1.42	1.48
3	E	305	IMH	C2-N1	3.48	1.41	1.35
3	F	306	IMH	C4'-N4'	-3.37	1.43	1.48
3	F	306	IMH	C3'-C4'	-3.30	1.50	1.53
3	F	306	IMH	C2-N1	3.28	1.41	1.35
3	E	305	IMH	C3'-C4'	-3.24	1.50	1.53
3	B	302	IMH	C4'-N4'	-3.24	1.43	1.48
3	C	303	IMH	C4'-N4'	-3.23	1.43	1.48
3	A	301	IMH	C3'-C4'	-3.12	1.50	1.53
3	E	305	IMH	C4'-N4'	-3.09	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	419	SO4	O1-S	3.07	1.63	1.44
2	E	416	SO4	O1-S	3.05	1.63	1.44
2	B	407	SO4	O1-S	3.01	1.62	1.44
2	F	406	SO4	O1-S	3.01	1.62	1.44
2	F	415	SO4	O1-S	3.01	1.62	1.44
2	F	414	SO4	O1-S	3.00	1.62	1.44
3	B	302	IMH	C2-N1	2.99	1.40	1.35
3	D	304	IMH	C4'-N4'	-2.98	1.43	1.48
2	B	402	SO4	O1-S	2.96	1.62	1.44
2	D	417	SO4	O1-S	2.90	1.62	1.44
3	A	301	IMH	C1'-N4'	-2.88	1.42	1.46
2	A	401	SO4	O1-S	2.88	1.62	1.44
3	A	301	IMH	C2-N1	2.87	1.40	1.35
3	C	303	IMH	C2-N1	2.85	1.40	1.35
3	B	302	IMH	C3'-C4'	-2.78	1.50	1.53
3	D	304	IMH	C2-N1	2.77	1.40	1.35
3	F	306	IMH	C1'-N4'	-2.64	1.42	1.46
3	D	304	IMH	C8-N7	-2.61	1.30	1.36
3	C	303	IMH	C3'-C4'	-2.56	1.50	1.53
3	B	302	IMH	C8-N7	-2.55	1.31	1.36
3	C	303	IMH	C8-N7	-2.54	1.31	1.36
3	F	306	IMH	C8-N7	-2.54	1.31	1.36
3	E	305	IMH	C5-C4	2.43	1.40	1.38
2	B	402	SO4	O2-S	-2.39	1.30	1.44
3	B	302	IMH	C1'-N4'	-2.36	1.43	1.46
2	F	415	SO4	O2-S	-2.35	1.31	1.44
2	A	412	SO4	O1-S	-2.33	1.31	1.44
2	B	410	SO4	O1-S	-2.32	1.31	1.44
2	E	419	SO4	O2-S	-2.32	1.31	1.44
2	C	403	SO4	O1-S	-2.31	1.31	1.44
2	A	411	SO4	O1-S	-2.30	1.31	1.44
3	E	305	IMH	C8-N7	-2.26	1.31	1.36
3	A	301	IMH	C5-C4	2.25	1.40	1.38
3	A	301	IMH	C8-N7	-2.24	1.31	1.36
2	C	418	SO4	O1-S	-2.24	1.31	1.44
2	E	405	SO4	O3-S	-2.16	1.30	1.48
2	A	401	SO4	O3-S	-2.14	1.30	1.48
3	F	306	IMH	C5-C4	2.14	1.40	1.38
2	F	406	SO4	O3-S	-2.13	1.30	1.48
2	D	404	SO4	O3-S	-2.12	1.30	1.48
2	A	413	SO4	O3-S	-2.05	1.31	1.48
2	E	416	SO4	O3-S	-2.04	1.31	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	409	SO4	O3-S	-2.03	1.31	1.48
2	F	414	SO4	O3-S	-2.02	1.31	1.48

All (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
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
3	C	303	IMH	C9-C8-N7	4.38	115.01	108.70
3	E	305	IMH	C8-N7-C5	-3.84	104.76	109.49
3	A	301	IMH	C8-N7-C5	-3.77	104.85	109.49
3	D	304	IMH	C8-N7-C5	-3.71	104.92	109.49
3	F	306	IMH	C8-N7-C5	-3.69	104.94	109.49
3	B	302	IMH	C8-N7-C5	-3.49	105.19	109.49
3	C	303	IMH	C8-N7-C5	-3.44	105.25	109.49
3	E	305	IMH	C4-C5-N7	3.42	110.56	105.57
3	A	301	IMH	C4-C5-N7	3.38	110.49	105.57
3	F	306	IMH	C4-C5-N7	3.35	110.45	105.57
3	D	304	IMH	C4-C5-N7	3.29	110.37	105.57
3	B	302	IMH	C4-C5-N7	3.26	110.32	105.57
3	C	303	IMH	C4-C5-N7	3.20	110.23	105.57
3	D	304	IMH	O3'-C3'-C4'	-2.81	105.41	112.92
3	E	305	IMH	O3'-C3'-C4'	-2.68	105.74	112.92
3	C	303	IMH	N1-C2-N3	-2.66	122.43	125.50
3	A	301	IMH	O3'-C3'-C4'	-2.64	105.86	112.92
3	A	301	IMH	N1-C2-N3	-2.62	122.48	125.50
3	E	305	IMH	N1-C2-N3	-2.62	122.48	125.50
3	F	306	IMH	N1-C2-N3	-2.60	122.50	125.50
3	F	306	IMH	O3'-C3'-C4'	-2.60	105.97	112.92
3	B	302	IMH	N1-C2-N3	-2.59	122.52	125.50
3	B	302	IMH	O3'-C3'-C4'	-2.56	106.08	112.92
3	D	304	IMH	N1-C2-N3	-2.49	122.63	125.50
3	C	303	IMH	O3'-C3'-C4'	-2.47	106.30	112.92

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	IMH	C2'-C1'-C9-C8

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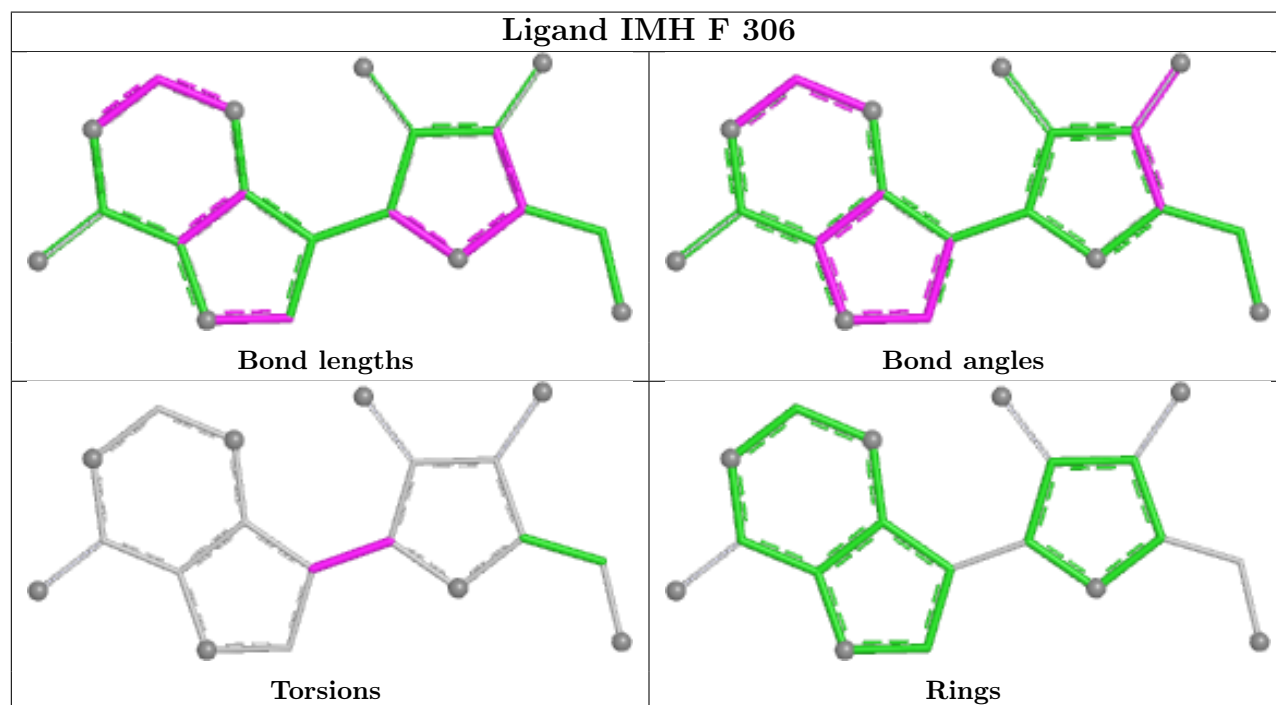
Mol	Chain	Res	Type	Atoms
3	A	301	IMH	C2'-C1'-C9-C4
3	B	302	IMH	C2'-C1'-C9-C8
3	B	302	IMH	C2'-C1'-C9-C4
3	C	303	IMH	C2'-C1'-C9-C8
3	C	303	IMH	C2'-C1'-C9-C4
3	D	304	IMH	C2'-C1'-C9-C8
3	D	304	IMH	C2'-C1'-C9-C4
3	E	305	IMH	C2'-C1'-C9-C8
3	E	305	IMH	C2'-C1'-C9-C4
3	F	306	IMH	C2'-C1'-C9-C8
3	F	306	IMH	C2'-C1'-C9-C4
3	A	301	IMH	N4'-C1'-C9-C8
3	B	302	IMH	N4'-C1'-C9-C8
3	C	303	IMH	N4'-C1'-C9-C8
3	D	304	IMH	N4'-C1'-C9-C8
3	E	305	IMH	N4'-C1'-C9-C8
3	F	306	IMH	N4'-C1'-C9-C8
3	A	301	IMH	N4'-C1'-C9-C4
3	B	302	IMH	N4'-C1'-C9-C4
3	C	303	IMH	N4'-C1'-C9-C4
3	D	304	IMH	N4'-C1'-C9-C4
3	E	305	IMH	N4'-C1'-C9-C4
3	F	306	IMH	N4'-C1'-C9-C4

There are no ring outliers.

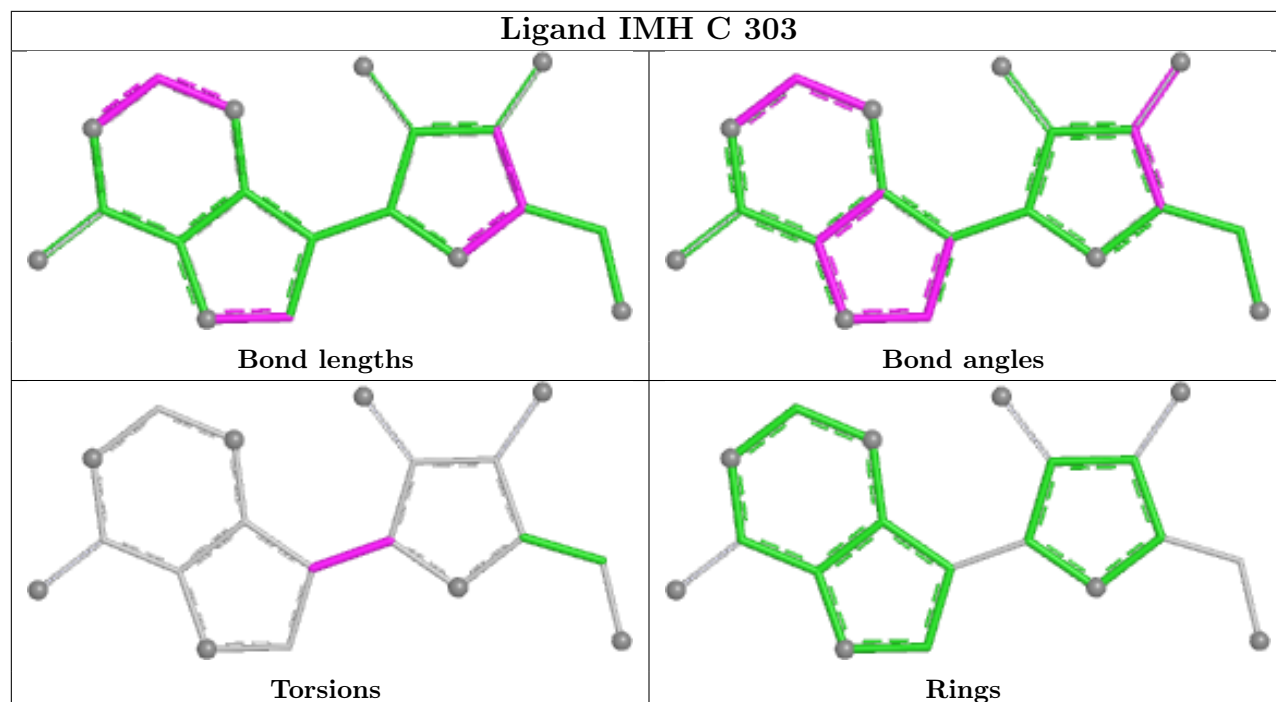
14 monomers are involved in 15 short contacts:

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

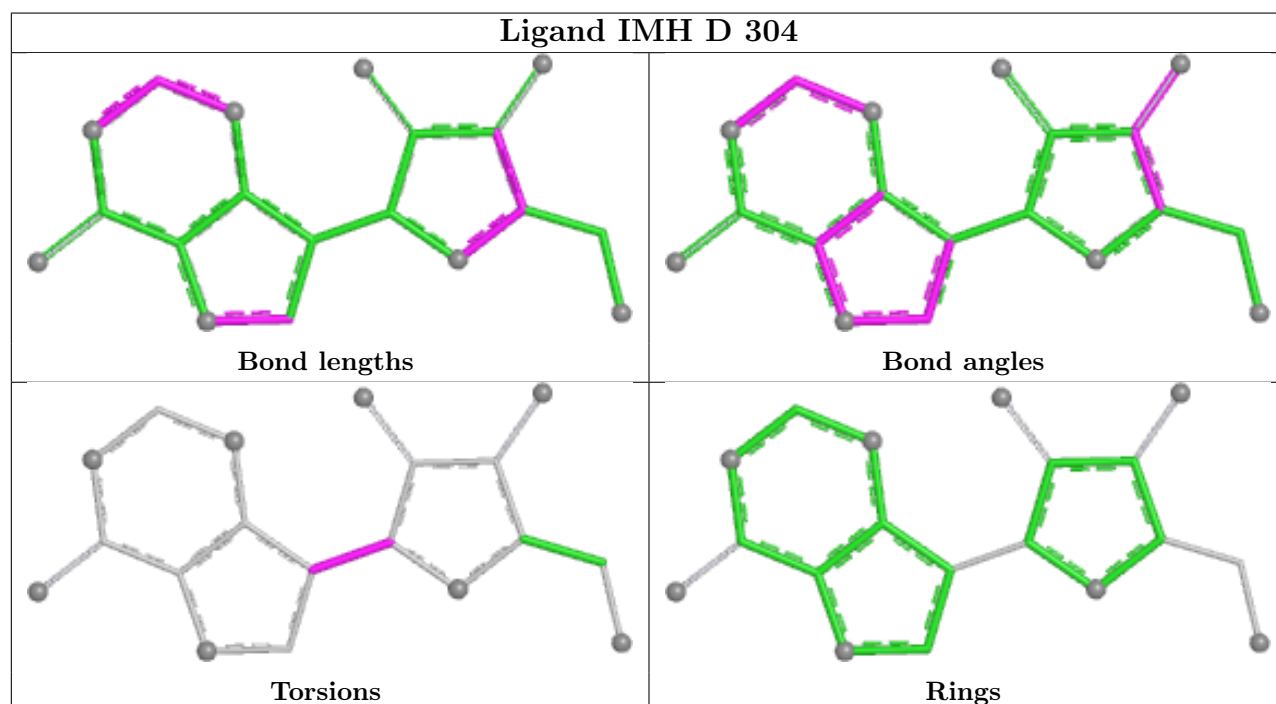
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



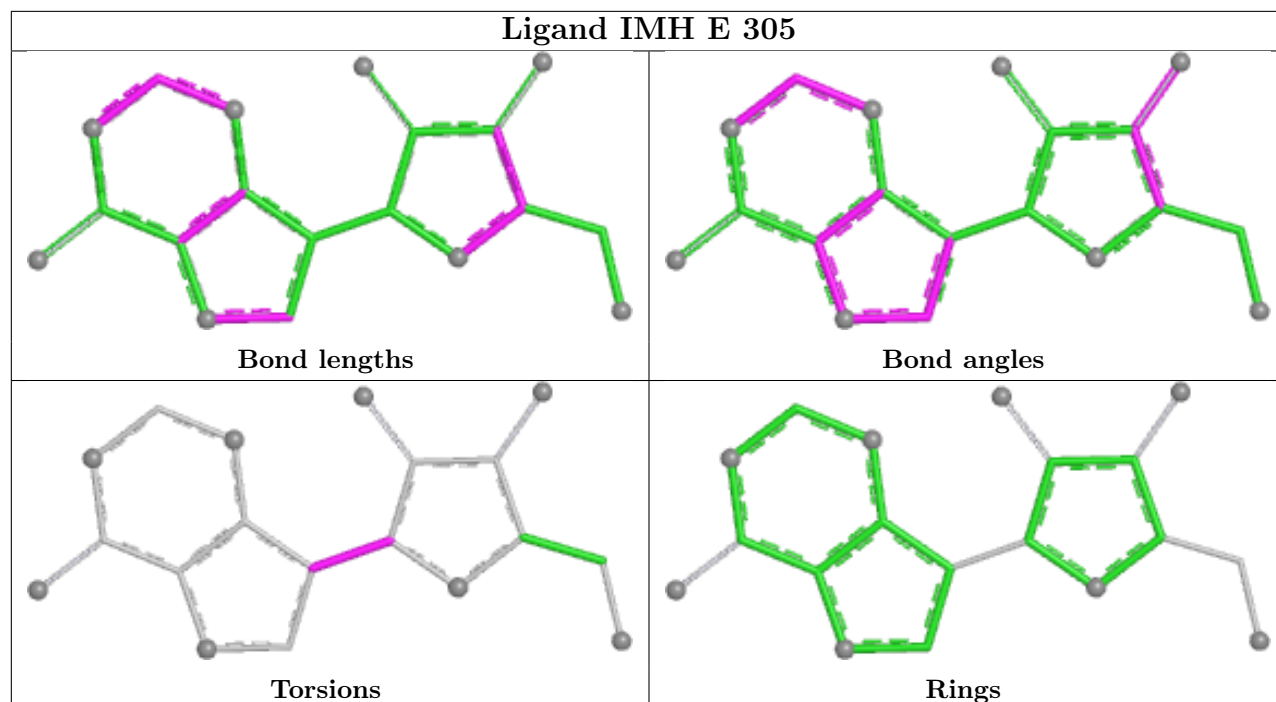
Ligand IMH C 303



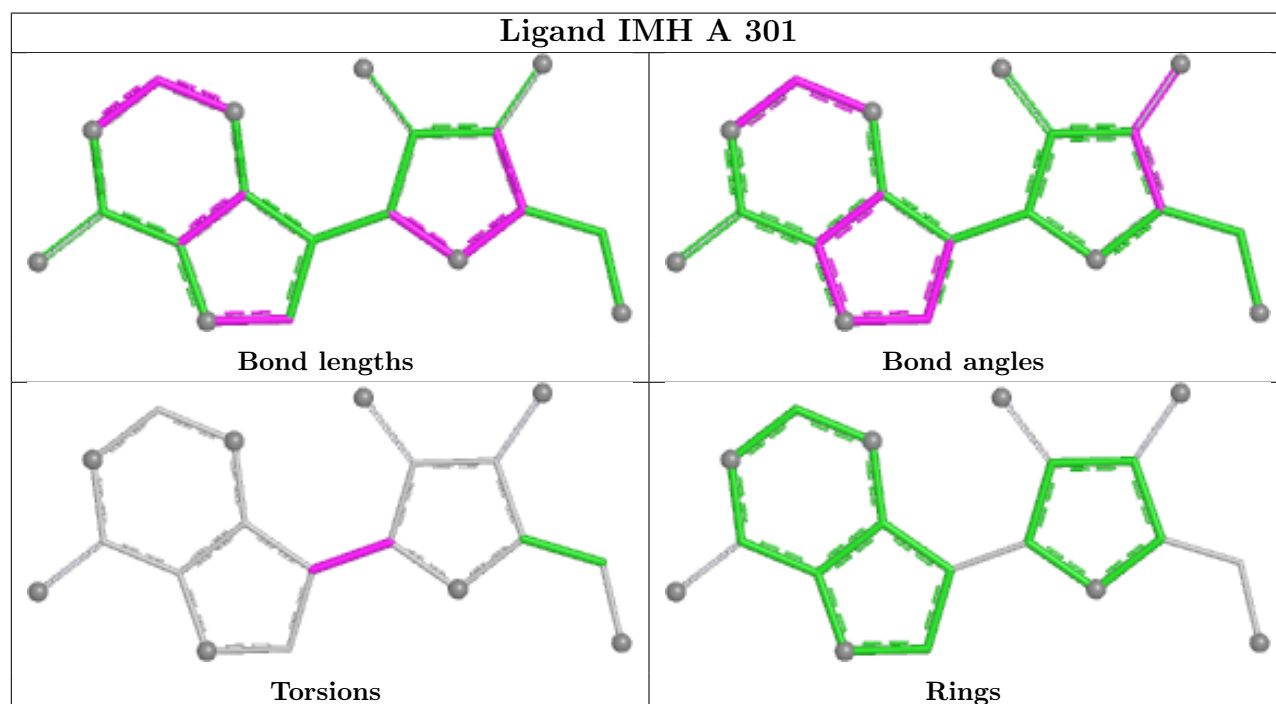
Ligand IMH D 304

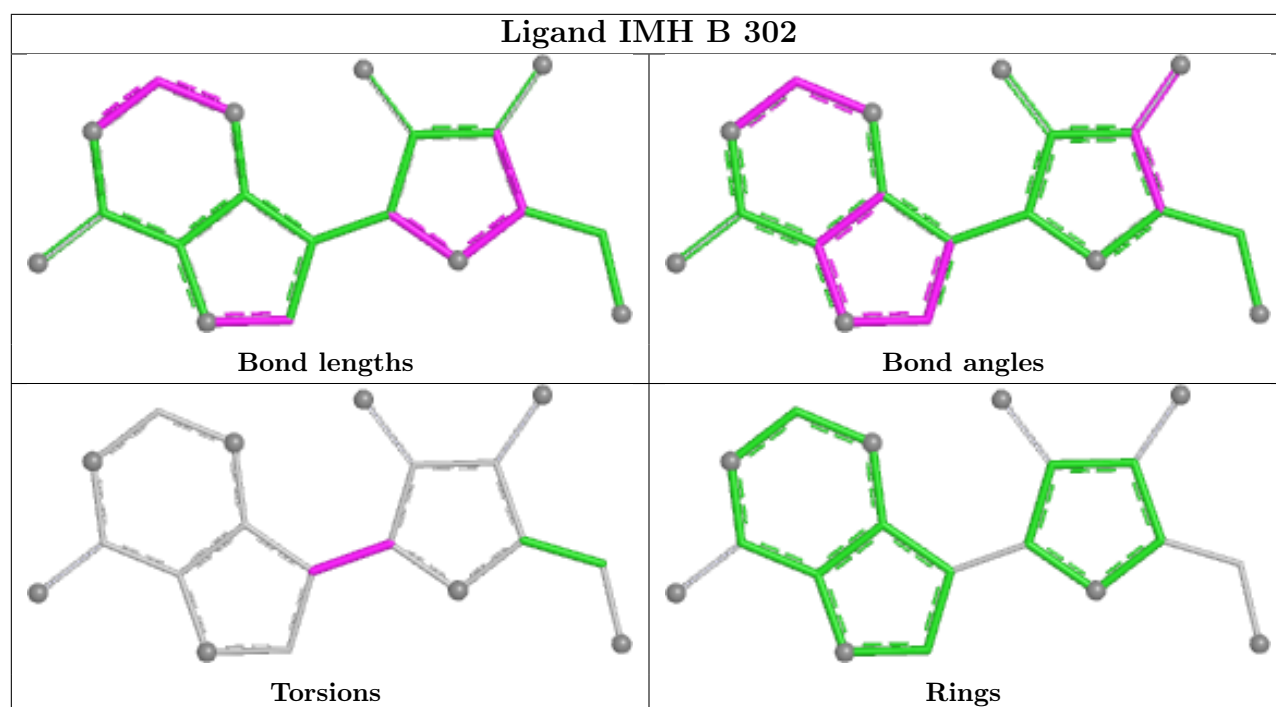


Ligand IMH E 305



Ligand IMH A 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	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

All (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
1	D	245	ALA	3.0
1	E	245	ALA	2.8
1	A	245	ALA	2.8
1	C	221	LEU	2.8
1	C	143	GLN	2.7
1	C	245	ALA	2.7
1	C	132	PHE	2.4
1	C	215	GLY	2.3
1	B	38	TYR	2.2
1	D	132	PHE	2.2
1	D	224	HIS	2.2
1	B	3	ASN	2.1
1	A	58	LYS	2.1
1	F	146	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	39	VAL	2.1
1	B	163	ASN	2.0
1	B	224	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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 ²)	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

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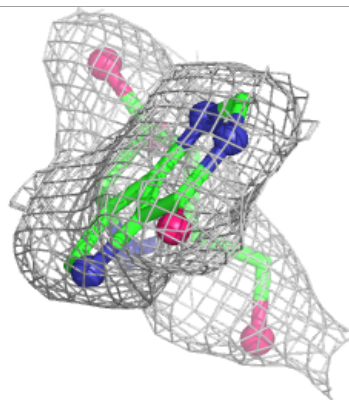
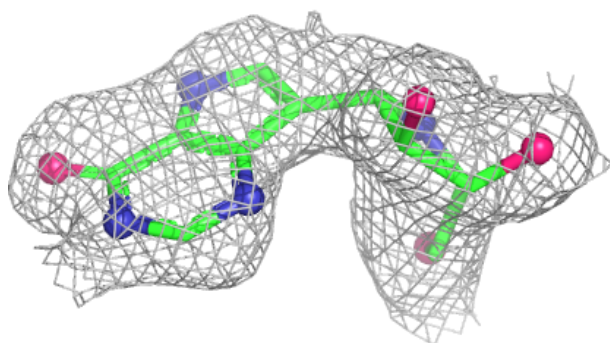
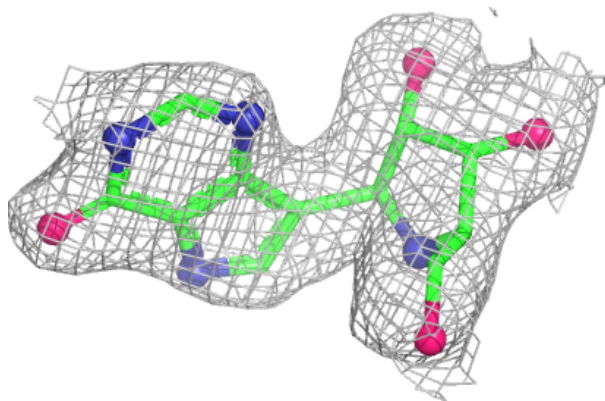
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IMH	D	304	19/19	0.93	0.07	17,21,28,28	0
3	IMH	A	301	19/19	0.94	0.07	27,28,31,31	0
2	SO4	E	419	5/5	0.95	0.07	54,54,56,57	0
3	IMH	B	302	19/19	0.95	0.07	31,35,38,39	0
3	IMH	F	306	19/19	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
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

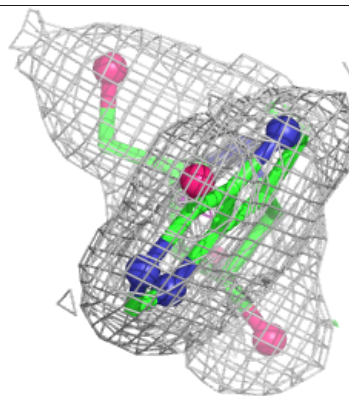
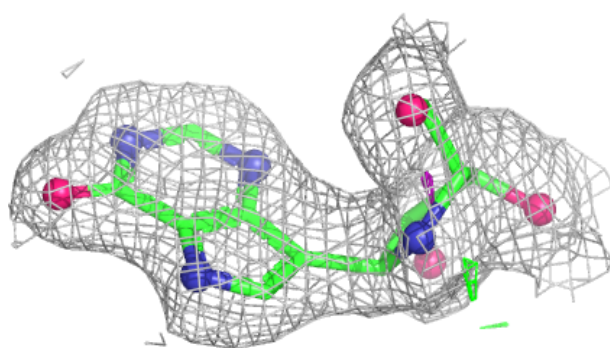
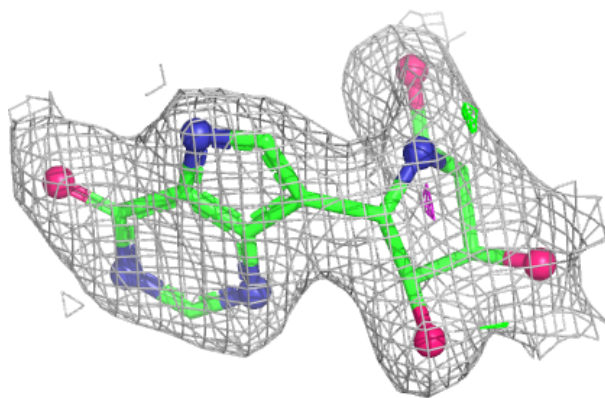
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IMH C 303:

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

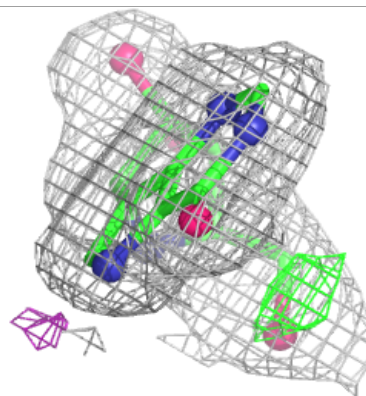
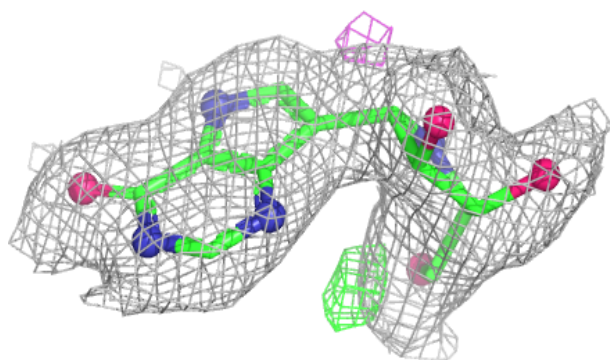
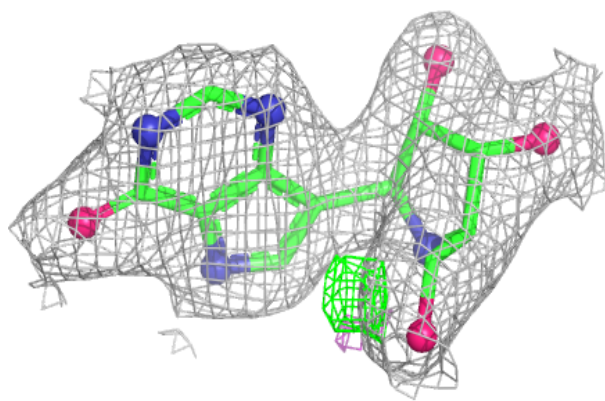
**Electron density around IMH E 305:**

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

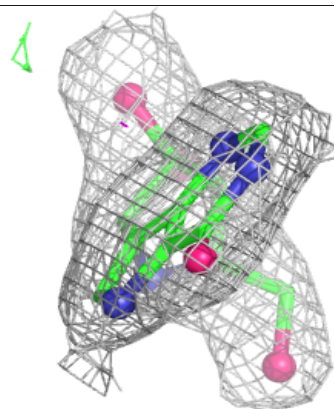
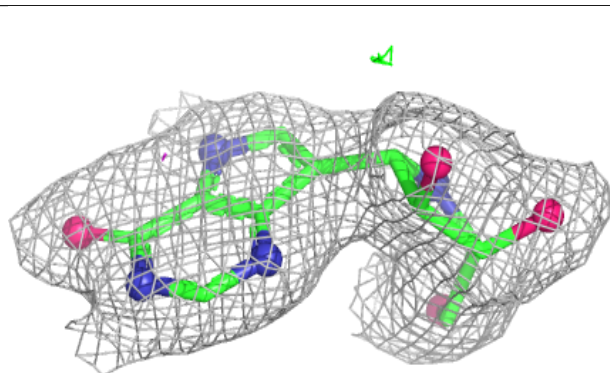
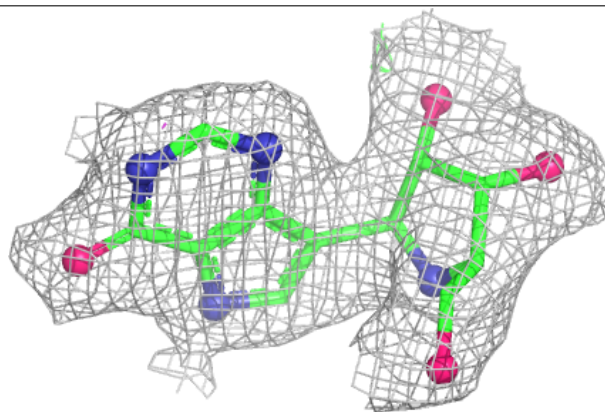


Electron density around IMH D 304:

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

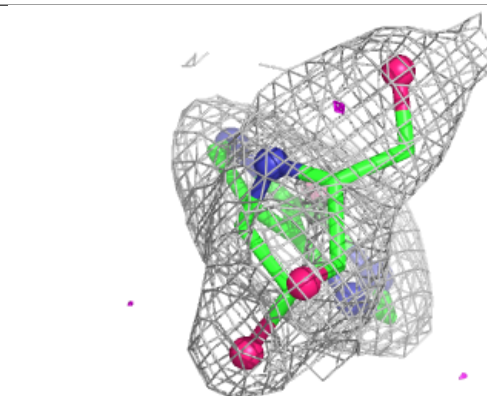
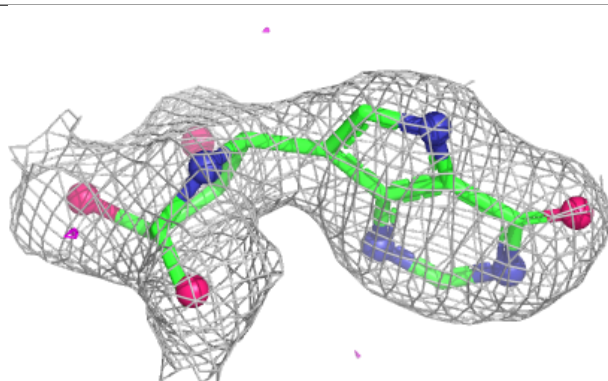
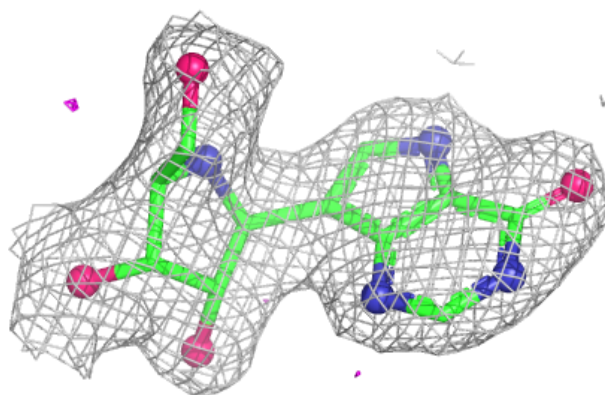
**Electron density around IMH A 301:**

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

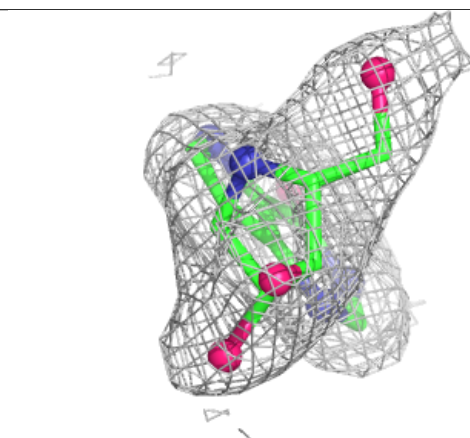
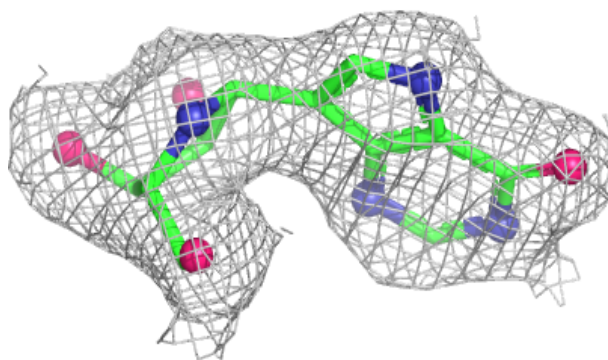
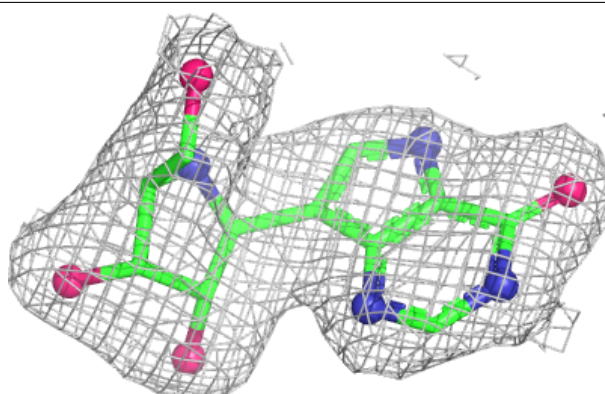


Electron density around IMH B 302:

$2mF_o-DF_c$ (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.