Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 12:04 AM EDT

PDB ID	:	1Q1G
Title	:	Crystal structure of Plasmodium falciparum PNP with 5'-methylthio-immucillin-H
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	:	2003-07-19
Resolution	:	2.02 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 (i) 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 (i)) were used in the production of this report:

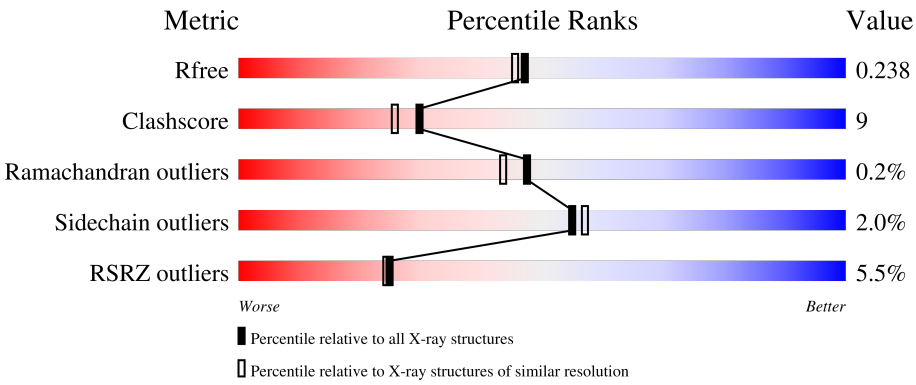
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 <=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	4% 72% 15% 12%
1	B	276	8% 71% 16% • 12%
1	C	276	6% 69% 18% • 12%
1	D	276	4% 67% 21% 12%

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Mol	Chain	Length	Quality of chain
1	E	276	5% 69% 18% • 12%
1	F	276	% 70% 17% • 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11789 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
			Total	C	N	O	S			
1	A	243	1861	1179	319	347	16	0	0	0
1	B	243	1861	1179	319	347	16	0	0	0
1	C	243	1861	1179	319	347	16	0	0	0
1	D	243	1861	1179	319	347	16	0	0	0
1	E	243	1861	1179	319	347	16	0	0	0
1	F	243	1861	1179	319	347	16	0	0	0

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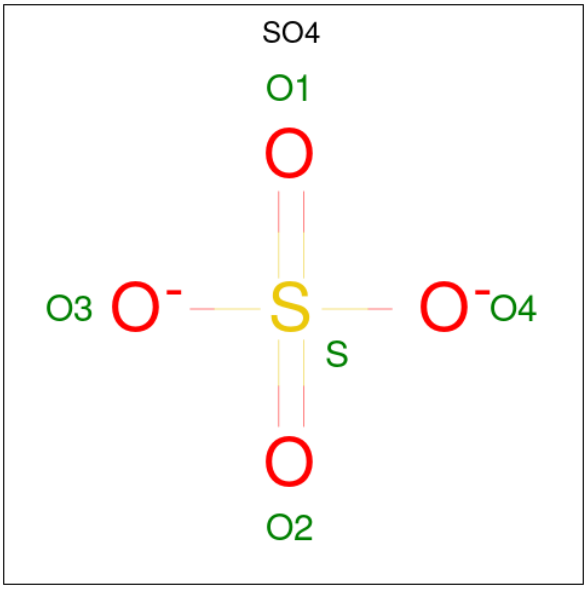
Chain	Residue	Modelled	Actual	Comment	Reference
F	274	HIS	-	expression tag	UNP Q8I3X4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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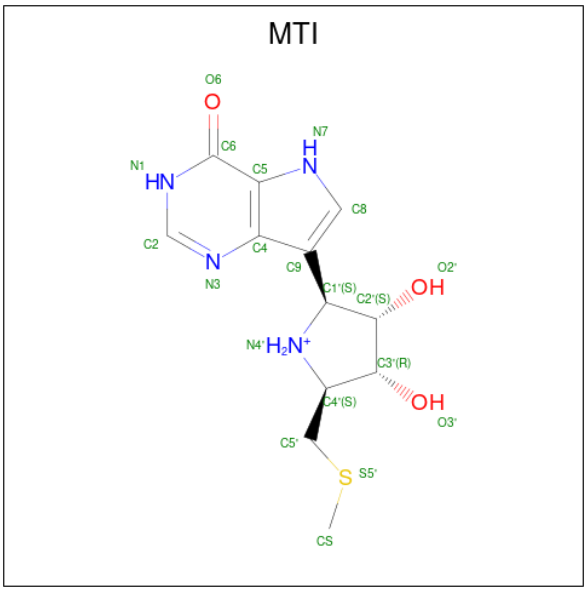
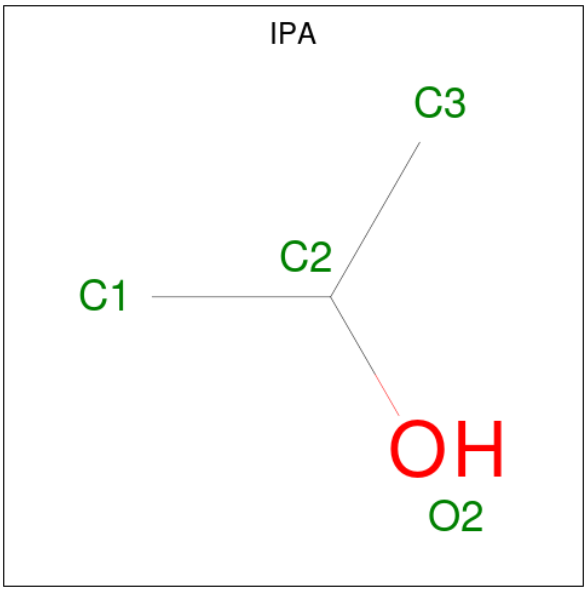
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	D	1	5	4	1		0	0
			Total	O	S			
2	D	1	5	4	1		0	0
			Total	O	S			
2	D	1	5	4	1		0	0
			Total	O	S			
2	D	1	5	4	1		0	0
			Total	O	S			
2	E	1	5	4	1		0	0
			Total	O	S			
2	E	1	5	4	1		0	0
			Total	O	S			
2	E	1	5	4	1		0	0
			Total	O	S			
2	F	1	5	4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

- Molecule 3 is 3,4-DIHYDROXY-2-[(METHYLSULFANYL)METHYL]-5-(4-OXO-4,5-DIHYDRO-3H-PYRROLO[3,2-D]PYRIMIDIN-7-YL)PYRROLIDINIUM (three-letter code: MTI) (formula: $C_{12}H_{17}N_4O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	20	12	4	3	1	0	0
3	B	1	20	12	4	3	1	0	0
3	C	1	20	12	4	3	1	0	0
3	D	1	20	12	4	3	1	0	0
3	E	1	20	12	4	3	1	0	0
3	F	1	20	12	4	3	1	0	0

- Molecule 4 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	E	1	4	3	1	0	0
			Total	C	O		
4	F	1	4	3	1	0	0
			Total	C	O		
4	F	1	4	3	1	0	0

- Molecule 5 is water.

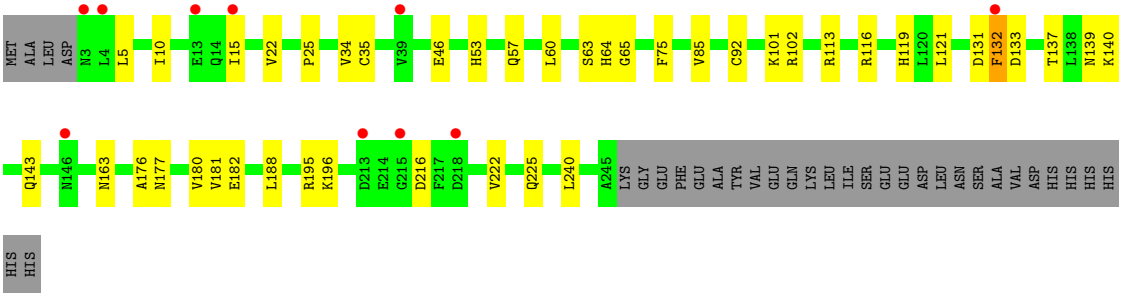
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	56	56	56	0	0
			Total	O		
5	B	45	45	45	0	0
			Total	O		
5	C	51	51	51	0	0
			Total	O		
5	D	61	61	61	0	0
			Total	O		
5	E	65	65	65	0	0
			Total	O		
5	F	79	79	79	0	0

3 Residue-property plots (i)

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.

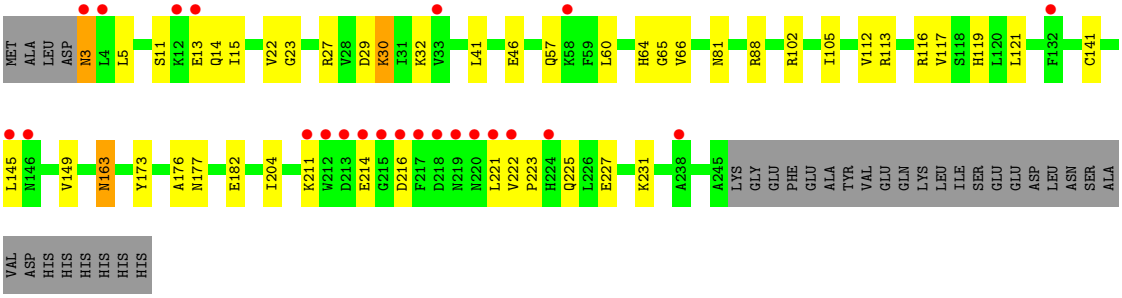
• Molecule 1: Uridine phosphorylase putative

Chain A:



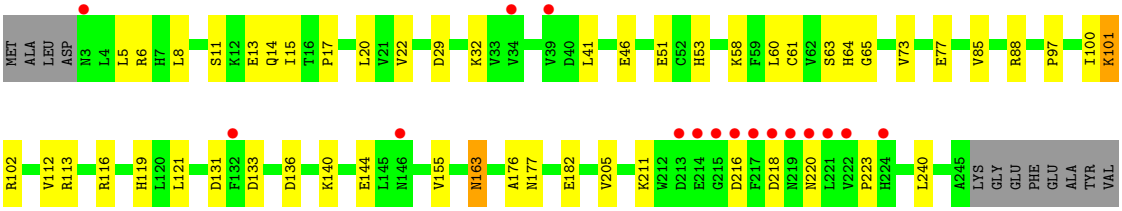
• Molecule 1: Uridine phosphorylase putative

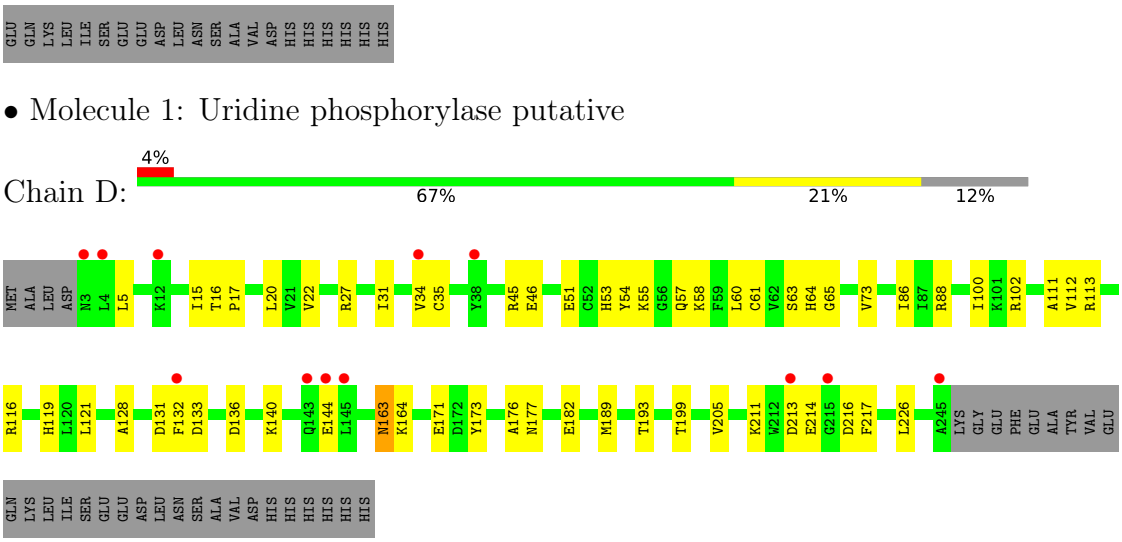
Chain B:

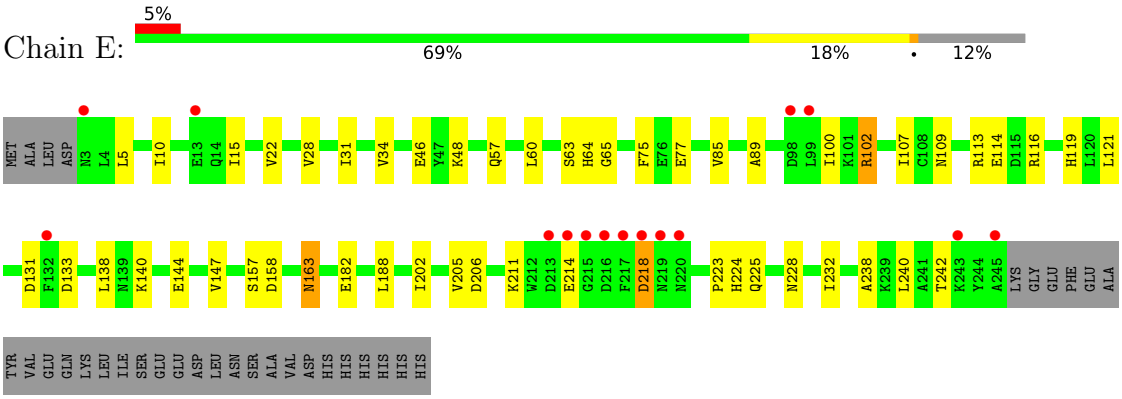


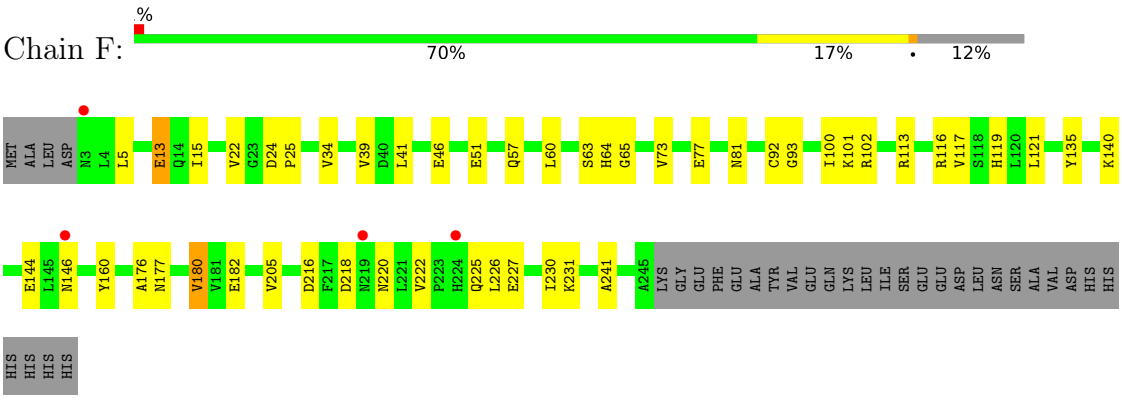
• Molecule 1: Uridine phosphorylase putative

Chain C:




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 D:
4%
67%
21%
12%
MET ALA LEU ASP N3 L4 L5 K12 I15 T16 P17 L20 V21 V22 R27 I31 V34 C35 Y38 R45 E46 E51 C52 H53 Y54 K55 G56 Q57 K58 F59 L60 C61 V62 S63 H64 G65 V73 I86 I87 R88 I100 K101 R102 A111 V112 R113
R116 H119 L120 L121 A128 D131 F132 D133 D136 K140 Q143 E144 L145 N163 K164 E171 D172 Y173 A176 N177 E182 M189 T193 T199 V205 K211 W212 D213 E214 G215 D216 F217 L226 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:
5%
69%
18%
12%
MET ALA LEU ASP N3 L4 L5 I10 E13 Q14 I15 V22 V28 I31 V34 E46 Y47 K48 Q57 L60 S63 H64 G65 F75 E76 E77 V85 A89 D98 L99 I100 K101 R102 I107 C108 N109 R113 E114 D115 R116 H119 L120 L121
D131 F132 D133 L138 N139 K140 E144 V147 S157 D158 N163 E182 L188 I202 V205 D206 K211 W212 D213 E214 G215 D216 F217 D218 N219 N220 P223 H224 Q225 N228 I232 A238 K239 L240 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 F:
%
70%
17%
12%
MET ALA LEU ASP N3 L4 L5 E13 Q14 I15 V22 G23 D24 P25 V34 V39 D40 L41 E46 E51 Q57 L60 S63 H64 G65 V73 E77 N81 C92 G93 I100 K101 R102 R113 R116 V117 S118 H119 L120 L121 Y135 K140
E144 L145 N146 Y160 A176 N177 V180 V181 E182 V205 D216 F217 D218 N219 N220 L221 V222 P223 H224 Q225 L226 E227 I230 K231 A241 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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.44Å 91.73Å 238.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.02 45.87 – 2.02	Depositor EDS
% Data completeness (in resolution range)	88.8 (30.00-2.02) 91.5 (45.87-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.97 (at 2.03Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.242 0.208 , 0.238	Depositor DCC
R_{free} test set	11403 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11789	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.32	0/1893	0.58	0/2561
1	B	0.30	0/1893	0.56	0/2561
1	C	0.31	0/1893	0.57	0/2561
1	D	0.31	0/1893	0.59	0/2561
1	E	0.33	0/1893	0.59	0/2561
1	F	0.33	0/1893	0.59	0/2561
All	All	0.32	0/11358	0.58	0/15366

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1861	0	1882	35	0
1	B	1861	0	1882	38	0
1	C	1861	0	1882	35	0
1	D	1861	0	1882	41	0
1	E	1861	0	1882	38	0
1	F	1861	0	1882	40	0
2	A	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	0	0	0
2	C	15	0	0	0	0
2	D	20	0	0	1	0
2	E	15	0	0	0	0
2	F	20	0	0	0	0
3	A	20	0	17	0	0
3	B	20	0	17	2	0
3	C	20	0	17	1	0
3	D	20	0	17	0	0
3	E	20	0	17	2	0
3	F	20	0	17	1	0
4	A	4	0	8	0	0
4	B	12	0	24	1	0
4	D	8	0	16	1	0
4	E	4	0	8	0	0
4	F	8	0	16	1	0
5	A	56	0	0	2	0
5	B	45	0	0	1	0
5	C	51	0	0	1	0
5	D	61	0	0	3	0
5	E	65	0	0	3	0
5	F	79	0	0	2	0
All	All	11789	0	11466	215	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 9.

All (215) 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:C:5:LEU:HD11	1:C:15:ILE:HD11	1.49	0.94
1:D:163:ASN:HD22	1:D:164:LYS:H	1.20	0.89
1:E:102:ARG:HH11	1:E:102:ARG:HB2	1.37	0.86
1:A:133:ASP:O	1:A:137:THR:HG23	1.76	0.84
1:B:5:LEU:HD11	1:B:15:ILE:HD11	1.61	0.83
1:F:92:CYS:SG	1:F:180:VAL:HG21	2.18	0.82
1:B:11:SER:HB2	1:B:13:GLU:OE2	1.80	0.80
1:B:117:VAL:O	1:B:121:LEU:HD13	1.82	0.79
1:A:5:LEU:HD11	1:A:15:ILE:HD11	1.67	0.77
1:A:46:GLU:HB3	1:B:46:GLU:HB3	1.70	0.74
5:E:828:HOH:O	1:F:117:VAL:HG23	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:GLY:O	1:F:180:VAL:HG22	1.90	0.72
1:D:64:HIS:HD2	1:D:65:GLY:O	1.73	0.71
1:B:141:CYS:O	1:B:145:LEU:HD13	1.92	0.70
1:E:158:ASP:HB3	1:F:117:VAL:HG22	1.73	0.70
1:C:53:HIS:HE1	1:C:58:LYS:HE2	1.56	0.70
1:F:5:LEU:HD11	1:F:15:ILE:HD11	1.72	0.69
1:B:13:GLU:CD	1:B:13:GLU:H	1.94	0.69
1:E:5:LEU:HD11	1:E:15:ILE:HD11	1.75	0.68
1:B:102:ARG:NH2	1:B:216:ASP:HA	2.08	0.67
1:F:140:LYS:O	1:F:144:GLU:HG3	1.93	0.67
1:A:163:ASN:HB3	5:A:691:HOH:O	1.93	0.67
1:B:3:ASN:N	1:B:3:ASN:HD22	1.92	0.66
1:D:31:ILE:O	1:D:34:VAL:HG12	1.95	0.66
1:F:102:ARG:HD2	1:F:216:ASP:OD1	1.94	0.66
1:E:31:ILE:O	1:E:34:VAL:HG22	1.95	0.66
1:E:163:ASN:C	1:E:163:ASN:HD22	1.98	0.66
1:E:46:GLU:HB3	1:F:46:GLU:HB3	1.76	0.66
1:B:11:SER:OG	1:B:14:GLN:HG3	1.95	0.65
1:A:92:CYS:HB2	1:A:180:VAL:HG13	1.77	0.65
1:C:13:GLU:CD	1:C:13:GLU:H	1.98	0.65
1:C:46:GLU:HB3	1:D:46:GLU:HB3	1.79	0.65
1:C:64:HIS:HD2	1:C:65:GLY:O	1.80	0.65
1:F:64:HIS:HD2	1:F:65:GLY:O	1.81	0.64
1:C:218:ASP:HB3	1:C:220:ASN:O	1.99	0.63
1:B:22:VAL:HG11	1:B:27:ARG:HG2	1.79	0.63
1:D:211:LYS:HE3	1:D:216:ASP:OD2	2.00	0.62
1:A:131:ASP:OD1	1:A:133:ASP:HB2	2.00	0.62
1:C:113:ARG:O	1:C:119:HIS:HE1	1.83	0.62
1:F:92:CYS:SG	1:F:180:VAL:CG2	2.88	0.62
1:B:64:HIS:HD2	1:B:65:GLY:O	1.83	0.61
1:B:163:ASN:HD22	1:B:163:ASN:H	1.48	0.61
1:D:163:ASN:ND2	1:D:164:LYS:H	1.95	0.60
1:A:64:HIS:HD2	1:A:65:GLY:O	1.84	0.60
1:F:146:ASN:HB3	5:F:954:HOH:O	2.01	0.60
1:E:102:ARG:HH11	1:E:102:ARG:CB	2.13	0.58
1:C:14:GLN:NE2	1:C:41:LEU:HD22	2.19	0.58
1:C:53:HIS:CE1	1:C:58:LYS:HE2	2.37	0.58
1:B:3:ASN:N	1:B:3:ASN:ND2	2.50	0.58
1:D:15:ILE:HA	1:D:60:LEU:HD11	1.86	0.58
1:B:227:GLU:HG2	1:B:231:LYS:HZ2	1.70	0.57
1:E:140:LYS:O	1:E:144:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:CG1	1:A:181:VAL:N	2.68	0.56
1:A:15:ILE:HA	1:A:60:LEU:HD11	1.86	0.56
1:D:113:ARG:O	1:D:119:HIS:HE1	1.89	0.56
3:E:305:MTI:HS3	1:F:73:VAL:HG21	1.88	0.55
1:D:51:GLU:OE2	1:D:58:LYS:HE3	2.07	0.55
1:E:85:VAL:HG11	1:E:240:LEU:HD13	1.87	0.55
1:D:22:VAL:O	1:D:63:SER:HA	2.07	0.55
1:C:100:ILE:HG22	1:C:205:VAL:HG21	1.88	0.55
1:A:85:VAL:HG11	1:A:240:LEU:HD13	1.88	0.54
1:D:189:MET:O	1:D:193:THR:HG23	2.05	0.54
1:C:116:ARG:HB2	1:D:116:ARG:HB2	1.88	0.54
1:A:116:ARG:HB2	1:B:116:ARG:HB2	1.90	0.54
1:C:85:VAL:HG11	1:C:240:LEU:HD13	1.88	0.54
1:E:64:HIS:HD2	1:E:65:GLY:O	1.90	0.54
1:D:5:LEU:HD11	1:D:15:ILE:HD11	1.88	0.54
1:A:57:GLN:NE2	1:A:57:GLN:HA	2.22	0.54
1:E:206:ASP:O	1:E:218:ASP:HB2	2.07	0.53
1:E:113:ARG:O	1:E:119:HIS:HE1	1.92	0.53
1:C:97:PRO:O	1:C:101:LYS:HE2	2.08	0.53
1:B:22:VAL:HG11	1:B:27:ARG:CG	2.38	0.53
1:E:5:LEU:HD13	1:E:77:GLU:HB3	1.90	0.53
1:D:116:ARG:HE	4:D:509:IPA:H13	1.74	0.53
1:D:213:ASP:OD2	1:D:214:GLU:HG3	2.09	0.53
1:E:163:ASN:C	1:E:163:ASN:ND2	2.62	0.53
1:C:102:ARG:HD2	1:C:218:ASP:OD2	2.09	0.52
1:C:140:LYS:O	1:C:144:GLU:HG3	2.10	0.52
1:B:113:ARG:O	1:B:119:HIS:HE1	1.93	0.52
1:E:211:LYS:HD3	1:E:214:GLU:OE1	2.09	0.52
1:B:163:ASN:H	1:B:163:ASN:ND2	2.07	0.51
1:F:116:ARG:HE	4:F:504:IPA:H13	1.76	0.51
1:A:222:VAL:HB	1:A:225:GLN:HB2	1.93	0.51
1:F:113:ARG:O	1:F:119:HIS:HE1	1.94	0.51
1:E:22:VAL:O	1:E:63:SER:HA	2.11	0.51
1:A:92:CYS:HB2	1:A:180:VAL:CG1	2.40	0.50
1:D:171:GLU:HG2	5:D:786:HOH:O	2.11	0.50
1:A:46:GLU:CB	1:B:46:GLU:HB3	2.41	0.50
1:B:22:VAL:HG12	5:B:780:HOH:O	2.12	0.50
1:A:180:VAL:HG13	1:A:181:VAL:N	2.27	0.49
1:B:105:ILE:HB	1:B:149:VAL:HG12	1.93	0.49
1:C:73:VAL:O	1:C:77:GLU:HG3	2.12	0.49
1:D:57:GLN:NE2	5:D:725:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:ASP:HB3	1:F:220:ASN:O	2.13	0.49
1:A:22:VAL:O	1:A:63:SER:HA	2.13	0.49
1:A:35:CYS:HB3	1:A:53:HIS:O	2.13	0.48
1:A:102:ARG:HD2	1:A:216:ASP:OD1	2.12	0.48
1:B:102:ARG:HH21	1:B:216:ASP:HA	1.75	0.48
1:D:140:LYS:O	1:D:144:GLU:HG3	2.13	0.48
1:F:5:LEU:HD22	1:F:81:ASN:ND2	2.28	0.48
1:C:176:ALA:O	1:C:177:ASN:HB2	2.13	0.48
1:E:116:ARG:HB2	1:F:116:ARG:HB2	1.94	0.48
1:E:158:ASP:HB3	1:F:117:VAL:CG2	2.43	0.48
1:B:211:LYS:HG2	1:B:214:GLU:OE1	2.13	0.48
1:A:25:PRO:HA	1:A:63:SER:HB3	1.95	0.48
1:B:227:GLU:HG2	1:B:231:LYS:NZ	2.29	0.48
1:D:136:ASP:OD2	1:D:140:LYS:HE3	2.14	0.48
1:F:93:GLY:O	1:F:180:VAL:CG2	2.61	0.47
1:F:100:ILE:HG22	1:F:205:VAL:HG21	1.97	0.47
1:B:14:GLN:NE2	1:B:41:LEU:HD22	2.30	0.47
1:B:222:VAL:HB	1:B:225:GLN:HB2	1.96	0.47
1:D:64:HIS:CD2	1:D:65:GLY:O	2.61	0.47
1:D:102:ARG:HD3	2:D:412:SO4:O3	2.14	0.47
1:F:34:VAL:HG12	1:F:34:VAL:O	2.14	0.47
1:D:34:VAL:HG22	1:D:34:VAL:O	2.14	0.47
1:D:176:ALA:O	1:D:177:ASN:HB2	2.15	0.47
1:A:132:PHE:CG	1:F:135:TYR:HE2	2.32	0.47
1:C:29:ASP:HA	1:C:32:LYS:HE2	1.97	0.47
1:E:100:ILE:HG22	1:E:205:VAL:HG21	1.97	0.47
1:E:131:ASP:OD1	1:E:133:ASP:HB2	2.14	0.47
1:A:113:ARG:O	1:A:119:HIS:HE1	1.97	0.47
1:B:112:VAL:HG11	1:B:173:TYR:CZ	2.50	0.47
1:D:16:THR:HB	1:D:17:PRO:HD2	1.97	0.47
1:C:51:GLU:HA	1:C:60:LEU:HD23	1.97	0.47
1:D:54:TYR:CE2	1:D:55:LYS:HE2	2.50	0.46
1:D:132:PHE:CE1	1:E:109:ASN:HB2	2.50	0.46
1:C:64:HIS:HE1	1:C:88:ARG:HH11	1.63	0.46
1:B:176:ALA:O	1:B:177:ASN:HB2	2.15	0.46
1:C:136:ASP:OD2	1:C:140:LYS:HE3	2.15	0.46
1:A:139:ASN:O	1:A:143:GLN:HG3	2.16	0.46
1:B:14:GLN:O	1:B:60:LEU:HD11	2.16	0.46
1:D:102:ARG:HD2	1:D:216:ASP:OD1	2.14	0.46
1:B:5:LEU:HD22	1:B:81:ASN:ND2	2.31	0.46
1:E:107:ILE:HD13	1:E:138:LEU:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:VAL:O	1:C:63:SER:HA	2.15	0.46
1:F:176:ALA:O	1:F:177:ASN:HB2	2.16	0.46
1:E:57:GLN:OE1	1:E:242:THR:HG22	2.15	0.46
1:E:224:HIS:CE1	1:E:228:ASN:HD21	2.33	0.46
1:F:22:VAL:O	1:F:63:SER:HA	2.15	0.45
1:C:5:LEU:HD13	1:C:77:GLU:HB3	1.99	0.45
1:C:101:LYS:HD2	1:C:101:LYS:N	2.31	0.45
1:D:100:ILE:HG22	1:D:205:VAL:HG21	1.98	0.45
1:E:46:GLU:HB3	1:F:46:GLU:CB	2.43	0.45
1:F:5:LEU:HD13	1:F:77:GLU:HB3	1.98	0.45
3:C:303:MTI:HS3	1:D:73:VAL:HG21	1.98	0.45
1:D:64:HIS:HE1	1:D:88:ARG:HH11	1.63	0.45
1:E:238:ALA:O	1:E:242:THR:HG23	2.16	0.45
1:E:211:LYS:HB3	1:E:214:GLU:HG2	1.99	0.45
1:A:132:PHE:CZ	1:A:133:ASP:OD2	2.71	0.44
1:A:57:GLN:HA	1:A:57:GLN:HE21	1.82	0.44
1:C:11:SER:HB2	1:C:13:GLU:OE2	2.18	0.44
1:C:6:ARG:HD3	1:D:217:PHE:CZ	2.52	0.44
1:D:51:GLU:CD	1:D:58:LYS:HE3	2.37	0.44
1:F:13:GLU:CD	1:F:13:GLU:H	2.20	0.44
1:A:92:CYS:SG	1:A:180:VAL:HG11	2.58	0.44
1:C:163:ASN:ND2	1:C:163:ASN:H	2.16	0.44
1:D:20:LEU:O	1:D:61:CYS:HA	2.18	0.44
1:E:114:GLU:HB3	1:E:157:SER:HA	2.00	0.44
1:C:20:LEU:O	1:C:61:CYS:HA	2.18	0.43
1:F:227:GLU:HG2	1:F:231:LYS:HE3	1.99	0.43
1:F:51:GLU:HA	1:F:60:LEU:HD23	1.99	0.43
1:F:64:HIS:CD2	1:F:65:GLY:O	2.67	0.43
1:D:45:ARG:HB3	1:D:46:GLU:OE2	2.18	0.43
1:D:86:ILE:O	1:D:199:THR:HA	2.19	0.43
1:E:46:GLU:CB	1:F:46:GLU:HB3	2.46	0.43
1:A:5:LEU:HG	1:A:10:ILE:O	2.19	0.43
1:B:22:VAL:HG12	1:B:23:GLY:N	2.34	0.43
1:B:116:ARG:HE	4:B:501:IPA:H13	1.84	0.43
1:A:140:LYS:O	1:A:143:GLN:HB2	2.19	0.43
1:D:112:VAL:HG11	1:D:173:TYR:CZ	2.54	0.43
1:E:228:ASN:O	1:E:232:ILE:HG13	2.18	0.43
1:E:15:ILE:HA	1:E:60:LEU:HD11	2.00	0.43
3:E:305:MTI:H3	5:E:884:HOH:O	2.18	0.43
1:D:35:CYS:HB3	1:D:53:HIS:O	2.19	0.43
1:F:57:GLN:HG3	1:F:241:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ASP:OD1	1:D:133:ASP:HB2	2.19	0.42
1:A:176:ALA:O	1:A:177:ASN:HB2	2.19	0.42
1:E:89:ALA:HA	1:E:202:ILE:O	2.18	0.42
1:E:119:HIS:HD2	5:E:833:HOH:O	2.01	0.42
1:B:64:HIS:HE1	1:B:88:ARG:HH11	1.68	0.42
1:E:28:VAL:HG21	1:E:48:LYS:HG2	2.01	0.42
1:E:75:PHE:CE1	1:E:188:LEU:HB2	2.54	0.42
1:F:160:TYR:CD1	3:F:306:MTI:HS1	2.54	0.42
1:A:75:PHE:CE1	1:A:188:LEU:HB2	2.54	0.42
1:C:211:LYS:HE3	1:C:216:ASP:OD2	2.19	0.42
1:F:41:LEU:HD11	1:F:51:GLU:HB2	2.01	0.41
1:E:147:VAL:HG11	1:E:232:ILE:HD11	2.01	0.41
1:A:101:LYS:HB3	2:A:413:SO4:O3	2.21	0.41
1:C:8:LEU:HG	1:C:77:GLU:OE1	2.20	0.41
1:F:24:ASP:HA	1:F:25:PRO:HD2	1.96	0.41
1:A:195:ARG:O	1:A:196:LYS:HB2	2.20	0.41
1:C:100:ILE:CG2	1:C:205:VAL:HG21	2.50	0.41
1:A:34:VAL:O	1:A:34:VAL:HG12	2.21	0.41
1:A:132:PHE:CG	1:A:133:ASP:N	2.88	0.41
1:C:64:HIS:CE1	1:C:88:ARG:HH11	2.38	0.41
1:F:119:HIS:HD2	5:F:836:HOH:O	2.04	0.41
1:B:30:LYS:NZ	1:B:30:LYS:HB3	2.36	0.41
1:E:225:GLN:HA	1:E:225:GLN:OE1	2.20	0.41
1:A:119:HIS:HD2	5:A:834:HOH:O	2.02	0.41
3:B:302:MTI:N3	3:B:302:MTI:H1	2.36	0.41
1:C:17:PRO:HG2	5:C:667:HOH:O	2.21	0.41
1:D:193:THR:HG21	5:D:649:HOH:O	2.21	0.41
1:E:5:LEU:HG	1:E:10:ILE:O	2.21	0.41
1:F:57:GLN:CG	1:F:241:ALA:HB3	2.50	0.41
1:B:23:GLY:HA2	1:B:64:HIS:CD2	2.56	0.40
1:B:66:VAL:HG11	3:B:302:MTI:HS3	2.03	0.40
1:B:204:ILE:HG21	1:B:221:LEU:HD13	2.04	0.40
1:C:112:VAL:HB	1:C:155:VAL:HA	2.03	0.40
1:C:131:ASP:OD1	1:C:133:ASP:HB2	2.21	0.40
1:F:226:LEU:O	1:F:230:ILE:HG13	2.21	0.40
1:F:222:VAL:HB	1:F:225:GLN:HB2	2.03	0.40
1:F:39:VAL:O	1:F:41:LEU:HD12	2.21	0.40
1:B:29:ASP:O	1:B:32:LYS:HG2	2.21	0.40
1:D:27:ARG:NH1	1:D:226:LEU:HD21	2.37	0.40
1:D:111:ALA:O	1:D:128:ALA:HB3	2.22	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%)	231 (96%)	10 (4%)	0	100	100
1	B	241/276 (87%)	234 (97%)	6 (2%)	1 (0%)	34	28
1	C	241/276 (87%)	228 (95%)	12 (5%)	1 (0%)	34	28
1	D	241/276 (87%)	230 (95%)	11 (5%)	0	100	100
1	E	241/276 (87%)	234 (97%)	6 (2%)	1 (0%)	34	28
1	F	241/276 (87%)	233 (97%)	8 (3%)	0	100	100
All	All	1446/1656 (87%)	1390 (96%)	53 (4%)	3 (0%)	47	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	223	PRO
1	E	223	PRO
1	C	223	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/235 (88%)	203 (98%)	3 (2%)	65	68
1	B	206/235 (88%)	201 (98%)	5 (2%)	49	49
1	C	206/235 (88%)	202 (98%)	4 (2%)	57	59
1	D	206/235 (88%)	203 (98%)	3 (2%)	65	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	206/235 (88%)	201 (98%)	5 (2%)	49	49
1	F	206/235 (88%)	201 (98%)	5 (2%)	49	49
All	All	1236/1410 (88%)	1211 (98%)	25 (2%)	55	57

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LEU
1	A	132	PHE
1	A	182	GLU
1	B	3	ASN
1	B	30	LYS
1	B	57	GLN
1	B	163	ASN
1	B	182	GLU
1	C	101	LYS
1	C	121	LEU
1	C	163	ASN
1	C	182	GLU
1	D	121	LEU
1	D	163	ASN
1	D	182	GLU
1	E	102	ARG
1	E	121	LEU
1	E	163	ASN
1	E	182	GLU
1	E	218	ASP
1	F	13	GLU
1	F	101	LYS
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 (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	64	HIS
1	A	80	GLN
1	A	119	HIS

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Mol	Chain	Res	Type
1	A	151	ASN
1	B	64	HIS
1	B	119	HIS
1	B	139	ASN
1	C	44	ASN
1	C	53	HIS
1	C	57	GLN
1	C	64	HIS
1	C	119	HIS
1	C	228	ASN
1	D	44	ASN
1	D	57	GLN
1	D	64	HIS
1	D	119	HIS
1	D	151	ASN
1	D	163	ASN
1	E	44	ASN
1	E	53	HIS
1	E	64	HIS
1	E	119	HIS
1	E	163	ASN
1	E	228	ASN
1	F	53	HIS
1	F	64	HIS
1	F	119	HIS
1	F	151	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

37 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	B	417	-	4,4,4	1.86	2 (50%)	6,6,6	0.90	0
2	SO4	D	404	-	4,4,4	1.86	2 (50%)	6,6,6	0.87	0
3	MTI	A	301	-	20,22,22	2.55	8 (40%)	14,32,32	2.16	3 (21%)
3	MTI	E	305	-	20,22,22	2.51	9 (45%)	14,32,32	2.18	3 (21%)
3	MTI	D	304	-	20,22,22	2.53	10 (50%)	14,32,32	2.20	3 (21%)
4	IPA	B	508	-	3,3,3	0.37	0	3,3,3	0.37	0
3	MTI	F	306	-	20,22,22	2.47	8 (40%)	14,32,32	2.21	3 (21%)
2	SO4	A	414	-	4,4,4	1.87	2 (50%)	6,6,6	0.82	0
2	SO4	E	415	-	4,4,4	1.82	2 (50%)	6,6,6	0.90	0
4	IPA	B	502	-	3,3,3	0.34	0	3,3,3	0.36	0
2	SO4	F	419	-	4,4,4	1.89	2 (50%)	6,6,6	0.92	0
2	SO4	C	403	-	4,4,4	1.84	2 (50%)	6,6,6	0.83	0
4	IPA	F	505	-	3,3,3	0.33	0	3,3,3	0.36	0
2	SO4	C	416	-	4,4,4	1.87	1 (25%)	6,6,6	0.86	0
2	SO4	B	402	-	4,4,4	1.82	2 (50%)	6,6,6	0.90	0
4	IPA	B	501	-	3,3,3	0.31	0	3,3,3	0.36	0
2	SO4	A	401	-	4,4,4	1.84	2 (50%)	6,6,6	0.87	0
3	MTI	C	303	-	20,22,22	2.54	9 (45%)	14,32,32	2.24	3 (21%)
2	SO4	D	412	-	4,4,4	1.86	2 (50%)	6,6,6	0.91	0
2	SO4	A	413	-	4,4,4	1.88	2 (50%)	6,6,6	0.90	0
2	SO4	F	411	-	4,4,4	1.80	2 (50%)	6,6,6	0.91	0
2	SO4	B	407	-	4,4,4	1.85	1 (25%)	6,6,6	0.94	0
2	SO4	D	421	-	4,4,4	1.91	2 (50%)	6,6,6	0.91	0
4	IPA	E	506	-	3,3,3	0.25	0	3,3,3	0.33	0
3	MTI	B	302	-	20,22,22	2.59	9 (45%)	14,32,32	2.19	3 (21%)
4	IPA	D	507	-	3,3,3	0.30	0	3,3,3	0.35	0
4	IPA	D	509	-	3,3,3	0.32	0	3,3,3	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	IPA	F	504	-	3,3,3	0.30	0	3,3,3	0.33	0
2	SO4	D	408	-	4,4,4	1.80	1 (25%)	6,6,6	0.85	0
2	SO4	F	409	-	4,4,4	1.85	2 (50%)	6,6,6	0.89	0
2	SO4	A	418	-	4,4,4	1.90	2 (50%)	6,6,6	0.90	0
2	SO4	C	422	-	4,4,4	1.88	2 (50%)	6,6,6	0.90	0
2	SO4	F	406	-	4,4,4	1.82	2 (50%)	6,6,6	0.82	0
2	SO4	E	405	-	4,4,4	1.86	2 (50%)	6,6,6	0.87	0
2	SO4	B	410	-	4,4,4	1.88	2 (50%)	6,6,6	0.90	0
4	IPA	A	503	-	3,3,3	0.33	0	3,3,3	0.38	0
2	SO4	E	420	-	4,4,4	1.89	2 (50%)	6,6,6	0.91	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	MTI	C	303	-	-	2/3/23/23	0/3/3/3
3	MTI	A	301	-	-	1/3/23/23	0/3/3/3
3	MTI	E	305	-	-	2/3/23/23	0/3/3/3
3	MTI	D	304	-	-	0/3/23/23	0/3/3/3
3	MTI	B	302	-	-	2/3/23/23	0/3/3/3
3	MTI	F	306	-	-	2/3/23/23	0/3/3/3

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	MTI	C6-N1	6.16	1.43	1.33
3	A	301	MTI	C6-N1	6.14	1.43	1.33
3	C	303	MTI	C6-N1	6.11	1.43	1.33
3	D	304	MTI	C6-N1	6.07	1.43	1.33
3	F	306	MTI	C6-N1	5.86	1.43	1.33
3	E	305	MTI	C6-N1	5.81	1.43	1.33
3	C	303	MTI	C2-N3	4.42	1.39	1.32
3	F	306	MTI	C2-N3	4.33	1.39	1.32
3	C	303	MTI	C4-N3	4.32	1.42	1.37
3	E	305	MTI	C2-N3	4.32	1.39	1.32
3	D	304	MTI	C4-N3	4.29	1.42	1.37
3	F	306	MTI	C2-N1	4.29	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	MTI	C2-N3	4.29	1.39	1.32
3	B	302	MTI	C2-N1	4.29	1.41	1.33
3	E	305	MTI	C2-N1	4.25	1.41	1.33
3	D	304	MTI	C2-N1	4.23	1.41	1.33
3	F	306	MTI	C4-N3	4.20	1.42	1.37
3	C	303	MTI	C2-N1	4.17	1.41	1.33
3	D	304	MTI	C2-N3	4.17	1.38	1.32
3	B	302	MTI	C2-N3	4.16	1.38	1.32
3	A	301	MTI	C4-N3	4.13	1.42	1.37
3	B	302	MTI	C4-N3	4.08	1.42	1.37
3	A	301	MTI	C2-N1	4.05	1.41	1.33
3	E	305	MTI	C4-N3	3.57	1.41	1.37
2	D	421	SO4	O1-S	3.20	1.63	1.46
2	A	418	SO4	O1-S	3.19	1.63	1.46
2	C	416	SO4	O1-S	3.17	1.63	1.46
2	E	420	SO4	O1-S	3.17	1.63	1.46
2	F	419	SO4	O1-S	3.16	1.63	1.46
2	A	413	SO4	O1-S	3.15	1.63	1.46
2	B	407	SO4	O1-S	3.15	1.63	1.46
2	B	410	SO4	O1-S	3.13	1.63	1.46
2	A	414	SO4	O1-S	3.11	1.62	1.46
2	C	422	SO4	O1-S	3.10	1.62	1.46
2	E	405	SO4	O1-S	3.10	1.62	1.46
2	B	417	SO4	O1-S	3.09	1.62	1.46
2	F	409	SO4	O1-S	3.09	1.62	1.46
2	D	404	SO4	O1-S	3.08	1.62	1.46
2	D	412	SO4	O1-S	3.07	1.62	1.46
2	D	408	SO4	O1-S	3.05	1.62	1.46
3	E	305	MTI	C5-C6	3.05	1.46	1.41
2	A	401	SO4	O1-S	3.04	1.62	1.46
2	C	403	SO4	O1-S	3.03	1.62	1.46
3	B	302	MTI	C5-C6	3.02	1.46	1.41
2	E	415	SO4	O1-S	3.01	1.62	1.46
2	F	406	SO4	O1-S	2.99	1.62	1.46
2	B	402	SO4	O1-S	2.97	1.62	1.46
3	B	302	MTI	O3'-C3'	2.95	1.49	1.43
2	F	411	SO4	O1-S	2.93	1.61	1.46
3	E	305	MTI	O3'-C3'	2.86	1.49	1.43
3	A	301	MTI	O3'-C3'	2.71	1.49	1.43
3	B	302	MTI	C3'-C2'	2.65	1.60	1.53
3	A	301	MTI	C8-N7	-2.63	1.31	1.36
3	C	303	MTI	O3'-C3'	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	305	MTI	C3'-C2'	2.60	1.60	1.53
3	D	304	MTI	O3'-C3'	2.58	1.49	1.43
3	A	301	MTI	C5-C6	2.55	1.45	1.41
3	C	303	MTI	C5-C6	2.55	1.45	1.41
3	A	301	MTI	C3'-C2'	2.54	1.60	1.53
3	F	306	MTI	C5-C6	2.52	1.45	1.41
3	C	303	MTI	C8-N7	-2.48	1.31	1.36
3	D	304	MTI	C3'-C2'	2.47	1.60	1.53
3	D	304	MTI	C8-N7	-2.45	1.31	1.36
3	F	306	MTI	C3'-C2'	2.40	1.59	1.53
3	C	303	MTI	C3'-C2'	2.35	1.59	1.53
3	B	302	MTI	C8-N7	-2.31	1.31	1.36
3	E	305	MTI	C8-N7	-2.30	1.31	1.36
3	D	304	MTI	C5-C6	2.21	1.45	1.41
3	F	306	MTI	C8-N7	-2.21	1.32	1.36
3	F	306	MTI	O3'-C3'	2.19	1.48	1.43
3	B	302	MTI	C2'-C1'	2.17	1.57	1.54
2	D	412	SO4	O3-S	-2.08	1.30	1.47
2	B	402	SO4	O3-S	-2.08	1.30	1.47
2	A	414	SO4	O3-S	-2.07	1.30	1.47
2	C	422	SO4	O3-S	-2.06	1.31	1.47
2	F	411	SO4	O3-S	-2.06	1.31	1.47
2	D	404	SO4	O3-S	-2.06	1.31	1.47
2	D	421	SO4	O3-S	-2.05	1.31	1.47
2	A	401	SO4	O3-S	-2.05	1.31	1.47
2	C	403	SO4	O3-S	-2.04	1.31	1.47
2	B	417	SO4	O3-S	-2.04	1.31	1.47
2	B	410	SO4	O3-S	-2.04	1.31	1.47
2	F	419	SO4	O3-S	-2.03	1.31	1.47
2	E	420	SO4	O3-S	-2.03	1.31	1.47
3	D	304	MTI	C2'-C1'	2.03	1.57	1.54
2	F	406	SO4	O3-S	-2.03	1.31	1.47
2	A	418	SO4	O3-S	-2.03	1.31	1.47
2	E	415	SO4	O3-S	-2.01	1.31	1.47
3	D	304	MTI	O2'-C2'	2.01	1.47	1.43
2	A	413	SO4	O3-S	-2.01	1.31	1.47
2	F	409	SO4	O3-S	-2.01	1.31	1.47
2	E	405	SO4	O3-S	-2.01	1.31	1.47
3	E	305	MTI	O2'-C2'	2.01	1.47	1.43
3	C	303	MTI	O2'-C2'	2.00	1.47	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	303	MTI	C2-N1-C6	5.26	124.69	115.88
3	F	306	MTI	C2-N1-C6	5.15	124.50	115.88
3	D	304	MTI	C2-N1-C6	5.10	124.42	115.88
3	B	302	MTI	C2-N1-C6	5.09	124.40	115.88
3	E	305	MTI	C2-N1-C6	5.03	124.30	115.88
3	A	301	MTI	C2-N1-C6	5.00	124.25	115.88
3	C	303	MTI	N3-C2-N1	-4.66	121.40	128.68
3	D	304	MTI	N3-C2-N1	-4.61	121.47	128.68
3	F	306	MTI	N3-C2-N1	-4.58	121.53	128.68
3	B	302	MTI	N3-C2-N1	-4.55	121.56	128.68
3	A	301	MTI	N3-C2-N1	-4.47	121.69	128.68
3	E	305	MTI	N3-C2-N1	-4.42	121.78	128.68
3	A	301	MTI	C9-C8-N7	3.58	115.62	108.79
3	C	303	MTI	C9-C8-N7	3.58	115.62	108.79
3	E	305	MTI	C9-C8-N7	3.53	115.52	108.79
3	F	306	MTI	C9-C8-N7	3.50	115.48	108.79
3	D	304	MTI	C9-C8-N7	3.50	115.48	108.79
3	B	302	MTI	C9-C8-N7	3.42	115.31	108.79

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	MTI	C4'-C5'-S5'-CS
3	C	303	MTI	C4'-C5'-S5'-CS
3	C	303	MTI	C3'-C4'-C5'-S5'
3	E	305	MTI	C4'-C5'-S5'-CS
3	E	305	MTI	C3'-C4'-C5'-S5'
3	F	306	MTI	C4'-C5'-S5'-CS
3	A	301	MTI	C4'-C5'-S5'-CS
3	B	302	MTI	C3'-C4'-C5'-S5'
3	F	306	MTI	C3'-C4'-C5'-S5'

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	305	MTI	2	0
3	F	306	MTI	1	0
4	B	501	IPA	1	0
3	C	303	MTI	1	0
2	D	412	SO4	1	0

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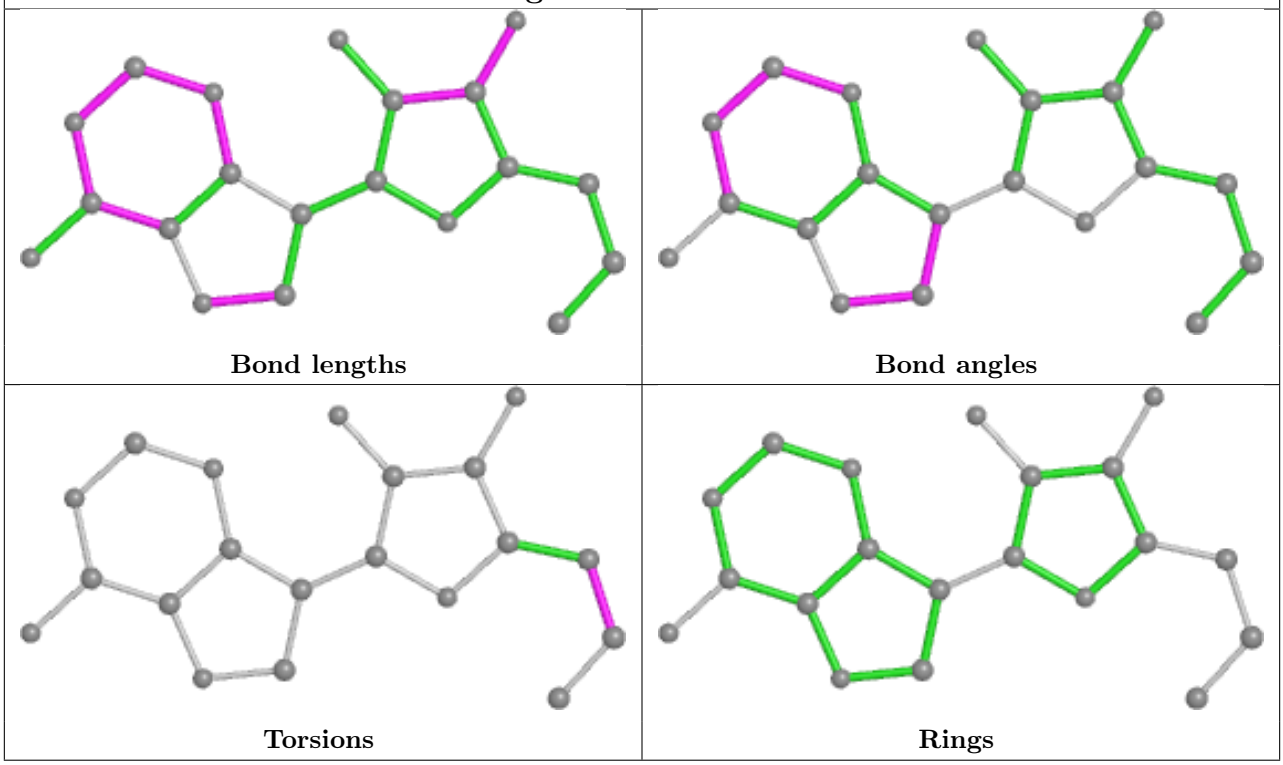
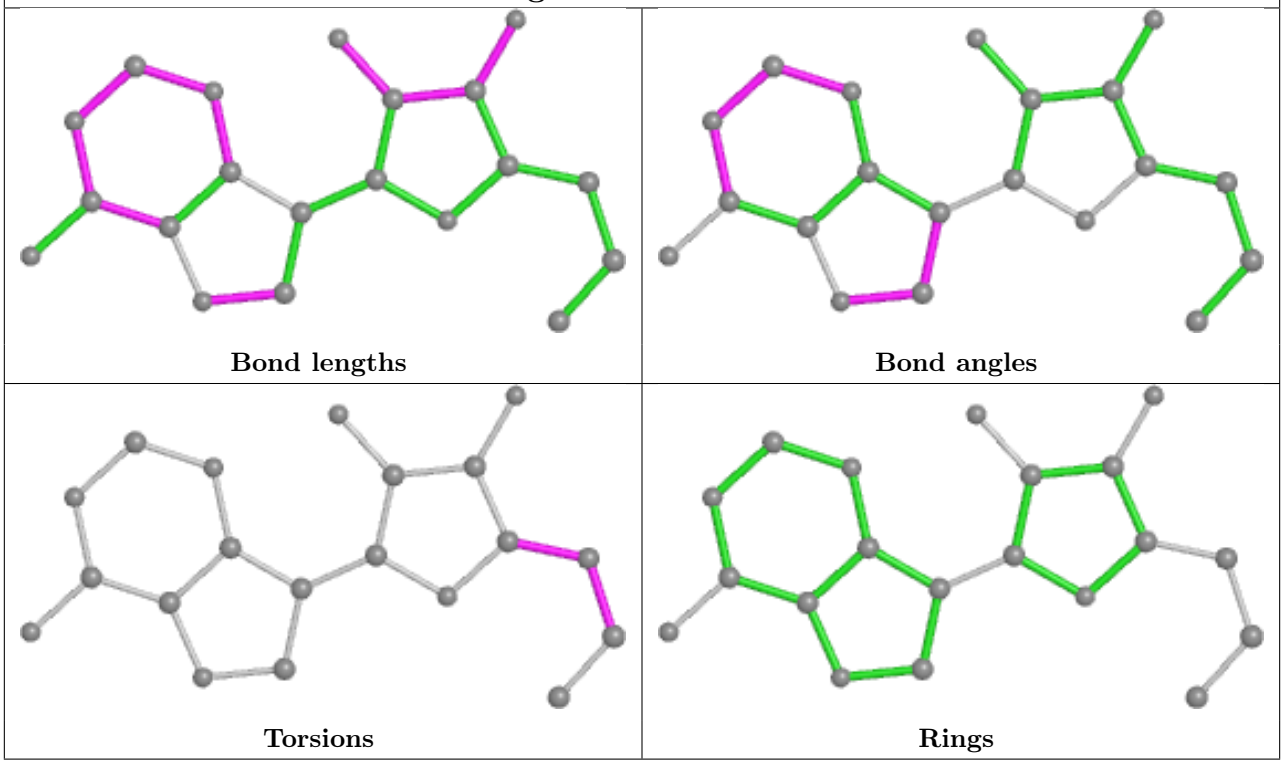
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	413	SO4	1	0
3	B	302	MTI	2	0
4	D	509	IPA	1	0
4	F	504	IPA	1	0

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 then 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.

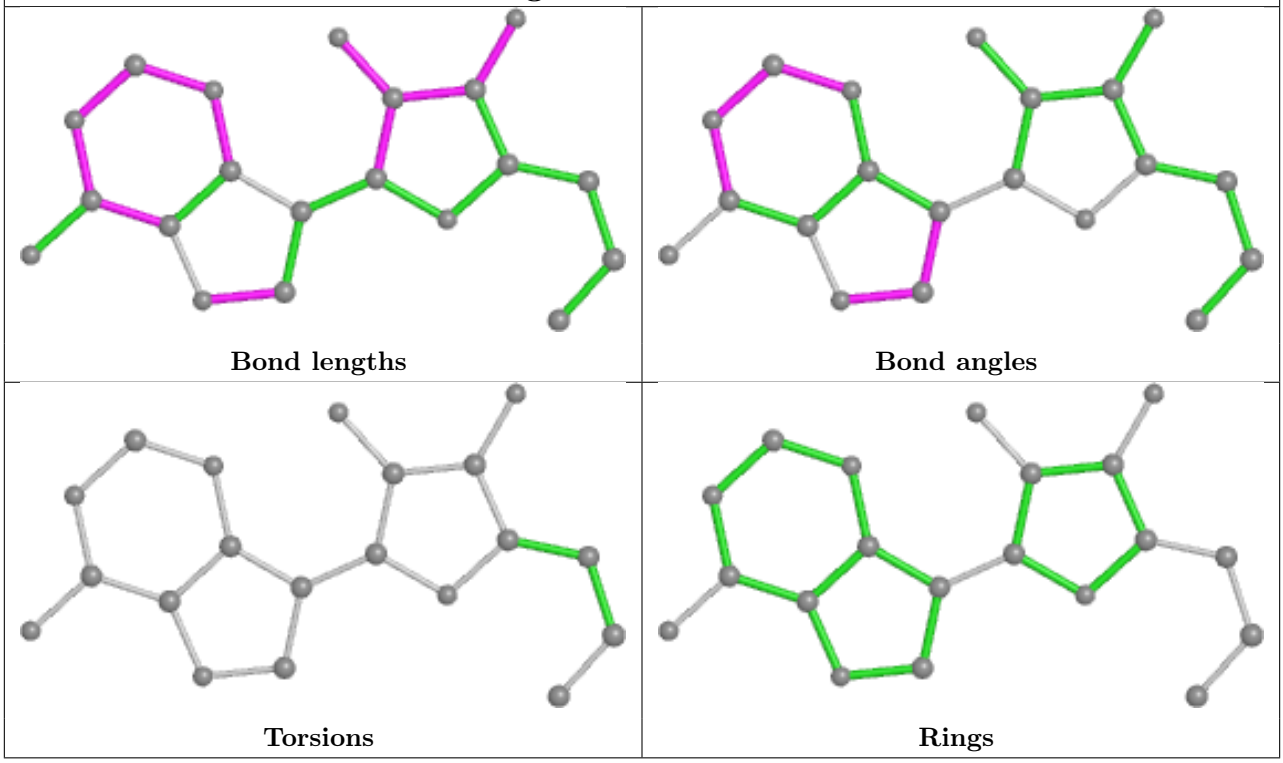
Ligand MTI A 301



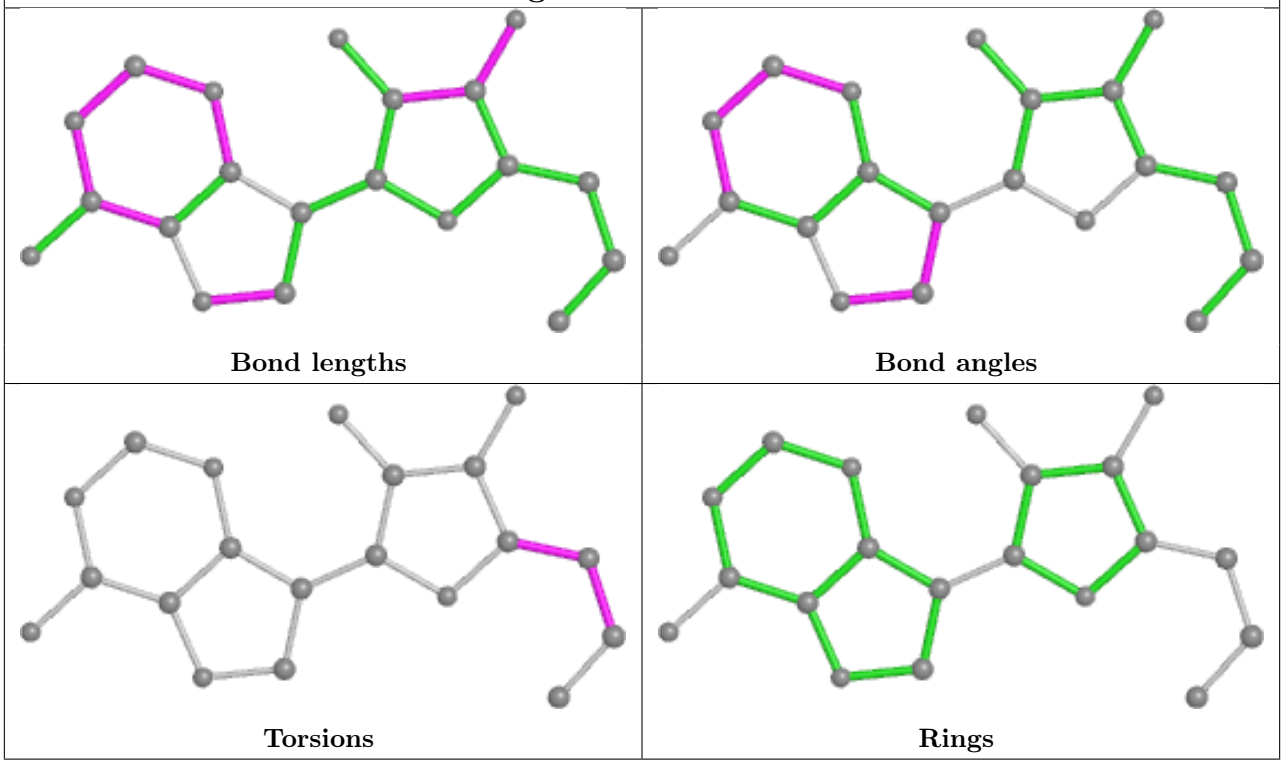
Ligand MTI E 305



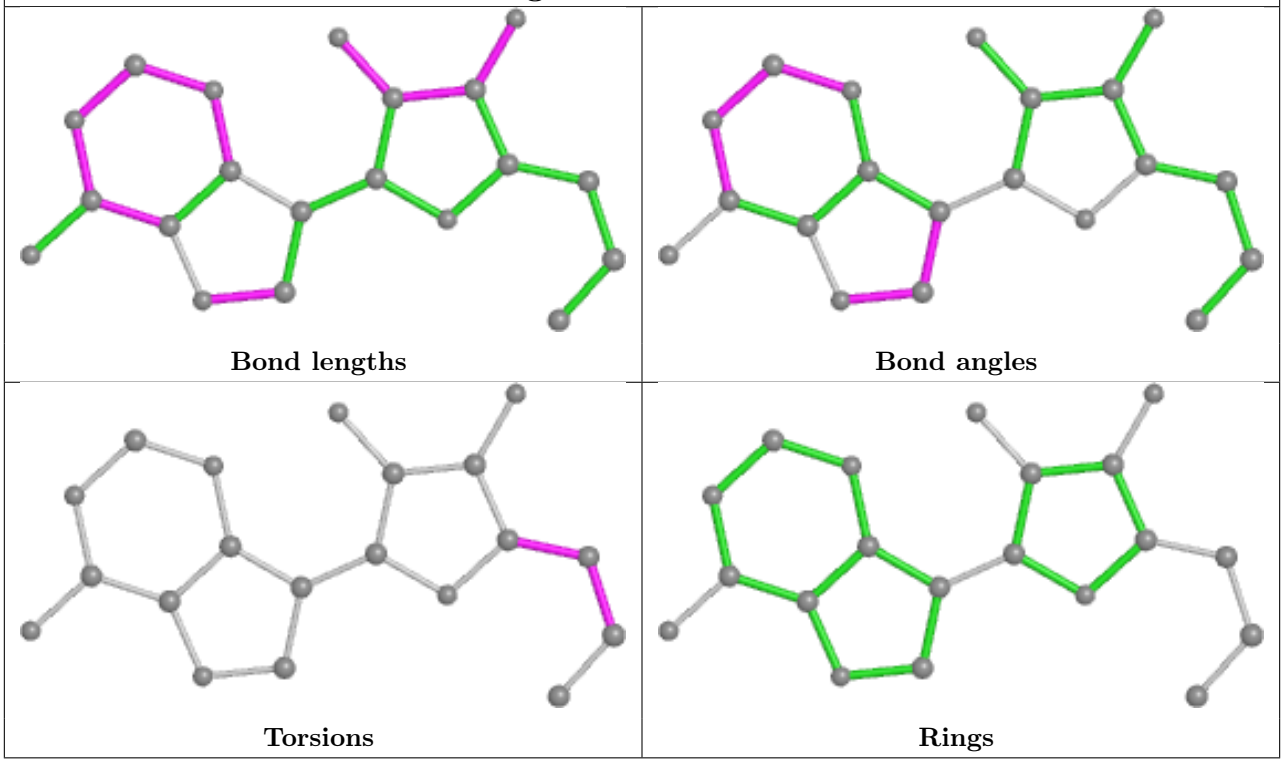
Ligand MTI D 304



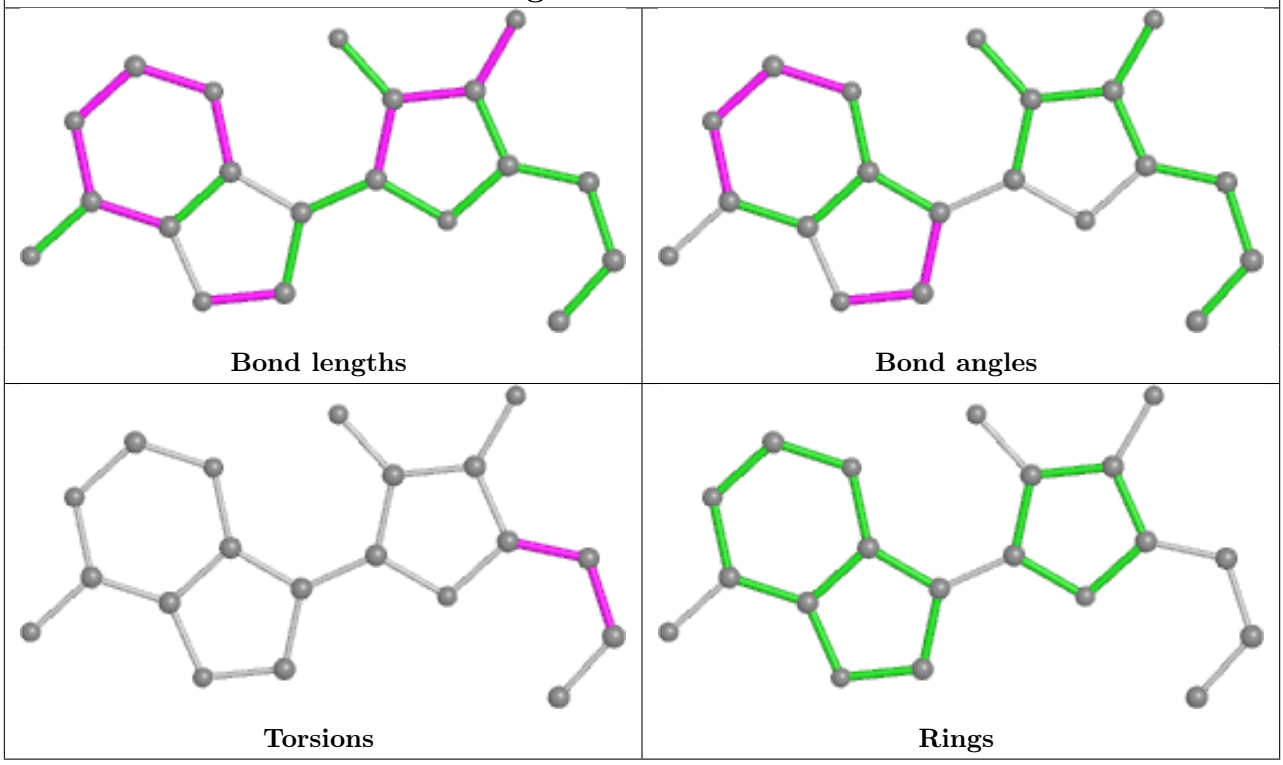
Ligand MTI F 306



Ligand MTI C 303



Ligand MTI B 302



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, 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%)	0.21	10 (4%)	37	37	14, 29, 47, 57	0
1	B	243/276 (88%)	0.56	23 (9%)	8	8	14, 33, 51, 62	0
1	C	243/276 (88%)	0.46	16 (6%)	18	17	12, 29, 48, 62	0
1	D	243/276 (88%)	0.36	12 (4%)	29	29	11, 28, 47, 58	0
1	E	243/276 (88%)	0.20	15 (6%)	20	19	10, 24, 45, 63	0
1	F	243/276 (88%)	0.19	4 (1%)	72	71	11, 24, 41, 51	0
All	All	1458/1656 (88%)	0.33	80 (5%)	25	24	10, 27, 48, 63	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ASN	5.3
1	C	3	ASN	5.3
1	A	132	PHE	5.1
1	E	213	ASP	5.0
1	C	219	ASN	4.9
1	C	215	GLY	4.8
1	E	219	ASN	4.7
1	E	3	ASN	4.4
1	D	3	ASN	4.3
1	B	214	GLU	4.3
1	C	217	PHE	4.3
1	C	221	LEU	4.3
1	A	3	ASN	4.2
1	B	132	PHE	4.0
1	E	217	PHE	4.0
1	F	3	ASN	4.0
1	D	4	LEU	4.0
1	B	219	ASN	3.9
1	C	218	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	218	ASP	3.9
1	B	220	ASN	3.8
1	B	215	GLY	3.7
1	B	146	ASN	3.7
1	B	222	VAL	3.7
1	C	220	ASN	3.5
1	D	245	ALA	3.5
1	B	213	ASP	3.5
1	B	217	PHE	3.4
1	B	221	LEU	3.4
1	B	216	ASP	3.4
1	C	214	GLU	3.4
1	E	216	ASP	3.3
1	B	212	TRP	3.3
1	C	222	VAL	3.2
1	A	4	LEU	3.2
1	B	224	HIS	3.2
1	A	213	ASP	3.2
1	C	34	VAL	3.2
1	D	34	VAL	3.2
1	E	214	GLU	3.1
1	D	213	ASP	3.0
1	A	215	GLY	3.0
1	A	146	ASN	2.9
1	F	219	ASN	2.8
1	C	146	ASN	2.8
1	F	146	ASN	2.8
1	A	13	GLU	2.8
1	C	213	ASP	2.7
1	E	99	LEU	2.7
1	A	15	ILE	2.7
1	B	58	LYS	2.7
1	B	4	LEU	2.6
1	C	39	VAL	2.5
1	E	243	LYS	2.5
1	E	245	ALA	2.5
1	C	224	HIS	2.4
1	B	13	GLU	2.4
1	E	218	ASP	2.4
1	A	218	ASP	2.4
1	B	145	LEU	2.4
1	B	33	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	211	LYS	2.3
1	B	12	LYS	2.3
1	C	132	PHE	2.3
1	D	145	LEU	2.3
1	A	39	VAL	2.3
1	D	12	LYS	2.2
1	D	144	GLU	2.2
1	C	216	ASP	2.2
1	F	224	HIS	2.2
1	E	215	GLY	2.2
1	D	132	PHE	2.1
1	D	38	TYR	2.1
1	D	215	GLY	2.1
1	E	98	ASP	2.1
1	E	220	ASN	2.0
1	E	132	PHE	2.0
1	E	13	GLU	2.0
1	B	238	ALA	2.0
1	D	143	GLN	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 monosaccharides 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	B	501	4/4	0.49	0.30	29,30,30,31	0
4	IPA	D	509	4/4	0.62	0.27	24,24,24,27	0
4	IPA	F	505	4/4	0.66	0.28	24,26,27,28	0
4	IPA	B	508	4/4	0.73	0.23	24,24,25,26	0

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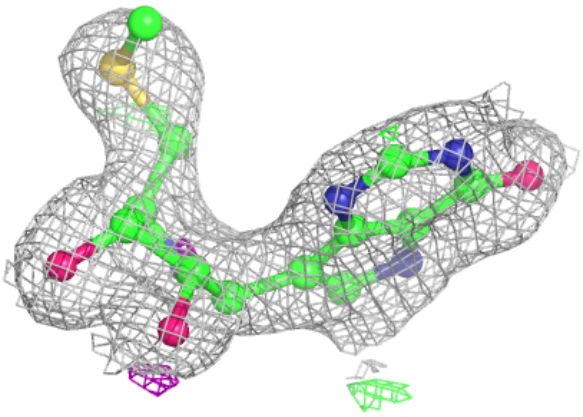
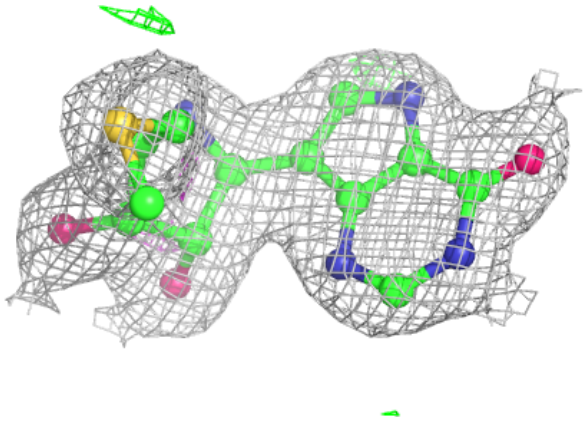
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	IPA	F	504	4/4	0.79	0.25	15,18,21,23	0
4	IPA	B	502	4/4	0.82	0.20	21,21,22,24	0
4	IPA	E	506	4/4	0.83	0.20	23,24,26,26	0
4	IPA	A	503	4/4	0.85	0.15	23,24,25,26	0
4	IPA	D	507	4/4	0.88	0.16	19,21,22,22	0
2	SO4	B	410	5/5	0.90	0.25	69,70,70,70	0
2	SO4	A	413	5/5	0.91	0.33	65,65,66,66	0
2	SO4	F	419	5/5	0.92	0.18	48,51,52,52	0
3	MTI	B	302	20/20	0.92	0.13	27,34,46,48	0
3	MTI	C	303	20/20	0.92	0.15	25,30,41,44	0
3	MTI	E	305	20/20	0.93	0.14	26,28,37,42	0
2	SO4	B	417	5/5	0.93	0.16	69,70,70,71	0
2	SO4	E	420	5/5	0.94	0.14	44,46,47,48	0
2	SO4	A	418	5/5	0.94	0.16	59,59,59,62	0
3	MTI	A	301	20/20	0.94	0.12	19,22,34,36	0
3	MTI	F	306	20/20	0.95	0.14	18,20,32,34	0
2	SO4	C	422	5/5	0.95	0.10	44,45,48,48	0
2	SO4	D	412	5/5	0.95	0.16	52,52,54,54	0
3	MTI	D	304	20/20	0.95	0.15	19,20,33,36	0
2	SO4	D	421	5/5	0.95	0.19	56,57,58,58	0
2	SO4	F	406	5/5	0.96	0.10	23,24,26,27	0
2	SO4	F	411	5/5	0.96	0.13	40,41,44,44	0
2	SO4	B	402	5/5	0.96	0.11	40,40,42,42	0
2	SO4	A	401	5/5	0.97	0.12	32,32,35,35	0
2	SO4	D	404	5/5	0.97	0.12	29,29,30,30	0
2	SO4	D	408	5/5	0.97	0.09	18,25,25,27	0
2	SO4	C	403	5/5	0.97	0.13	30,31,34,35	0
2	SO4	F	409	5/5	0.98	0.06	20,23,29,30	0
2	SO4	A	414	5/5	0.98	0.08	22,26,28,29	0
2	SO4	E	405	5/5	0.98	0.11	26,27,27,28	0
2	SO4	E	415	5/5	0.98	0.09	20,22,26,27	0
2	SO4	C	416	5/5	0.98	0.07	25,26,27,29	0
2	SO4	B	407	5/5	0.98	0.10	25,27,29,31	0

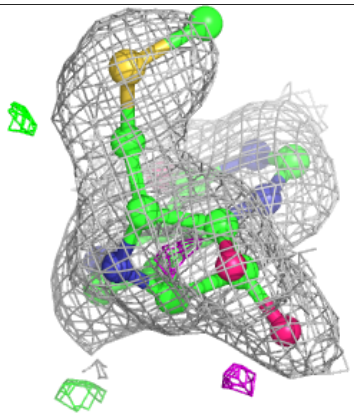
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MTI 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)

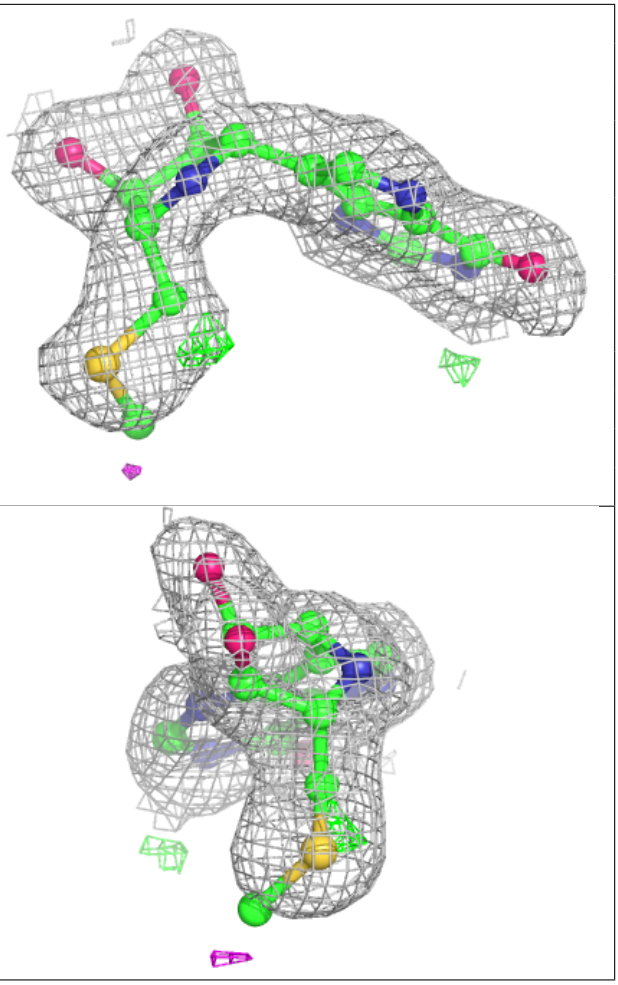


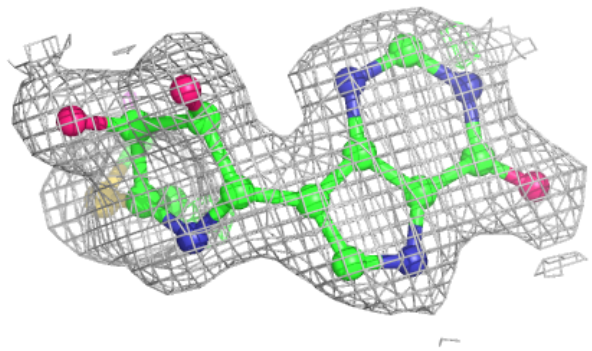




Electron density around MTI C 303:

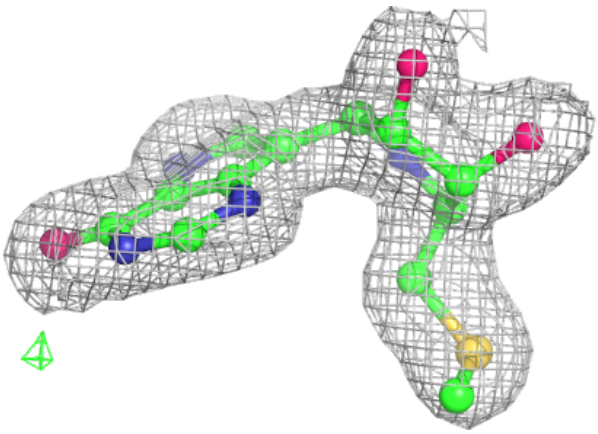
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

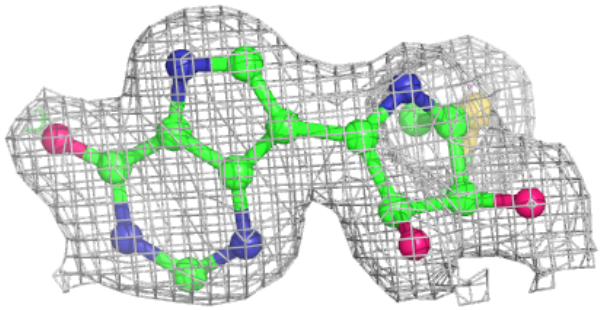


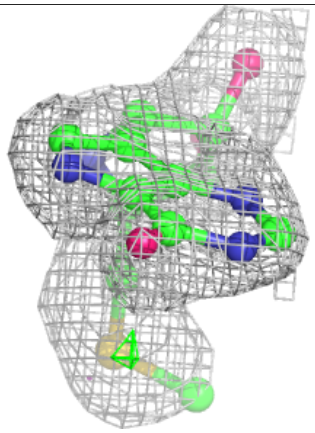


Electron density around MTI E 305:

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

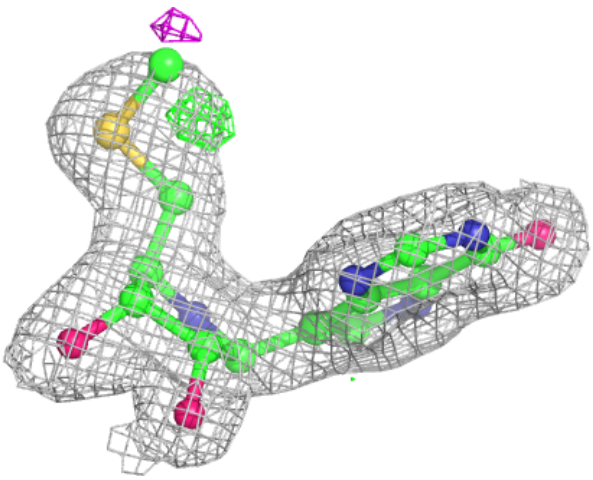


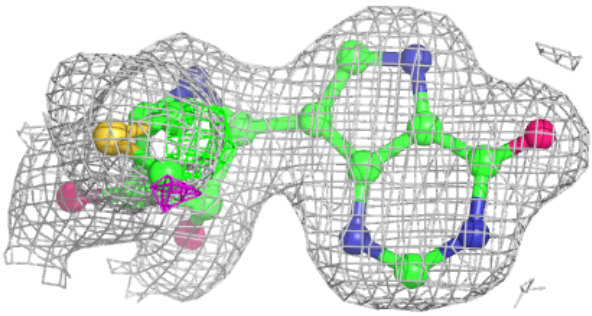


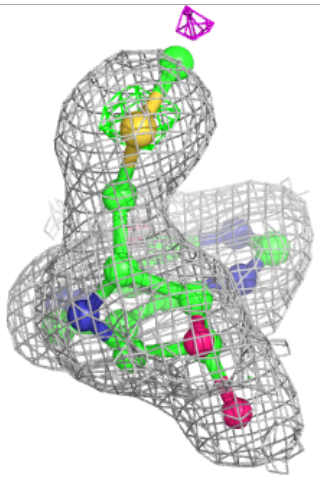


Electron density around MTI A 301:

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

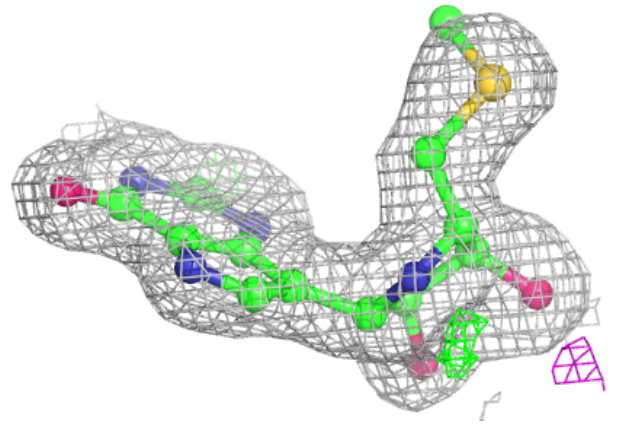


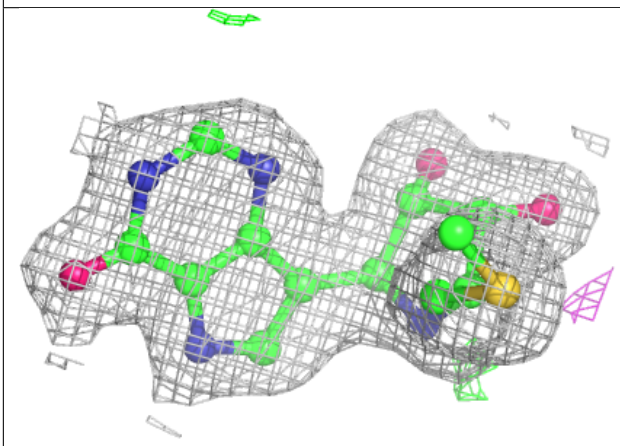


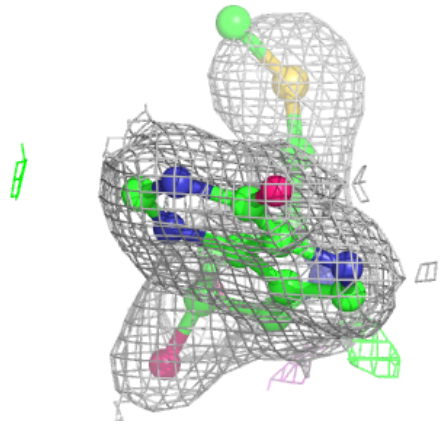


Electron density around MTI F 306:

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

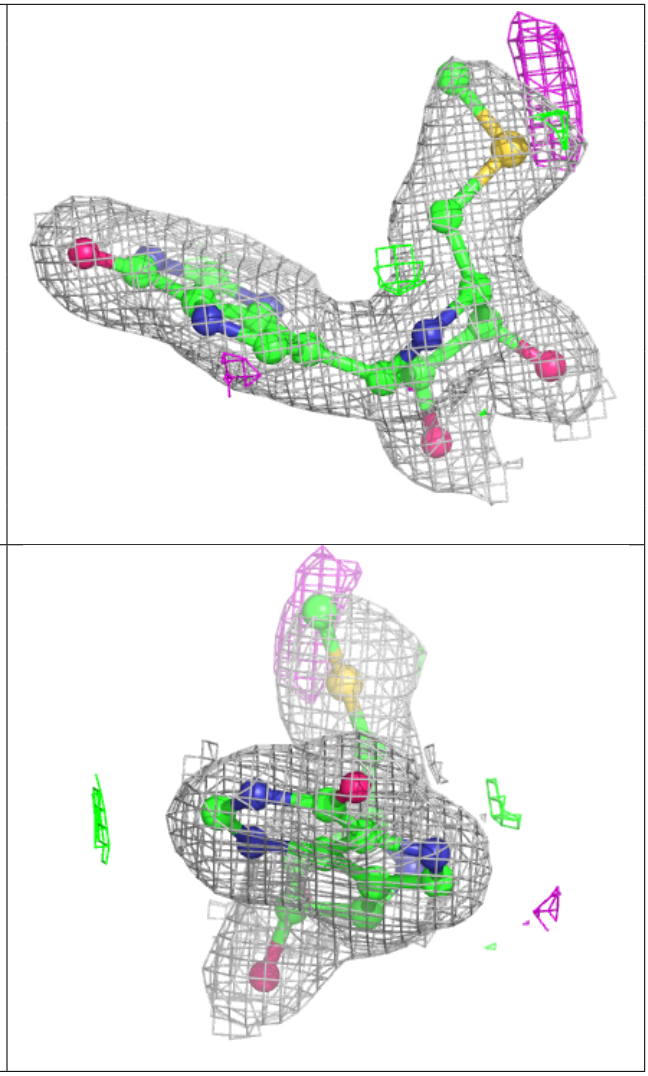






Electron density around MTI D 304:

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



6.5 Other polymers (i)

There are no such residues in this entry.