Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 07:21 PM EDT

PDB ID	:	4MYX
Title	:	Crystal Structure of the Inosine 5'-monophosphate Dehydrogenase, with a Internal Deletion of CBS Domain from Bacillus anthracis str. Ame complexed with P32
Authors	:	Kim, Y.; Makowska-Grzyska, M.; Gu, M.; Gorla, S.K.; Hedstrom, L.; Anderson, W.F.; Joachimiak, A.; CSGID; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2013-09-28
Resolution	:	2.70 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:

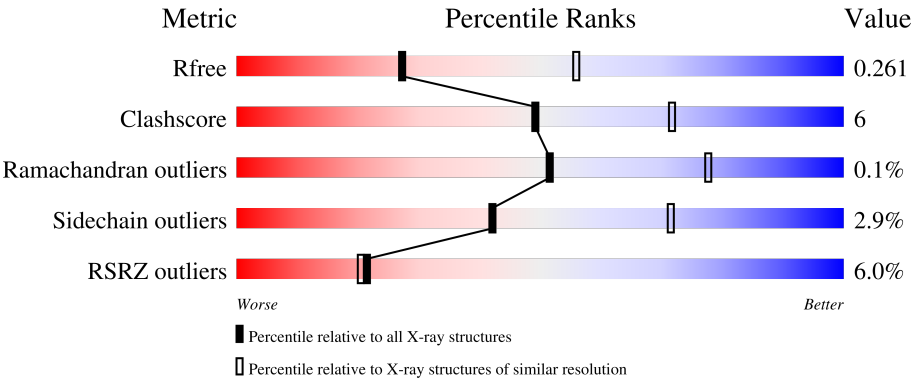
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	384	8% 79% 12% 9%
1	B	384	2% 77% 14% • 8%
1	C	384	2% 76% 15% 9%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

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Mol	Chain	Length	Quality of chain
1	D	384	7% 78% 13% 8%
1	E	384	6% 77% 13% 8%
1	F	384	8% 79% 11% 9%
1	G	384	6% 80% 13% 7%
1	H	384	7% 73% 17% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SO4	G	502	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 21740 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	7	0
			2637	1656	465	498	18			
1	B	355	Total	C	N	O	S	0	1	0
			2614	1641	458	499	16			
1	C	348	Total	C	N	O	S	0	4	0
			2587	1623	451	496	17			
1	D	352	Total	C	N	O	S	0	4	0
			2615	1639	459	501	16			
1	E	352	Total	C	N	O	S	0	2	0
			2597	1629	455	496	17			
1	F	350	Total	C	N	O	S	0	0	0
			2567	1612	450	489	16			
1	G	356	Total	C	N	O	S	0	2	0
			2627	1647	462	502	16			
1	H	350	Total	C	N	O	S	0	0	0
			2567	1612	450	489	16			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q81W29
A	-22	HIS	-	expression tag	UNP Q81W29
A	-21	HIS	-	expression tag	UNP Q81W29
A	-20	HIS	-	expression tag	UNP Q81W29
A	-19	HIS	-	expression tag	UNP Q81W29
A	-18	HIS	-	expression tag	UNP Q81W29
A	-17	HIS	-	expression tag	UNP Q81W29
A	-16	SER	-	expression tag	UNP Q81W29
A	-15	SER	-	expression tag	UNP Q81W29
A	-14	GLY	-	expression tag	UNP Q81W29
A	-13	VAL	-	expression tag	UNP Q81W29
A	-12	ASP	-	expression tag	UNP Q81W29
A	-11	LEU	-	expression tag	UNP Q81W29

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP Q81W29
A	-9	THR	-	expression tag	UNP Q81W29
A	-8	GLU	-	expression tag	UNP Q81W29
A	-7	ASN	-	expression tag	UNP Q81W29
A	-6	LEU	-	expression tag	UNP Q81W29
A	-5	TYR	-	expression tag	UNP Q81W29
A	-4	PHE	-	expression tag	UNP Q81W29
A	-3	GLN	-	expression tag	UNP Q81W29
A	-2	SER	-	expression tag	UNP Q81W29
A	-1	ASN	-	expression tag	UNP Q81W29
A	0	ALA	-	expression tag	UNP Q81W29
A	92	GLY	-	linker	UNP Q81W29
A	220	GLY	-	linker	UNP Q81W29
B	-23	MET	-	expression tag	UNP Q81W29
B	-22	HIS	-	expression tag	UNP Q81W29
B	-21	HIS	-	expression tag	UNP Q81W29
B	-20	HIS	-	expression tag	UNP Q81W29
B	-19	HIS	-	expression tag	UNP Q81W29
B	-18	HIS	-	expression tag	UNP Q81W29
B	-17	HIS	-	expression tag	UNP Q81W29
B	-16	SER	-	expression tag	UNP Q81W29
B	-15	SER	-	expression tag	UNP Q81W29
B	-14	GLY	-	expression tag	UNP Q81W29
B	-13	VAL	-	expression tag	UNP Q81W29
B	-12	ASP	-	expression tag	UNP Q81W29
B	-11	LEU	-	expression tag	UNP Q81W29
B	-10	GLY	-	expression tag	UNP Q81W29
B	-9	THR	-	expression tag	UNP Q81W29
B	-8	GLU	-	expression tag	UNP Q81W29
B	-7	ASN	-	expression tag	UNP Q81W29
B	-6	LEU	-	expression tag	UNP Q81W29
B	-5	TYR	-	expression tag	UNP Q81W29
B	-4	PHE	-	expression tag	UNP Q81W29
B	-3	GLN	-	expression tag	UNP Q81W29
B	-2	SER	-	expression tag	UNP Q81W29
B	-1	ASN	-	expression tag	UNP Q81W29
B	0	ALA	-	expression tag	UNP Q81W29
B	92	GLY	-	linker	UNP Q81W29
B	220	GLY	-	linker	UNP Q81W29
C	-23	MET	-	expression tag	UNP Q81W29
C	-22	HIS	-	expression tag	UNP Q81W29
C	-21	HIS	-	expression tag	UNP Q81W29

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	expression tag	UNP Q81W29
C	-19	HIS	-	expression tag	UNP Q81W29
C	-18	HIS	-	expression tag	UNP Q81W29
C	-17	HIS	-	expression tag	UNP Q81W29
C	-16	SER	-	expression tag	UNP Q81W29
C	-15	SER	-	expression tag	UNP Q81W29
C	-14	GLY	-	expression tag	UNP Q81W29
C	-13	VAL	-	expression tag	UNP Q81W29
C	-12	ASP	-	expression tag	UNP Q81W29
C	-11	LEU	-	expression tag	UNP Q81W29
C	-10	GLY	-	expression tag	UNP Q81W29
C	-9	THR	-	expression tag	UNP Q81W29
C	-8	GLU	-	expression tag	UNP Q81W29
C	-7	ASN	-	expression tag	UNP Q81W29
C	-6	LEU	-	expression tag	UNP Q81W29
C	-5	TYR	-	expression tag	UNP Q81W29
C	-4	PHE	-	expression tag	UNP Q81W29
C	-3	GLN	-	expression tag	UNP Q81W29
C	-2	SER	-	expression tag	UNP Q81W29
C	-1	ASN	-	expression tag	UNP Q81W29
C	0	ALA	-	expression tag	UNP Q81W29
C	92	GLY	-	linker	UNP Q81W29
C	220	GLY	-	linker	UNP Q81W29
D	-23	MET	-	expression tag	UNP Q81W29
D	-22	HIS	-	expression tag	UNP Q81W29
D	-21	HIS	-	expression tag	UNP Q81W29
D	-20	HIS	-	expression tag	UNP Q81W29
D	-19	HIS	-	expression tag	UNP Q81W29
D	-18	HIS	-	expression tag	UNP Q81W29
D	-17	HIS	-	expression tag	UNP Q81W29
D	-16	SER	-	expression tag	UNP Q81W29
D	-15	SER	-	expression tag	UNP Q81W29
D	-14	GLY	-	expression tag	UNP Q81W29
D	-13	VAL	-	expression tag	UNP Q81W29
D	-12	ASP	-	expression tag	UNP Q81W29
D	-11	LEU	-	expression tag	UNP Q81W29
D	-10	GLY	-	expression tag	UNP Q81W29
D	-9	THR	-	expression tag	UNP Q81W29
D	-8	GLU	-	expression tag	UNP Q81W29
D	-7	ASN	-	expression tag	UNP Q81W29
D	-6	LEU	-	expression tag	UNP Q81W29
D	-5	TYR	-	expression tag	UNP Q81W29

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	PHE	-	expression tag	UNP Q81W29
D	-3	GLN	-	expression tag	UNP Q81W29
D	-2	SER	-	expression tag	UNP Q81W29
D	-1	ASN	-	expression tag	UNP Q81W29
D	0	ALA	-	expression tag	UNP Q81W29
D	92	GLY	-	linker	UNP Q81W29
D	220	GLY	-	linker	UNP Q81W29
E	-23	MET	-	expression tag	UNP Q81W29
E	-22	HIS	-	expression tag	UNP Q81W29
E	-21	HIS	-	expression tag	UNP Q81W29
E	-20	HIS	-	expression tag	UNP Q81W29
E	-19	HIS	-	expression tag	UNP Q81W29
E	-18	HIS	-	expression tag	UNP Q81W29
E	-17	HIS	-	expression tag	UNP Q81W29
E	-16	SER	-	expression tag	UNP Q81W29
E	-15	SER	-	expression tag	UNP Q81W29
E	-14	GLY	-	expression tag	UNP Q81W29
E	-13	VAL	-	expression tag	UNP Q81W29
E	-12	ASP	-	expression tag	UNP Q81W29
E	-11	LEU	-	expression tag	UNP Q81W29
E	-10	GLY	-	expression tag	UNP Q81W29
E	-9	THR	-	expression tag	UNP Q81W29
E	-8	GLU	-	expression tag	UNP Q81W29
E	-7	ASN	-	expression tag	UNP Q81W29
E	-6	LEU	-	expression tag	UNP Q81W29
E	-5	TYR	-	expression tag	UNP Q81W29
E	-4	PHE	-	expression tag	UNP Q81W29
E	-3	GLN	-	expression tag	UNP Q81W29
E	-2	SER	-	expression tag	UNP Q81W29
E	-1	ASN	-	expression tag	UNP Q81W29
E	0	ALA	-	expression tag	UNP Q81W29
E	92	GLY	-	linker	UNP Q81W29
E	220	GLY	-	linker	UNP Q81W29
F	-23	MET	-	expression tag	UNP Q81W29
F	-22	HIS	-	expression tag	UNP Q81W29
F	-21	HIS	-	expression tag	UNP Q81W29
F	-20	HIS	-	expression tag	UNP Q81W29
F	-19	HIS	-	expression tag	UNP Q81W29
F	-18	HIS	-	expression tag	UNP Q81W29
F	-17	HIS	-	expression tag	UNP Q81W29
F	-16	SER	-	expression tag	UNP Q81W29
F	-15	SER	-	expression tag	UNP Q81W29

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	GLY	-	expression tag	UNP Q81W29
F	-13	VAL	-	expression tag	UNP Q81W29
F	-12	ASP	-	expression tag	UNP Q81W29
F	-11	LEU	-	expression tag	UNP Q81W29
F	-10	GLY	-	expression tag	UNP Q81W29
F	-9	THR	-	expression tag	UNP Q81W29
F	-8	GLU	-	expression tag	UNP Q81W29
F	-7	ASN	-	expression tag	UNP Q81W29
F	-6	LEU	-	expression tag	UNP Q81W29
F	-5	TYR	-	expression tag	UNP Q81W29
F	-4	PHE	-	expression tag	UNP Q81W29
F	-3	GLN	-	expression tag	UNP Q81W29
F	-2	SER	-	expression tag	UNP Q81W29
F	-1	ASN	-	expression tag	UNP Q81W29
F	0	ALA	-	expression tag	UNP Q81W29
F	92	GLY	-	linker	UNP Q81W29
F	220	GLY	-	linker	UNP Q81W29
G	-23	MET	-	expression tag	UNP Q81W29
G	-22	HIS	-	expression tag	UNP Q81W29
G	-21	HIS	-	expression tag	UNP Q81W29
G	-20	HIS	-	expression tag	UNP Q81W29
G	-19	HIS	-	expression tag	UNP Q81W29
G	-18	HIS	-	expression tag	UNP Q81W29
G	-17	HIS	-	expression tag	UNP Q81W29
G	-16	SER	-	expression tag	UNP Q81W29
G	-15	SER	-	expression tag	UNP Q81W29
G	-14	GLY	-	expression tag	UNP Q81W29
G	-13	VAL	-	expression tag	UNP Q81W29
G	-12	ASP	-	expression tag	UNP Q81W29
G	-11	LEU	-	expression tag	UNP Q81W29
G	-10	GLY	-	expression tag	UNP Q81W29
G	-9	THR	-	expression tag	UNP Q81W29
G	-8	GLU	-	expression tag	UNP Q81W29
G	-7	ASN	-	expression tag	UNP Q81W29
G	-6	LEU	-	expression tag	UNP Q81W29
G	-5	TYR	-	expression tag	UNP Q81W29
G	-4	PHE	-	expression tag	UNP Q81W29
G	-3	GLN	-	expression tag	UNP Q81W29
G	-2	SER	-	expression tag	UNP Q81W29
G	-1	ASN	-	expression tag	UNP Q81W29
G	0	ALA	-	expression tag	UNP Q81W29
G	92	GLY	-	linker	UNP Q81W29

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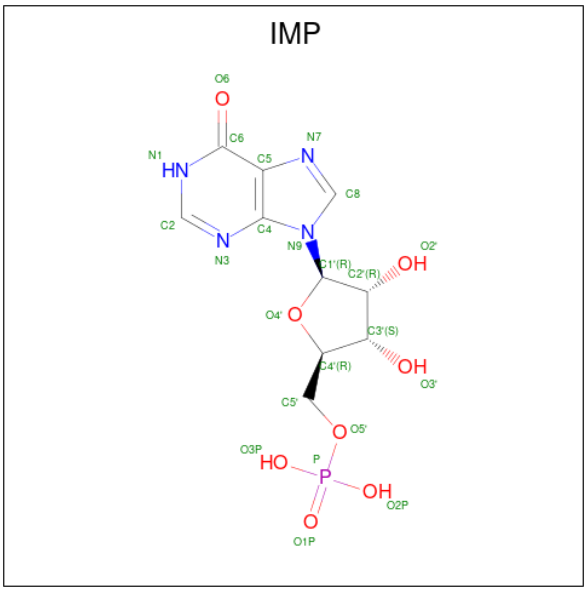
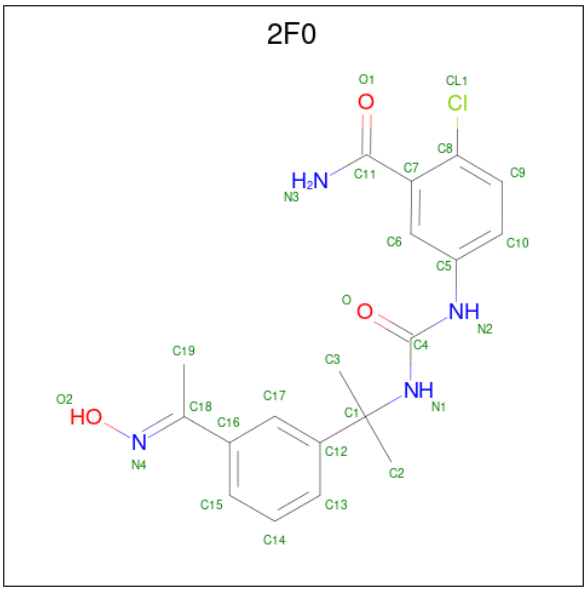
Chain	Residue	Modelled	Actual	Comment	Reference
G	220	GLY	-	linker	UNP Q81W29
H	-23	MET	-	expression tag	UNP Q81W29
H	-22	HIS	-	expression tag	UNP Q81W29
H	-21	HIS	-	expression tag	UNP Q81W29
H	-20	HIS	-	expression tag	UNP Q81W29
H	-19	HIS	-	expression tag	UNP Q81W29
H	-18	HIS	-	expression tag	UNP Q81W29
H	-17	HIS	-	expression tag	UNP Q81W29
H	-16	SER	-	expression tag	UNP Q81W29
H	-15	SER	-	expression tag	UNP Q81W29
H	-14	GLY	-	expression tag	UNP Q81W29
H	-13	VAL	-	expression tag	UNP Q81W29
H	-12	ASP	-	expression tag	UNP Q81W29
H	-11	LEU	-	expression tag	UNP Q81W29
H	-10	GLY	-	expression tag	UNP Q81W29
H	-9	THR	-	expression tag	UNP Q81W29
H	-8	GLU	-	expression tag	UNP Q81W29
H	-7	ASN	-	expression tag	UNP Q81W29
H	-6	LEU	-	expression tag	UNP Q81W29
H	-5	TYR	-	expression tag	UNP Q81W29
H	-4	PHE	-	expression tag	UNP Q81W29
H	-3	GLN	-	expression tag	UNP Q81W29
H	-2	SER	-	expression tag	UNP Q81W29
H	-1	ASN	-	expression tag	UNP Q81W29
H	0	ALA	-	expression tag	UNP Q81W29
H	92	GLY	-	linker	UNP Q81W29
H	220	GLY	-	linker	UNP Q81W29

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



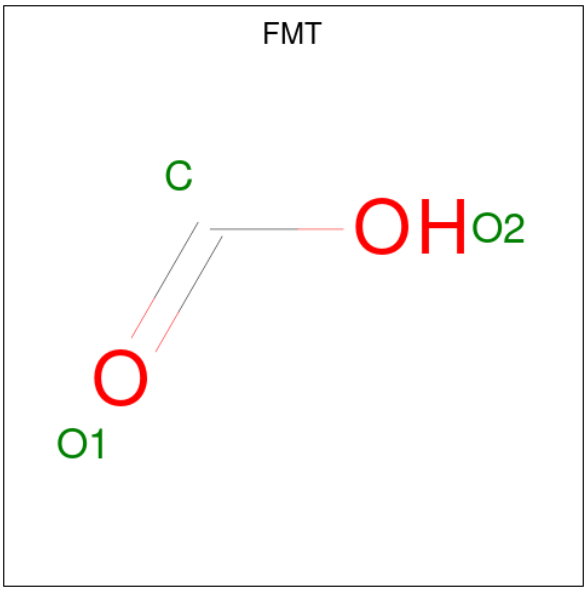
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	G	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	H	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is 2-chloro-5-{[(2-{3-[(1E)-N-hydroxyethanimidoyl]phenyl}propan-2-yl)carbamoyl]amino}benzamide (three-letter code: 2F0) (formula: $C_{19}H_{21}ClN_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	B	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	C	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	D	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	E	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	E	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	F	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	H	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	H	1	Total	C	O	0	0
			3	1	2		
4	H	1	Total	C	O	0	0
			3	1	2		
4	H	1	Total	C	O	0	0
			3	1	2		

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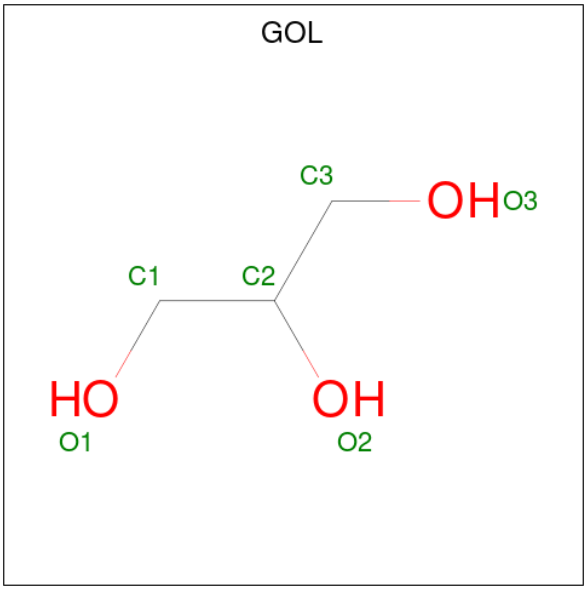
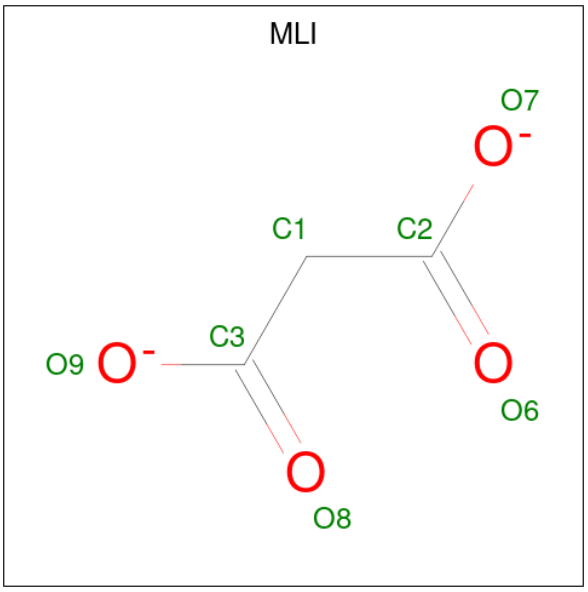
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 3 1 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



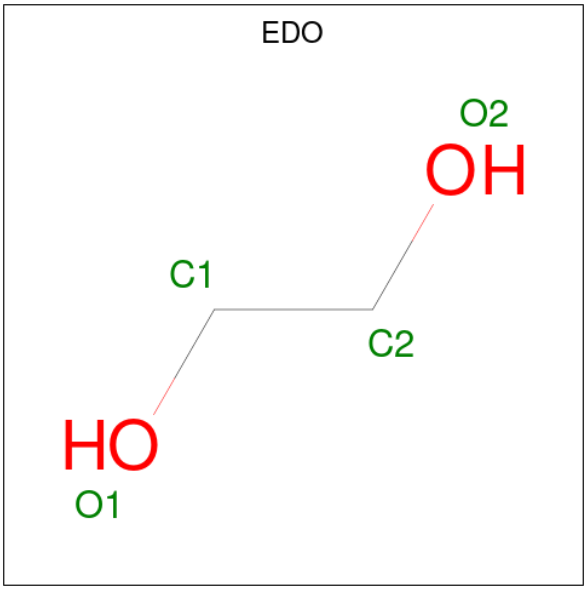
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 3 4	0	0
6	E	1	Total C O 7 3 4	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0

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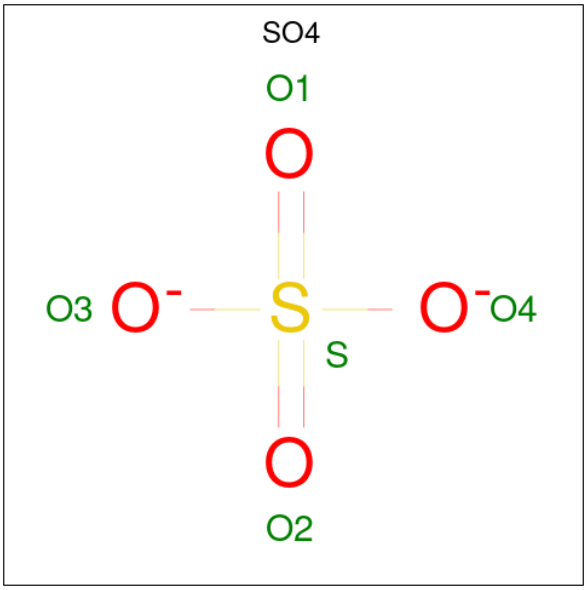
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0

- Molecule 9 is water.

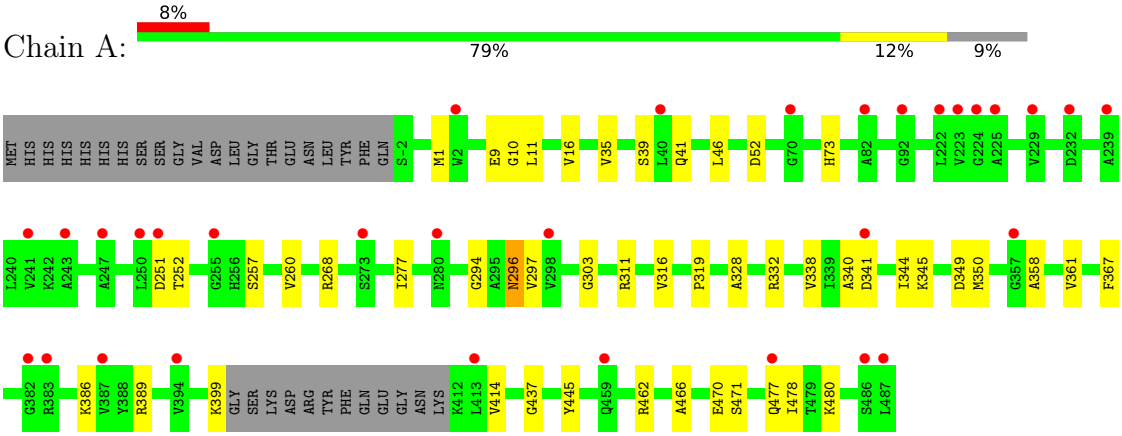
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	53	Total O 53 53	0	0
9	B	62	Total O 62 62	0	0
9	C	52	Total O 52 52	0	0
9	D	49	Total O 49 49	0	0
9	E	48	Total O 48 48	0	0
9	F	37	Total O 37 37	0	0
9	G	48	Total O 48 48	0	0
9	H	54	Total O 54 54	0	0

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.

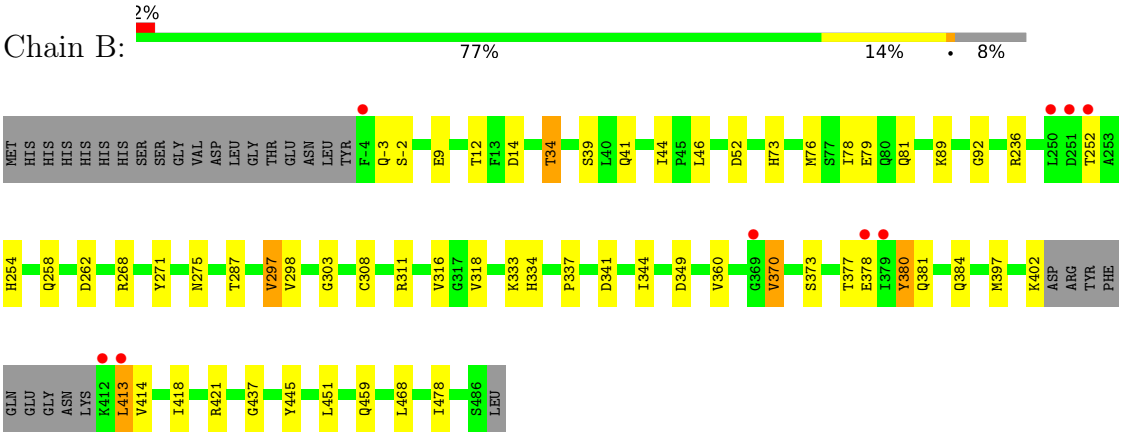
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain A:



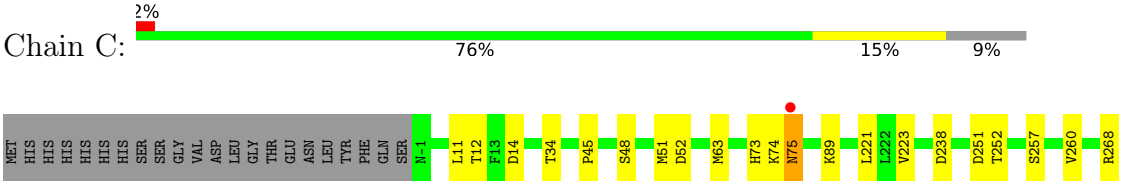
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

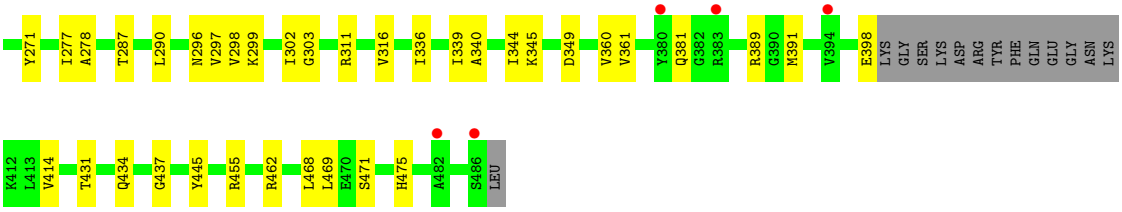
Chain B:



• Molecule 1: Inosine-5'-monophosphate dehydrogenase

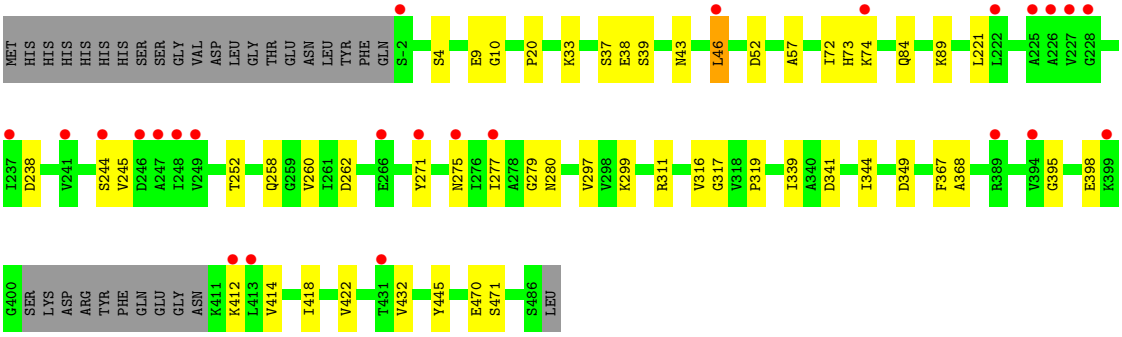
Chain C:





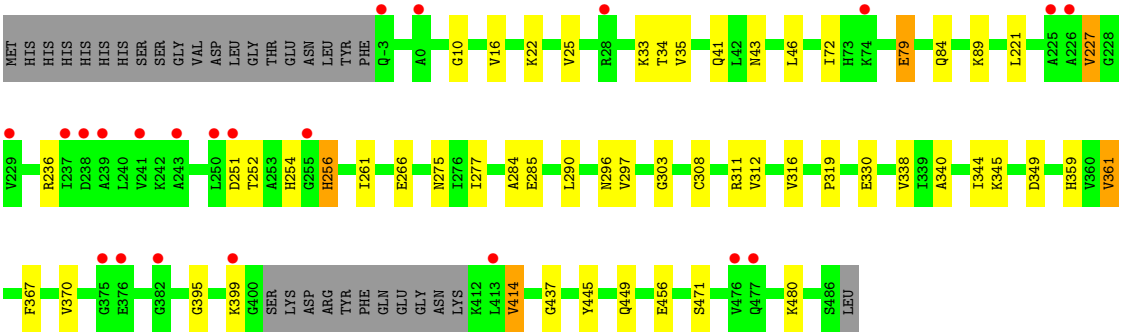
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain D:



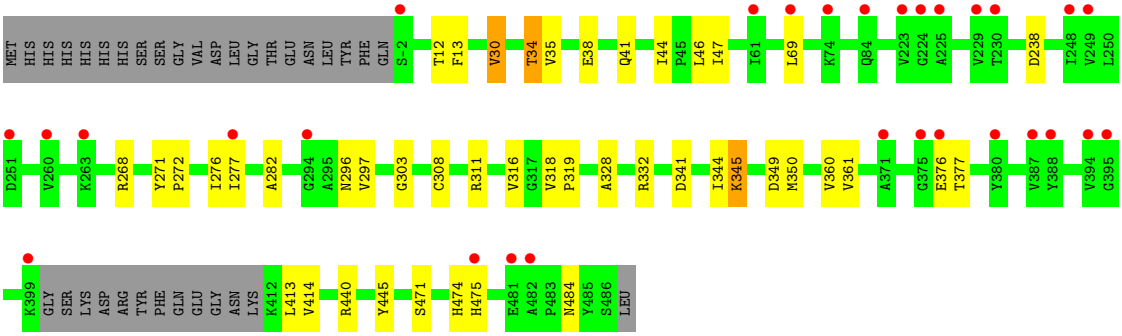
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain E:



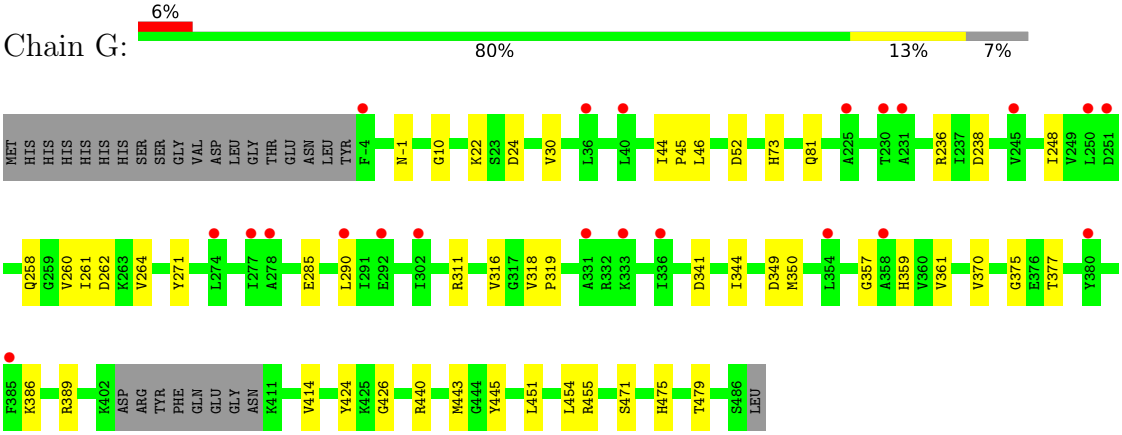
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain F:



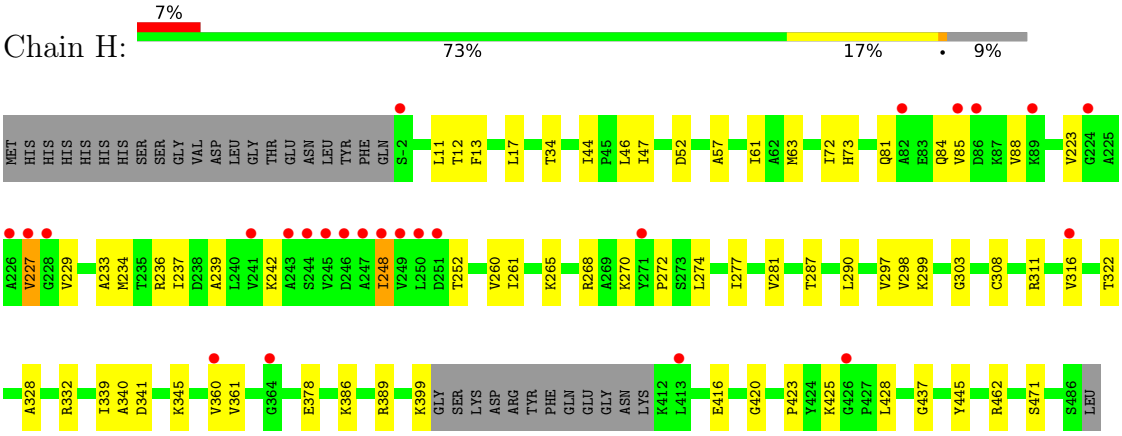
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain G:



• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	85.36Å 89.82Å 104.50Å 81.41° 90.42° 83.50°	Depositor
Resolution (Å)	41.90 – 2.70 48.17 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (41.90-2.70) 98.1 (48.17-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1161)	Depositor
R, R_{free}	0.218 , 0.260 0.219 , 0.261	Depositor DCC
R_{free} test set	4101 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	21740	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.58% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, 2F0, GOL, SO4, EDO, MLI, IMP

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	0.20	0/2673	0.39	0/3610
1	B	0.21	0/2651	0.41	0/3581
1	C	0.20	0/2623	0.40	0/3545
1	D	0.21	0/2651	0.40	0/3581
1	E	0.21	0/2633	0.39	0/3557
1	F	0.21	0/2603	0.39	0/3518
1	G	0.20	0/2663	0.38	0/3596
1	H	0.20	0/2603	0.39	0/3518
All	All	0.21	0/21100	0.39	0/28506

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2637	0	2702	35	0
1	B	2614	0	2667	41	0
1	C	2587	0	2631	36	0
1	D	2615	0	2664	29	0
1	E	2597	0	2651	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2567	0	2626	26	0
1	G	2627	0	2682	32	0
1	H	2567	0	2626	44	0
2	A	23	0	11	1	0
2	B	23	0	11	2	0
2	C	23	0	11	1	0
2	D	23	0	11	1	0
2	E	23	0	11	0	0
2	F	23	0	11	1	0
2	G	23	0	11	1	0
2	H	23	0	11	1	0
3	A	27	0	21	3	0
3	B	27	0	21	2	0
3	C	27	0	21	1	0
3	D	27	0	21	3	0
3	E	54	0	42	6	0
3	F	27	0	21	2	0
3	H	27	0	21	4	0
4	A	6	0	2	0	0
4	B	3	0	1	0	0
4	C	3	0	1	0	0
4	D	6	0	2	0	0
4	E	9	0	3	0	0
4	F	6	0	2	0	0
4	H	12	0	4	0	0
5	A	6	0	8	0	0
5	E	6	0	8	0	0
6	A	7	0	2	0	0
6	E	7	0	2	0	0
7	B	4	0	6	0	0
7	C	8	0	12	4	0
7	D	12	0	18	0	0
7	E	4	0	6	0	0
7	F	12	0	18	2	0
8	C	5	0	0	0	0
8	G	10	0	0	0	0
9	A	53	0	0	0	0
9	B	62	0	0	1	0
9	C	52	0	0	0	0
9	D	49	0	0	0	0
9	E	48	0	0	0	0
9	F	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	48	0	0	1	0
9	H	54	0	0	1	0
All	All	21740	0	21600	253	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 6.

All (253) 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)
3:H:505:2F0:H3	3:H:505:2F0:O	1.89	0.72
3:F:502:2F0:H3	3:F:502:2F0:O	1.89	0.72
1:A:414:VAL:HG21	1:C:437:GLY:HA3	1.72	0.71
3:A:502:2F0:O	3:A:502:2F0:H13	1.93	0.68
1:E:344:ILE:HG23	1:E:349:ASP:HB2	1.75	0.68
1:A:340:ALA:HB3	1:A:361:VAL:HG12	1.76	0.68
1:A:268[A]:ARG:NH2	1:A:296:ASN:OD1	2.28	0.67
1:B:297:VAL:HG13	1:B:337:PRO:HG2	1.77	0.66
1:A:389:ARG:HH22	1:A:399:LYS:HD2	1.60	0.66
3:E:502:2F0:O	3:E:502:2F0:H13	1.95	0.66
1:D:57:ALA:HB2	1:D:84:GLN:HB2	1.78	0.65
1:C:278:ALA:HB3	1:C:290:LEU:HD21	1.79	0.65
1:A:344[A]:ILE:HG23	1:A:349:ASP:HB2	1.79	0.63
1:H:389:ARG:HH22	1:H:399:LYS:HD2	1.63	0.63
1:B:459:GLN:NE2	1:D:4:SER:O	2.31	0.62
1:A:437:GLY:HA3	1:B:414:VAL:HG21	1.82	0.62
1:E:72:ILE:HD13	1:E:84:GLN:HB3	1.80	0.62
1:A:462:ARG:NH1	1:B:9:GLU:OE1	2.33	0.61
1:D:258:GLN:NE2	1:D:262:ASP:OD2	2.32	0.61
1:H:227:VAL:HG12	1:H:236:ARG:HD2	1.81	0.61
1:E:456:GLU:OE1	1:G:-1:ASN:ND2	2.33	0.61
1:H:239:ALA:HA	1:H:242:LYS:HE3	1.82	0.61
1:B:258:GLN:NE2	1:B:262:ASP:OD1	2.31	0.60
1:C:299:LYS:HG3	1:C:339:ILE:HB	1.82	0.60
1:A:277:ILE:HG13	1:A:297:VAL:HB	1.83	0.60
1:A:341:ASP:OD2	2:A:501:IMP:O2'	2.20	0.58
1:C:51:MET:SD	2:C:502:IMP:H8	2.43	0.58
1:D:311:ARG:HD3	1:D:317:GLY:HA3	1.84	0.58
1:G:359:HIS:ND1	9:G:628:HOH:O	2.32	0.58
1:E:437:GLY:HA3	1:G:414:VAL:HG21	1.86	0.58
1:E:46:LEU:HD23	1:E:367:PHE:HZ	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:501:2F0:O	3:D:501:2F0:H13	2.04	0.57
1:F:277:ILE:HG12	1:F:297:VAL:HB	1.87	0.57
1:H:340:ALA:HB3	1:H:361:VAL:HG12	1.86	0.57
1:C:455:ARG:HH12	7:C:504:EDO:H22	1.69	0.57
1:B:380:TYR:HD2	1:B:381:GLN:H	1.52	0.56
1:F:34:THR:HG21	1:F:360:VAL:HG23	1.87	0.56
1:H:11:LEU:HD11	1:H:462:ARG:HD3	1.88	0.56
1:A:471:SER:HA	1:B:311:ARG:HD2	1.85	0.56
1:E:312:VAL:HG22	7:F:506:EDO:H12	1.87	0.56
1:H:281:VAL:HG11	1:H:290:LEU:HD11	1.86	0.56
1:B:44:ILE:HD12	1:B:46:LEU:HD12	1.87	0.55
1:F:35:VAL:HG13	1:F:41:GLN:HG2	1.88	0.55
1:G:30:VAL:O	1:G:440:ARG:NH1	2.40	0.55
1:H:277:ILE:HG12	1:H:297:VAL:HB	1.87	0.55
1:H:341:ASP:OD2	2:H:504:IMP:O2'	2.25	0.55
3:A:502:2F0:O	3:A:502:2F0:H3	2.06	0.55
1:B:344:ILE:HG23	1:B:349:ASP:HB2	1.88	0.55
1:G:375:GLY:O	1:G:386:LYS:NZ	2.31	0.55
1:C:316:VAL:HG11	1:D:445:TYR:HB3	1.89	0.55
1:E:10:GLY:HA3	1:E:319:PRO:HG2	1.89	0.55
1:H:423:PRO:HB2	1:H:425:LYS:HE3	1.89	0.55
1:B:341:ASP:OD2	2:B:500:IMP:O2'	2.24	0.54
1:D:277:ILE:HG12	1:D:297:VAL:HB	1.89	0.54
1:B:437:GLY:HA3	1:D:414:VAL:HG21	1.89	0.54
1:D:39:SER:HB2	1:D:275:ASN:HD21	1.71	0.54
1:G:81:GLN:OE1	1:G:236:ARG:NH1	2.35	0.54
1:B:380:TYR:CD2	1:B:381:GLN:N	2.76	0.54
1:E:311:ARG:HD2	1:F:471:SER:HA	1.89	0.54
1:F:47:ILE:HG12	1:F:69:LEU:HB3	1.90	0.54
1:H:299:LYS:HG3	1:H:339:ILE:HB	1.89	0.54
1:G:238:ASP:OD1	1:G:271:TYR:OH	2.25	0.53
1:C:431:THR:HG23	7:C:506:EDO:H22	1.91	0.53
1:A:11:LEU:HD11	1:A:462:ARG:HD3	1.91	0.53
1:E:22:LYS:NZ	1:G:285:GLU:OE1	2.41	0.53
1:D:72:ILE:HG23	1:D:84:GLN:HE21	1.74	0.53
1:F:341:ASP:OD2	2:F:501:IMP:O2'	2.26	0.53
1:H:44:ILE:HD12	1:H:46:LEU:HD12	1.91	0.53
1:B:397:MET:SD	3:B:501:2F0:H21	2.49	0.53
1:E:277:ILE:HG12	1:E:297:VAL:HB	1.91	0.53
1:G:341:ASP:OD2	2:G:501:IMP:O2'	2.25	0.53
1:A:46[B]:LEU:HD23	1:A:367:PHE:HZ	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ARG:NH2	1:C:296:ASN:OD1	2.42	0.52
1:H:72:ILE:HD13	1:H:84:GLN:HB3	1.92	0.52
1:E:227:VAL:HG13	1:E:236:ARG:HD2	1.92	0.52
1:G:445:TYR:HB3	1:H:316:VAL:HG11	1.91	0.52
1:C:252:THR:HG21	1:C:260:VAL:HG22	1.92	0.52
3:C:503:2F0:O	3:C:503:2F0:H3	2.09	0.52
1:F:311:ARG:HD2	1:H:471:SER:HA	1.92	0.51
1:E:445:TYR:HB2	1:G:316:VAL:HG21	1.92	0.51
1:B:76:MET:O	1:B:236:ARG:NH1	2.42	0.51
1:A:296:ASN:OD1	1:A:296:ASN:N	2.42	0.51
1:C:238:ASP:OD1	1:C:271:TYR:OH	2.26	0.51
1:F:44:ILE:HD12	1:F:46:LEU:HD12	1.93	0.51
1:A:9:GLU:OE2	1:C:462:ARG:NH1	2.45	0.50
1:F:12:THR:OG1	1:F:13:PHE:N	2.41	0.50
1:D:252:THR:HG21	1:D:260:VAL:HG21	1.93	0.50
1:G:10:GLY:HA3	1:G:319:PRO:HG2	1.92	0.50
1:B:333:LYS:HB2	1:B:334:HIS:HD2	1.76	0.50
3:E:502:2F0:O	3:E:502:2F0:H3	2.10	0.50
3:E:502:2F0:O1	3:E:502:2F0:CL1	2.66	0.50
3:E:509:2F0:O	3:E:509:2F0:H13	2.11	0.50
1:G:443:MET:HG2	1:G:454:LEU:HD22	1.94	0.50
1:B:478:ILE:HG12	1:D:418:ILE:HD13	1.94	0.50
3:B:501:2F0:H3	3:B:501:2F0:O	2.11	0.50
1:C:277:ILE:HG12	1:C:297:VAL:HB	1.94	0.50
1:C:302:ILE:HD12	1:D:20:PRO:HG3	1.93	0.50
1:G:311:ARG:NH2	1:G:318:VAL:O	2.44	0.50
1:B:445:TYR:HB3	1:D:316:VAL:HG11	1.94	0.50
1:E:35:VAL:HG13	1:E:41:GLN:HG2	1.94	0.50
3:E:502:2F0:O	3:E:502:2F0:C3	2.59	0.50
1:F:350:MET:HG3	1:F:361:VAL:HG21	1.94	0.50
3:H:505:2F0:O	3:H:505:2F0:H13	2.11	0.50
1:H:61:ILE:HD11	1:H:88:VAL:HA	1.93	0.49
1:A:252:THR:HG21	1:A:260:VAL:HG21	1.94	0.49
1:D:341:ASP:OD2	2:D:504:IMP:O2'	2.30	0.49
1:C:381:GLN:HG2	1:E:25:VAL:HG12	1.94	0.49
1:A:478:ILE:HG12	1:B:418:ILE:HD12	1.94	0.49
1:E:252:THR:HG22	1:E:254:HIS:H	1.77	0.49
1:E:25:VAL:HG11	1:E:449:GLN:HG2	1.95	0.49
1:G:475:HIS:NE2	1:H:345:LYS:HD2	2.27	0.49
1:B:377:THR:CG2	1:B:384:GLN:HB3	2.43	0.49
1:D:52:ASP:HA	1:D:73:HIS:CD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:316:VAL:HG11	1:H:445:TYR:HB3	1.95	0.48
1:D:46:LEU:HD12	1:D:367:PHE:HZ	1.78	0.48
1:G:471:SER:HA	1:H:311:ARG:HD2	1.95	0.48
1:A:257:SER:HB3	1:A:260:VAL:HG23	1.95	0.48
1:C:311:ARG:HD2	1:D:471:SER:HA	1.96	0.48
1:B:303:GLY:HA2	1:B:308:CYS:SG	2.53	0.48
1:B:268:ARG:NH1	1:B:271:TYR:O	2.47	0.47
1:H:229:VAL:HG11	1:H:260:VAL:HA	1.96	0.47
1:H:88:VAL:HG11	1:H:223:VAL:HB	1.96	0.47
1:A:303:GLY:HA3	1:A:311:ARG:HE	1.79	0.47
1:A:311:ARG:HD2	1:C:471:SER:HA	1.96	0.47
1:F:344:ILE:HG23	1:F:349:ASP:HB2	1.95	0.47
3:F:502:2F0:O	3:F:502:2F0:C6	2.54	0.47
1:H:328:ALA:O	1:H:332:ARG:HB2	2.14	0.47
1:E:33:LYS:HG2	1:E:43:ASN:HD22	1.80	0.47
1:G:260:VAL:O	1:G:264:VAL:HG12	2.14	0.47
1:C:11:LEU:HD11	1:C:462:ARG:HD3	1.96	0.47
1:C:340:ALA:HB3	1:C:361:VAL:HG12	1.96	0.47
1:G:424:TYR:CZ	1:G:426:GLY:HA2	2.49	0.47
1:E:275:ASN:HA	1:E:296:ASN:HD21	1.80	0.47
1:H:47:ILE:HG13	1:H:360:VAL:HG11	1.97	0.47
1:C:339:ILE:HD13	1:C:360:VAL:HG13	1.96	0.47
1:H:416:GLU:OE1	3:H:505:2F0:N2	2.32	0.47
1:E:471:SER:HA	1:G:311:ARG:HD2	1.96	0.46
1:F:238:ASP:OD1	1:F:271:TYR:OH	2.27	0.46
1:H:11:LEU:N	1:H:322:THR:OG1	2.39	0.46
1:F:30:VAL:O	1:F:440:ARG:NH1	2.48	0.46
1:A:345:LYS:HD2	1:C:475:HIS:CD2	2.50	0.46
1:D:299:LYS:HG3	1:D:339:ILE:HB	1.98	0.46
1:F:328:ALA:O	1:F:332:ARG:HB2	2.15	0.46
1:A:303:GLY:HA3	1:A:311:ARG:NE	2.31	0.46
1:A:445:TYR:HB3	1:B:316:VAL:HG11	1.98	0.46
3:A:502:2F0:O	3:A:502:2F0:C3	2.56	0.46
1:A:350:MET:HG3	1:A:361:VAL:HG21	1.98	0.46
1:C:12:THR:OG1	1:D:470:GLU:OE1	2.34	0.46
1:C:75:ASN:HB2	1:C:391:MET:HE1	1.98	0.46
1:C:34:THR:HA	7:C:504:EDO:H21	1.98	0.45
1:G:261:ILE:HD13	1:G:290:LEU:HD23	1.97	0.45
1:D:238:ASP:OD1	1:D:271:TYR:OH	2.27	0.45
1:G:52:ASP:HA	1:G:73:HIS:CD2	2.52	0.45
1:B:377:THR:HG21	1:B:384:GLN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:501:2F0:O	3:D:501:2F0:H3	2.16	0.45
1:E:311:ARG:O	7:F:506:EDO:O2	2.33	0.45
1:B:252:THR:HG22	1:B:254:HIS:H	1.80	0.45
1:F:319:PRO:HD3	1:H:17:LEU:HD12	1.97	0.45
1:A:344[B]:ILE:HB	1:A:349:ASP:HB2	1.99	0.45
1:E:316:VAL:HG11	1:F:445:TYR:HB3	1.99	0.45
1:H:52:ASP:HA	1:H:73:HIS:CD2	2.52	0.45
1:B:81:GLN:OE1	1:B:236:ARG:NE	2.48	0.45
1:B:52:ASP:HA	1:B:73:HIS:CD2	2.52	0.45
1:B:413:LEU:O	9:B:645:HOH:O	2.20	0.45
1:F:303:GLY:HA2	1:F:308:CYS:SG	2.56	0.45
1:H:265:LYS:NZ	9:H:633:HOH:O	2.50	0.45
1:A:52:ASP:HA	1:A:73:HIS:CD2	2.52	0.45
1:G:45:PRO:HG3	1:G:451:LEU:HD11	1.99	0.44
1:C:52:ASP:HA	1:C:73:HIS:CD2	2.51	0.44
1:C:434:GLN:HB2	7:C:506:EDO:H12	2.00	0.44
1:H:248:ILE:HD12	1:H:274:LEU:HD21	1.99	0.44
1:D:344:ILE:HG23	1:D:349:ASP:HB2	2.00	0.44
3:D:501:2F0:O	3:D:501:2F0:C3	2.66	0.44
1:E:303:GLY:HA2	1:E:308:CYS:SG	2.57	0.44
1:A:328:ALA:O	1:A:332:ARG:N	2.46	0.44
1:D:89:LYS:HD2	1:D:244:SER:O	2.17	0.44
1:F:414:VAL:HG21	1:H:437:GLY:HA3	1.98	0.44
1:H:81:GLN:O	1:H:85:VAL:HG12	2.17	0.44
1:B:378:GLU:OE1	1:B:421:ARG:NH2	2.50	0.44
3:H:505:2F0:O1	3:H:505:2F0:CL1	2.72	0.44
1:F:276:ILE:H	1:F:296:ASN:HB2	1.83	0.44
1:H:268:ARG:HD3	1:H:272:PRO:HA	1.99	0.43
1:E:285:GLU:OE1	1:E:285:GLU:N	2.47	0.43
1:E:395:GLY:O	1:E:399:LYS:HD3	2.18	0.43
1:E:480:LYS:HE3	1:E:480:LYS:HB2	1.73	0.43
1:F:38:GLU:CD	1:F:38:GLU:H	2.21	0.43
1:H:57:ALA:O	1:H:61:ILE:HG12	2.17	0.43
1:G:258[B]:GLN:NE2	1:G:262:ASP:OD1	2.43	0.43
1:H:303:GLY:HA2	1:H:308:CYS:SG	2.58	0.43
1:B:308:CYS:SG	2:B:500:IMP:H2	2.59	0.43
1:D:10:GLY:HA3	1:D:319:PRO:HG2	1.99	0.43
1:G:44:ILE:HD12	1:G:46:LEU:HD12	1.99	0.43
1:B:39:SER:OG	1:B:275:ASN:ND2	2.52	0.43
1:E:414:VAL:HG23	1:F:484:ASN:HD22	1.84	0.43
1:F:268:ARG:NH1	1:F:272:PRO:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:233:ALA:O	1:H:237:ILE:HG12	2.18	0.43
1:E:284:ALA:HB1	1:E:330:GLU:HB2	2.01	0.43
1:C:48:SER:HB2	1:C:63:MET:HG3	2.01	0.42
1:E:79:GLU:CD	1:E:79:GLU:H	2.22	0.42
1:G:344:ILE:HG23	1:G:349:ASP:HB2	2.00	0.42
1:H:234:MET:HE1	1:H:270:LYS:HD3	2.01	0.42
1:B:34:THR:HG23	1:B:451:LEU:HD12	2.01	0.42
1:C:344:ILE:HG23	1:C:349:ASP:HB2	2.01	0.42
1:D:37:SER:OG	1:D:38:GLU:N	2.53	0.42
1:B:311:ARG:NH2	1:B:318:VAL:O	2.53	0.42
1:E:340:ALA:HB3	1:E:361:VAL:HG22	2.01	0.42
1:G:479:THR:HG23	1:H:420:GLY:HA2	2.01	0.42
1:H:237:ILE:HG23	1:H:248:ILE:HD13	2.02	0.42
1:H:287:THR:HG23	1:H:298:VAL:HG11	2.02	0.42
1:D:395:GLY:O	1:D:398[A]:GLU:HG2	2.20	0.42
1:D:33:LYS:HG2	1:D:43:ASN:HA	2.02	0.42
1:H:12:THR:OG1	1:H:13:PHE:N	2.51	0.42
1:E:445:TYR:HB3	1:G:316:VAL:HG11	2.00	0.42
1:G:357:GLY:HA2	1:G:455:ARG:HG2	2.01	0.42
1:A:10:GLY:HA3	1:A:319:PRO:HG2	2.02	0.42
1:A:345:LYS:HD2	1:C:475:HIS:NE2	2.34	0.42
1:E:89:LYS:HD3	1:E:89:LYS:HA	1.88	0.42
1:G:445:TYR:HB2	1:H:316:VAL:HG21	2.02	0.42
1:H:61:ILE:HD13	1:H:88:VAL:HG13	2.01	0.42
1:A:466:ALA:HB1	1:B:14:ASP:HB2	2.02	0.41
1:A:470:GLU:OE1	1:B:12:THR:OG1	2.32	0.41
1:C:45:PRO:C	1:C:360:VAL:HG23	2.40	0.41
3:E:509:2F0:O	3:E:509:2F0:H3	2.20	0.41
1:C:14:ASP:HB3	1:C:468:LEU:HD22	2.02	0.41
1:F:282:ALA:HB1	1:F:318:VAL:HB	2.01	0.41
1:H:34:THR:HG21	1:H:360:VAL:HG22	2.01	0.41
1:A:35:VAL:HG13	1:A:41:GLN:HG2	2.02	0.41
1:B:78:ILE:H	1:B:78:ILE:HD12	1.85	0.41
1:G:22:LYS:HE2	1:H:261:ILE:HD12	2.02	0.41
1:A:345:LYS:HE2	1:A:345:LYS:HB2	1.89	0.41
1:E:254:HIS:CE1	1:E:256:HIS:HB3	2.55	0.41
1:F:345:LYS:H	1:F:345:LYS:HG3	1.71	0.41
1:D:368:ALA:HB3	1:D:422:VAL:HG21	2.02	0.41
1:H:63:MET:SD	1:H:428:LEU:HD21	2.60	0.41
1:C:89:LYS:HE3	1:C:221:LEU:O	2.21	0.41
1:D:279:GLY:HA3	1:D:280:ASN:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:ASP:OD1	1:G:24:ASP:N	2.53	0.41
1:A:338:VAL:HG23	1:A:358:ALA:HA	2.01	0.41
1:E:345:LYS:HZ3	1:F:474:HIS:CD2	2.38	0.41
1:B:14:ASP:HB3	1:B:468:LEU:HD22	2.03	0.41
1:C:296:ASN:O	1:C:336:ILE:HG23	2.21	0.41
1:A:268[A]:ARG:NH2	1:A:294:GLY:O	2.54	0.41
1:A:316:VAL:HG11	1:C:445:TYR:HB3	2.03	0.40
1:C:287:THR:HG23	1:C:298:VAL:HG21	2.03	0.40
1:G:350:MET:HG3	1:G:361:VAL:HG21	2.03	0.40
1:B:370:VAL:O	1:B:373:SER:HB3	2.22	0.40
1:C:303:GLY:HA3	1:C:311:ARG:HG3	2.03	0.40
1:E:261:ILE:HD13	1:E:290:LEU:HD23	2.03	0.40
1:B:89:LYS:HD2	1:B:89:LYS:HA	1.76	0.40
1:B:445:TYR:HB2	1:D:316:VAL:HG21	2.04	0.40
1:B:451:LEU:HD23	1:B:451:LEU:HA	1.94	0.40
1:B:287:THR:HG23	1:B:298:VAL:HG21	2.04	0.40
1:C:257:SER:OG	1:C:260:VAL:HG23	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	354/384 (92%)	342 (97%)	12 (3%)	0	100	100
1	B	352/384 (92%)	343 (97%)	8 (2%)	1 (0%)	41	66
1	C	348/384 (91%)	338 (97%)	10 (3%)	0	100	100
1	D	352/384 (92%)	340 (97%)	11 (3%)	1 (0%)	41	66
1	E	350/384 (91%)	342 (98%)	8 (2%)	0	100	100
1	F	346/384 (90%)	336 (97%)	10 (3%)	0	100	100
1	G	354/384 (92%)	350 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	346/384 (90%)	337 (97%)	9 (3%)	0	100 100
All	All	2802/3072 (91%)	2728 (97%)	72 (3%)	2 (0%)	51 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	GLY
1	D	412	LYS

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	276/298 (93%)	268 (97%)	8 (3%)	42 71
1	B	273/298 (92%)	262 (96%)	11 (4%)	31 60
1	C	270/298 (91%)	261 (97%)	9 (3%)	38 67
1	D	273/298 (92%)	267 (98%)	6 (2%)	52 79
1	E	271/298 (91%)	258 (95%)	13 (5%)	25 53
1	F	268/298 (90%)	261 (97%)	7 (3%)	46 75
1	G	274/298 (92%)	270 (98%)	4 (2%)	65 86
1	H	268/298 (90%)	263 (98%)	5 (2%)	57 82
All	All	2173/2384 (91%)	2110 (97%)	63 (3%)	42 71

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	VAL
1	A	39	SER
1	A	251	ASP
1	A	296	ASN
1	A	386	LYS

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Mol	Chain	Res	Type
1	A	477	GLN
1	A	480	LYS
1	B	-3	GLN
1	B	-2	SER
1	B	34	THR
1	B	41	GLN
1	B	79	GLU
1	B	297	VAL
1	B	360	VAL
1	B	370	VAL
1	B	380	TYR
1	B	402	LYS
1	B	413	LEU
1	C	74	LYS
1	C	75	ASN
1	C	223	VAL
1	C	251	ASP
1	C	345	LYS
1	C	389	ARG
1	C	398	GLU
1	C	414	VAL
1	C	469	LEU
1	D	9	GLU
1	D	46	LEU
1	D	74	LYS
1	D	221	LEU
1	D	245	VAL
1	D	432	VAL
1	E	16	VAL
1	E	34	THR
1	E	79	GLU
1	E	221	LEU
1	E	227	VAL
1	E	251	ASP
1	E	256	HIS
1	E	266	GLU
1	E	338	VAL
1	E	359	HIS
1	E	361	VAL
1	E	370	VAL
1	E	414	VAL
1	F	30	VAL

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Mol	Chain	Res	Type
1	F	34	THR
1	F	345	LYS
1	F	376	GLU
1	F	377	THR
1	F	413	LEU
1	F	475	HIS
1	G	248	ILE
1	G	370	VAL
1	G	377	THR
1	G	389	ARG
1	H	227	VAL
1	H	248	ILE
1	H	252	THR
1	H	378	GLU
1	H	386	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	GLN
1	B	275	ASN
1	B	334	HIS
1	C	75	ASN
1	C	475	HIS
1	D	84	GLN
1	E	43	ASN
1	E	474	HIS
1	E	475	HIS
1	E	477	GLN
1	F	474	HIS
1	G	459	GLN
1	G	474	HIS
1	H	434	GLN

5.3.3 RNA

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)

48 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	$\#\|Z\| > 2$
8	SO4	C	505	-	4,4,4	0.14	0	6,6,6	0.05	0
2	IMP	E	501	-	21,25,25	1.47	2 (9%)	24,38,38	1.27	4 (16%)
2	IMP	D	504	-	21,25,25	1.46	2 (9%)	24,38,38	1.26	4 (16%)
4	FMT	D	506	-	2,2,2	0.71	0	1,1,1	0.23	0
4	FMT	H	501	-	2,2,2	0.72	0	1,1,1	0.25	0
3	2F0	F	502	-	28,28,28	1.57	5 (17%)	40,40,40	1.48	3 (7%)
7	EDO	F	504	-	3,3,3	0.47	0	2,2,2	0.33	0
3	2F0	H	505	-	28,28,28	1.48	3 (10%)	40,40,40	1.50	6 (15%)
5	GOL	E	506	-	5,5,5	0.39	0	5,5,5	0.21	0
6	MLI	A	506	-	6,6,6	1.20	0	7,7,7	1.31	0
6	MLI	E	508	-	6,6,6	1.21	0	7,7,7	1.29	0
2	IMP	H	504	-	21,25,25	1.47	2 (9%)	24,38,38	1.30	4 (16%)
3	2F0	E	509	-	28,28,28	1.73	4 (14%)	40,40,40	1.18	2 (5%)
4	FMT	F	507	-	2,2,2	0.71	0	1,1,1	0.24	0
7	EDO	D	503	-	3,3,3	0.47	0	2,2,2	0.31	0
7	EDO	F	506	-	3,3,3	0.45	0	2,2,2	0.31	0
7	EDO	C	506	-	3,3,3	0.46	0	2,2,2	0.27	0
3	2F0	E	502	-	28,28,28	1.58	5 (17%)	40,40,40	1.23	5 (12%)
2	IMP	F	501	-	21,25,25	1.47	2 (9%)	24,38,38	1.28	4 (16%)
3	2F0	A	502	-	28,28,28	1.67	6 (21%)	40,40,40	1.13	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FMT	A	503	-	2,2,2	0.72	0	1,1,1	0.24	0
4	FMT	F	503	-	2,2,2	0.72	0	1,1,1	0.24	0
4	FMT	B	503	-	2,2,2	0.73	0	1,1,1	0.23	0
2	IMP	A	501	-	21,25,25	1.55	2 (9%)	24,38,38	1.30	4 (16%)
4	FMT	H	503	-	2,2,2	0.73	0	1,1,1	0.24	0
8	SO4	G	502	-	4,4,4	0.14	0	6,6,6	0.06	0
7	EDO	F	505	-	3,3,3	0.46	0	2,2,2	0.32	0
3	2F0	C	503	-	28,28,28	1.59	5 (17%)	40,40,40	1.26	3 (7%)
7	EDO	D	502	-	3,3,3	0.46	0	2,2,2	0.33	0
2	IMP	C	502	-	21,25,25	1.48	2 (9%)	24,38,38	1.28	4 (16%)
2	IMP	G	501	-	21,25,25	1.47	2 (9%)	24,38,38	1.29	4 (16%)
4	FMT	A	504	-	2,2,2	0.72	0	1,1,1	0.23	0
4	FMT	E	507	-	2,2,2	0.73	0	1,1,1	0.26	0
7	EDO	B	502	-	3,3,3	0.45	0	2,2,2	0.37	0
7	EDO	E	505	-	3,3,3	0.47	0	2,2,2	0.32	0
2	IMP	B	500	-	21,25,25	1.45	2 (9%)	24,38,38	1.28	3 (12%)
4	FMT	H	502	-	2,2,2	0.71	0	1,1,1	0.24	0
5	GOL	A	505	-	5,5,5	0.36	0	5,5,5	0.33	0
4	FMT	D	507	-	2,2,2	0.72	0	1,1,1	0.23	0
8	SO4	G	503	-	4,4,4	0.14	0	6,6,6	0.05	0
4	FMT	E	504	-	2,2,2	0.72	0	1,1,1	0.23	0
4	FMT	H	506	-	2,2,2	0.72	0	1,1,1	0.23	0
3	2F0	B	501	-	28,28,28	1.73	4 (14%)	40,40,40	1.11	2 (5%)
4	FMT	E	503	-	2,2,2	0.71	0	1,1,1	0.23	0
7	EDO	C	504	-	3,3,3	0.46	0	2,2,2	0.33	0
7	EDO	D	505	-	3,3,3	0.47	0	2,2,2	0.33	0
3	2F0	D	501	-	28,28,28	1.42	4 (14%)	40,40,40	1.64	7 (17%)
4	FMT	C	501	-	2,2,2	0.72	0	1,1,1	0.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	E	501	-	-	0/6/26/26	0/3/3/3
2	IMP	D	504	-	-	0/6/26/26	0/3/3/3
3	2F0	F	502	-	-	4/25/25/25	0/2/2/2
7	EDO	F	504	-	-	0/1/1/1	-
3	2F0	H	505	-	-	0/25/25/25	0/2/2/2
5	GOL	E	506	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MLI	A	506	-	-	0/4/4/4	-
6	MLI	E	508	-	-	4/4/4/4	-
2	IMP	H	504	-	-	0/6/26/26	0/3/3/3
3	2F0	E	509	-	-	5/25/25/25	0/2/2/2
7	EDO	D	503	-	-	0/1/1/1	-
7	EDO	F	506	-	-	0/1/1/1	-
7	EDO	C	506	-	-	0/1/1/1	-
3	2F0	E	502	-	-	3/25/25/25	0/2/2/2
2	IMP	F	501	-	-	0/6/26/26	0/3/3/3
3	2F0	A	502	-	-	3/25/25/25	0/2/2/2
2	IMP	A	501	-	-	0/6/26/26	0/3/3/3
7	EDO	F	505	-	-	0/1/1/1	-
3	2F0	C	503	-	-	4/25/25/25	0/2/2/2
7	EDO	D	502	-	-	0/1/1/1	-
2	IMP	C	502	-	-	0/6/26/26	0/3/3/3
2	IMP	G	501	-	-	0/6/26/26	0/3/3/3
7	EDO	E	505	-	-	0/1/1/1	-
7	EDO	B	502	-	-	0/1/1/1	-
2	IMP	B	500	-	-	0/6/26/26	0/3/3/3
5	GOL	A	505	-	-	2/4/4/4	-
3	2F0	B	501	-	-	4/25/25/25	0/2/2/2
7	EDO	C	504	-	-	0/1/1/1	-
7	EDO	D	505	-	-	0/1/1/1	-
3	2F0	D	501	-	-	3/25/25/25	0/2/2/2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IMP	C2-N3	5.13	1.39	1.29
3	B	501	2F0	C1-C12	-4.97	1.47	1.53
3	E	509	2F0	C1-C12	-4.94	1.47	1.53
3	C	503	2F0	C1-C12	-4.78	1.47	1.53
3	F	502	2F0	C1-C12	-4.78	1.47	1.53
2	F	501	IMP	C2-N3	4.76	1.38	1.29
2	G	501	IMP	C2-N3	4.75	1.38	1.29
2	C	502	IMP	C2-N3	4.74	1.38	1.29
2	E	501	IMP	C2-N3	4.71	1.38	1.29
2	D	504	IMP	C2-N3	4.70	1.38	1.29
2	H	504	IMP	C2-N3	4.69	1.38	1.29
2	B	500	IMP	C2-N3	4.65	1.38	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	2F0	C1-C12	-4.46	1.48	1.53
2	A	501	IMP	C5-C6	-4.05	1.39	1.47
2	E	501	IMP	C5-C6	-3.97	1.39	1.47
2	C	502	IMP	C5-C6	-3.97	1.39	1.47
3	A	502	2F0	C1-N1	-3.97	1.43	1.47
3	E	509	2F0	C1-N1	-3.95	1.43	1.47
2	H	504	IMP	C5-C6	-3.94	1.39	1.47
2	B	500	IMP	C5-C6	-3.90	1.39	1.47
3	E	502	2F0	C1-C12	-3.90	1.48	1.53
2	F	501	IMP	C5-C6	-3.90	1.39	1.47
2	G	501	IMP	C5-C6	-3.90	1.39	1.47
2	D	504	IMP	C5-C6	-3.82	1.39	1.47
3	H	505	2F0	C1-C12	-3.78	1.49	1.53
3	D	501	2F0	C1-C12	-3.77	1.49	1.53
3	B	501	2F0	C1-N1	-3.76	1.43	1.47
3	E	502	2F0	C1-N1	-3.46	1.43	1.47
3	C	503	2F0	C1-N1	-3.20	1.43	1.47
3	H	505	2F0	C1-N1	-3.18	1.44	1.47
3	B	501	2F0	C18-N4	-3.08	1.23	1.28
3	F	502	2F0	C4-N2	-2.99	1.31	1.37
3	B	501	2F0	C4-N2	-2.73	1.31	1.37
3	F	502	2F0	C1-N1	-2.67	1.44	1.47
3	C	503	2F0	C4-N2	-2.62	1.32	1.37
3	E	509	2F0	C4-N2	-2.57	1.32	1.37
3	E	502	2F0	C4-N2	-2.52	1.32	1.37
3	H	505	2F0	C4-N2	-2.51	1.32	1.37
3	E	509	2F0	C18-N4	-2.50	1.24	1.28
3	A	502	2F0	C4-N2	-2.48	1.32	1.37
3	D	501	2F0	C1-N1	-2.37	1.44	1.47
3	A	502	2F0	C18-N4	-2.34	1.24	1.28
3	E	502	2F0	C18-N4	-2.26	1.24	1.28
3	C	503	2F0	C2-C1	-2.17	1.50	1.53
3	C	503	2F0	C18-N4	-2.15	1.24	1.28
3	D	501	2F0	C4-N2	-2.14	1.33	1.37
3	E	502	2F0	C4-N1	-2.10	1.31	1.35
3	F	502	2F0	C18-N4	-2.09	1.24	1.28
3	F	502	2F0	C2-C1	-2.08	1.50	1.53
3	A	502	2F0	C2-C1	-2.08	1.50	1.53
3	A	502	2F0	C4-N1	-2.05	1.31	1.35
3	D	501	2F0	C18-N4	-2.01	1.25	1.28

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	501	2F0	O2-N4-C18	6.23	121.61	112.68
3	F	502	2F0	O2-N4-C18	5.85	121.06	112.68
3	H	505	2F0	O2-N4-C18	4.95	119.77	112.68
3	A	502	2F0	O2-N4-C18	4.51	119.15	112.68
3	H	505	2F0	C8-C7-C11	-4.13	116.09	122.59
3	D	501	2F0	C17-C16-C18	-4.12	114.82	120.54
3	E	502	2F0	O2-N4-C18	4.09	118.54	112.68
3	C	503	2F0	O2-N4-C18	3.94	118.32	112.68
3	E	509	2F0	O2-N4-C18	3.71	117.99	112.68
2	F	501	IMP	C5-C6-N1	3.22	119.63	113.95
2	A	501	IMP	C5-C6-N1	3.20	119.60	113.95
2	B	500	IMP	C8-N7-C5	3.12	108.93	102.99
2	E	501	IMP	C5-C6-N1	3.09	119.40	113.95
2	C	502	IMP	C5-C6-N1	3.07	119.38	113.95
2	B	500	IMP	C5-C6-N1	3.06	119.35	113.95
2	D	504	IMP	C8-N7-C5	3.05	108.80	102.99
2	F	501	IMP	C8-N7-C5	3.04	108.78	102.99
2	H	504	IMP	C8-N7-C5	3.03	108.75	102.99
2	G	501	IMP	C8-N7-C5	3.02	108.75	102.99
2	G	501	IMP	C5-C6-N1	3.01	119.27	113.95
2	D	504	IMP	C5-C6-N1	3.00	119.25	113.95
2	E	501	IMP	C8-N7-C5	3.00	108.70	102.99
2	C	502	IMP	C8-N7-C5	2.91	108.54	102.99
2	H	504	IMP	C5-C6-N1	2.87	119.02	113.95
3	H	505	2F0	C17-C16-C18	-2.83	116.61	120.54
2	H	504	IMP	O6-C6-C5	-2.76	118.97	124.37
2	A	501	IMP	C8-N7-C5	2.74	108.21	102.99
3	B	501	2F0	C19-C18-N4	-2.72	115.72	123.55
3	B	501	2F0	C19-C18-C16	2.71	124.05	119.43
2	A	501	IMP	O6-C6-C5	-2.71	119.08	124.37
3	D	501	2F0	C19-C18-C16	2.62	123.88	119.43
3	E	502	2F0	C8-C7-C11	-2.57	118.55	122.59
2	C	502	IMP	O6-C6-C5	-2.55	119.40	124.37
3	F	502	2F0	C1-N1-C4	2.51	129.49	124.17
2	G	501	IMP	O6-C6-C5	-2.45	119.59	124.37
3	H	505	2F0	C6-C7-C8	2.39	120.65	117.92
3	D	501	2F0	C8-C7-C11	-2.33	118.92	122.59
2	B	500	IMP	O6-C6-C5	-2.31	119.86	124.37
2	D	504	IMP	O6-C6-C5	-2.30	119.88	124.37
3	C	503	2F0	C1-N1-C4	2.24	128.92	124.17
3	D	501	2F0	C15-C16-C18	2.23	123.94	121.26
2	F	501	IMP	O6-C6-C5	-2.23	120.01	124.37
3	D	501	2F0	C17-C12-C1	-2.23	117.14	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	IMP	O6-C6-C5	-2.21	120.05	124.37
2	A	501	IMP	N1-C2-N3	-2.18	120.19	125.87
3	C	503	2F0	C8-C7-C11	-2.18	119.17	122.59
3	E	509	2F0	C6-C7-C8	2.16	120.39	117.92
2	G	501	IMP	N1-C2-N3	-2.14	120.30	125.87
3	D	501	2F0	C6-C7-C8	2.14	120.36	117.92
3	E	502	2F0	C19-C18-N4	-2.13	117.43	123.55
2	C	502	IMP	N1-C2-N3	-2.13	120.32	125.87
3	E	502	2F0	C19-C18-C16	2.12	123.05	119.43
2	F	501	IMP	N1-C2-N3	-2.12	120.34	125.87
3	H	505	2F0	C15-C16-C17	2.11	121.74	119.24
2	H	504	IMP	N1-C2-N3	-2.11	120.36	125.87
3	F	502	2F0	O1-C11-N3	-2.10	119.59	122.58
2	E	501	IMP	N1-C2-N3	-2.09	120.41	125.87
2	D	504	IMP	N1-C2-N3	-2.09	120.42	125.87
3	A	502	2F0	C17-C16-C18	-2.02	117.73	120.54
3	E	502	2F0	C6-C7-C8	2.01	120.22	117.92
3	H	505	2F0	C7-C8-CL1	-2.01	118.03	121.00

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	503	2F0	N3-C11-C7-C8
3	F	502	2F0	O1-C11-C7-C8
3	F	502	2F0	N3-C11-C7-C6
3	F	502	2F0	N3-C11-C7-C8
5	A	505	GOL	O1-C1-C2-C3
5	E	506	GOL	O1-C1-C2-C3
3	F	502	2F0	O1-C11-C7-C6
3	C	503	2F0	N3-C11-C7-C6
5	E	506	GOL	O1-C1-C2-O2
3	A	502	2F0	C3-C1-N1-C4
3	C	503	2F0	O1-C11-C7-C8
3	C	503	2F0	O1-C11-C7-C6
3	A	502	2F0	C2-C1-N1-C4
3	D	501	2F0	C3-C1-N1-C4
3	E	502	2F0	C2-C1-N1-C4
3	E	502	2F0	C3-C1-N1-C4
3	E	509	2F0	C3-C1-N1-C4
3	E	509	2F0	C2-C1-N1-C4
3	B	501	2F0	O1-C11-C7-C8

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Mol	Chain	Res	Type	Atoms
3	B	501	2F0	N3-C11-C7-C8
3	E	509	2F0	O1-C11-C7-C8
3	E	509	2F0	N3-C11-C7-C8
6	E	508	MLI	C2-C1-C3-O8
5	A	505	GOL	O1-C1-C2-O2
3	A	502	2F0	C12-C1-N1-C4
3	D	501	2F0	C2-C1-N1-C4
3	E	502	2F0	C12-C1-N1-C4
3	E	509	2F0	C12-C1-N1-C4
3	B	501	2F0	N3-C11-C7-C6
6	E	508	MLI	C2-C1-C3-O9
3	B	501	2F0	O1-C11-C7-C6
3	D	501	2F0	N3-C11-C7-C8
6	E	508	MLI	C3-C1-C2-O6
6	E	508	MLI	C3-C1-C2-O7

There are no ring outliers.

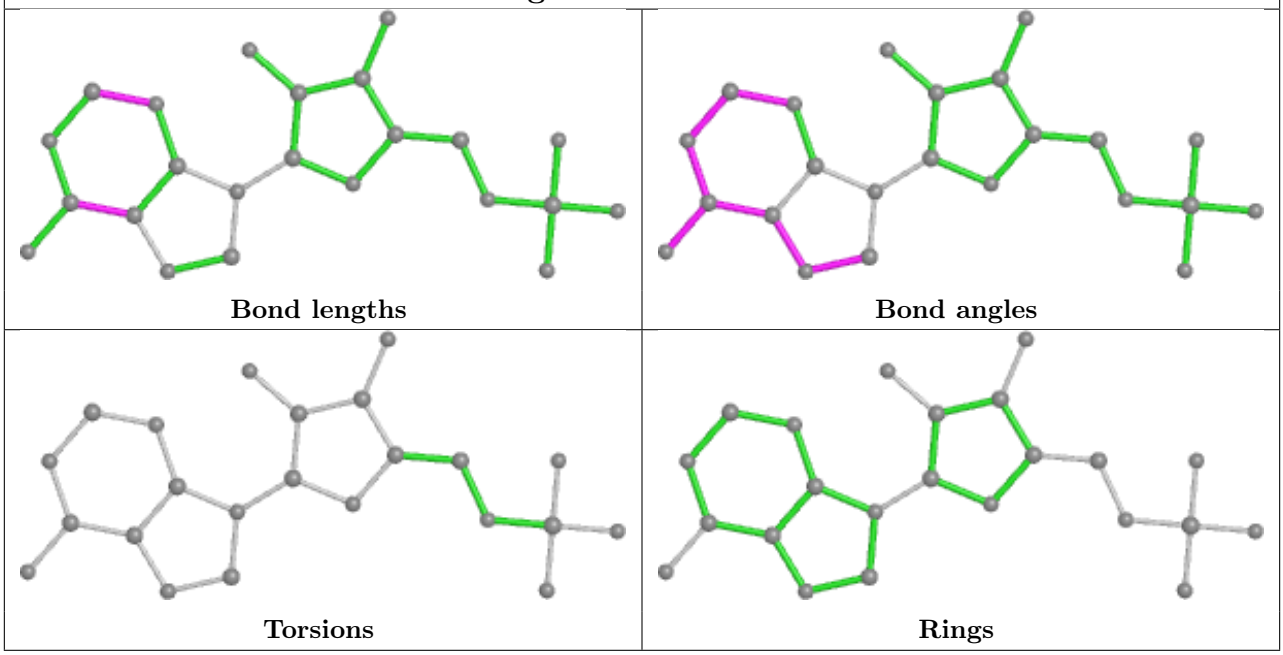
18 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	504	IMP	1	0
3	F	502	2F0	2	0
3	H	505	2F0	4	0
2	H	504	IMP	1	0
3	E	509	2F0	2	0
7	F	506	EDO	2	0
7	C	506	EDO	2	0
3	E	502	2F0	4	0
2	F	501	IMP	1	0
3	A	502	2F0	3	0
2	A	501	IMP	1	0
3	C	503	2F0	1	0
2	C	502	IMP	1	0
2	G	501	IMP	1	0
2	B	500	IMP	2	0
3	B	501	2F0	2	0
7	C	504	EDO	2	0
3	D	501	2F0	3	0

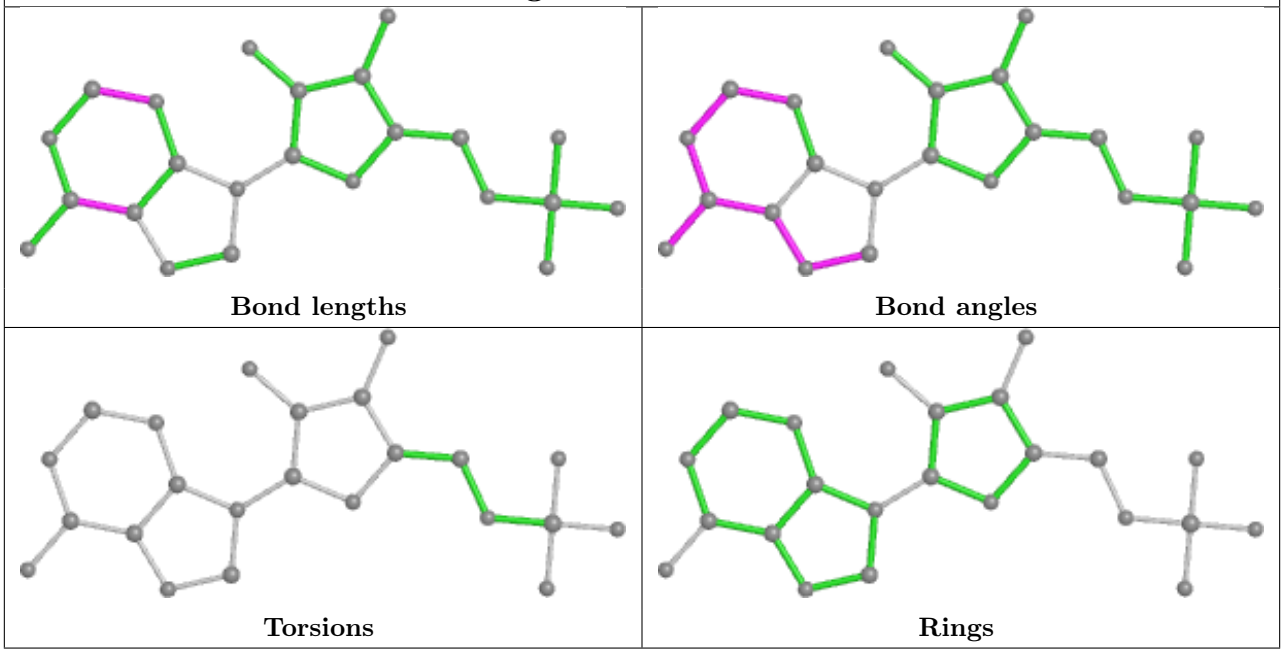
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

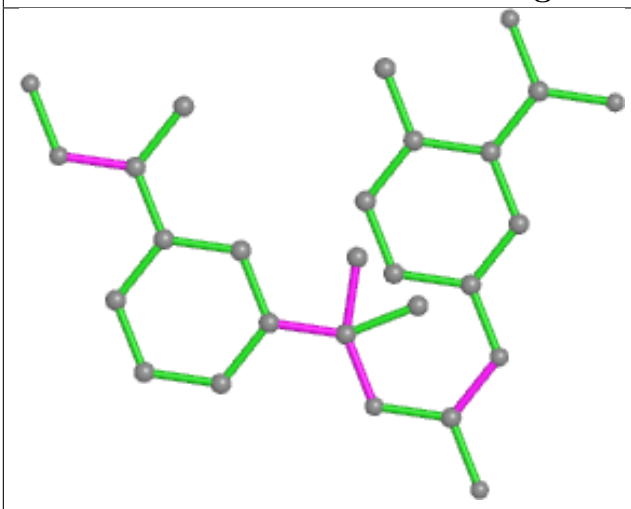
Ligand IMP E 501



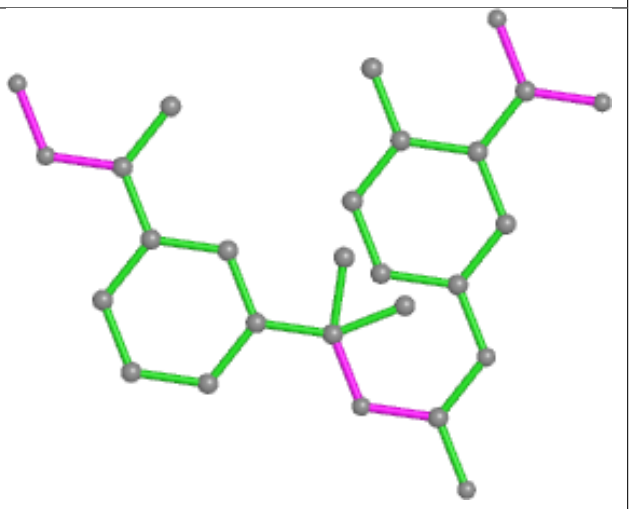
Ligand IMP D 504



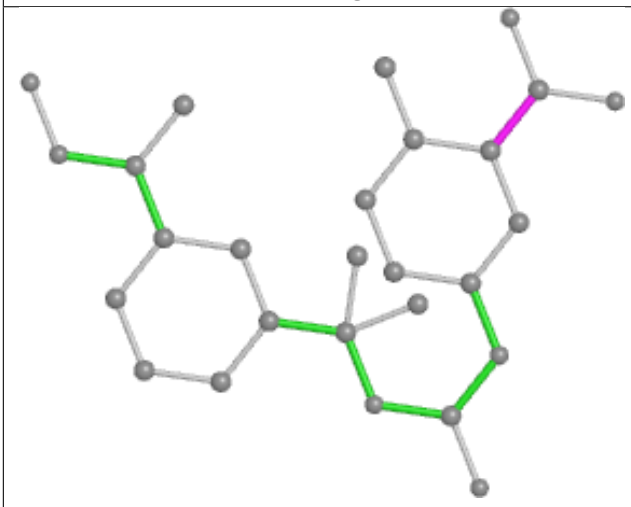
Ligand 2F0 F 502



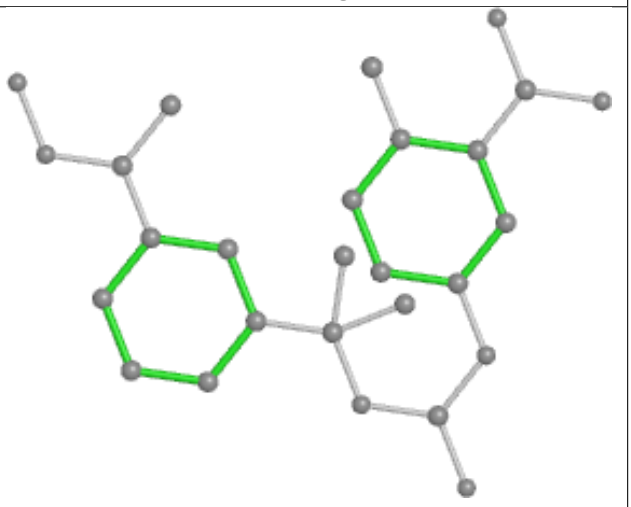
Bond lengths



Bond angles

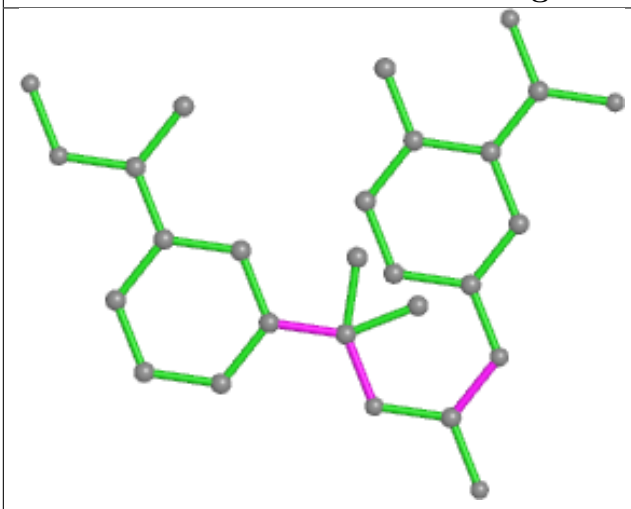


Torsions

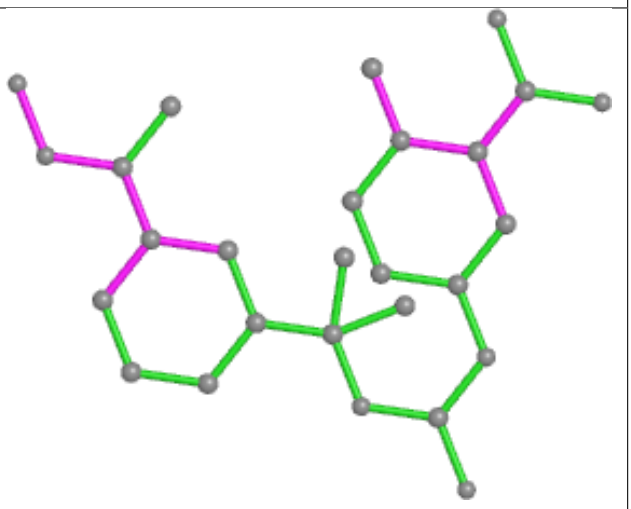


Rings

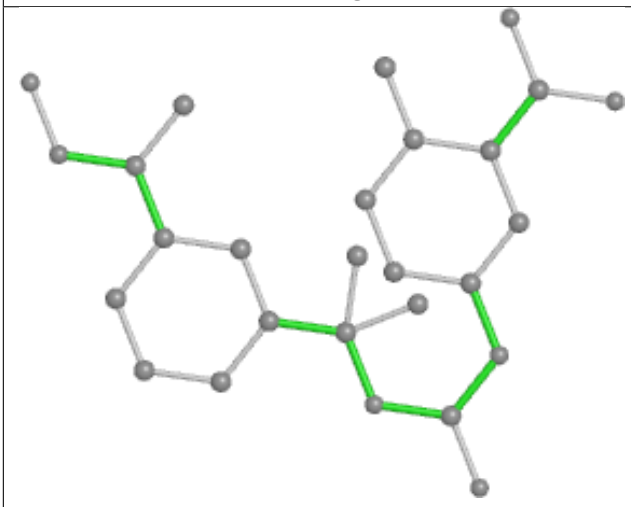
Ligand 2F0 H 505



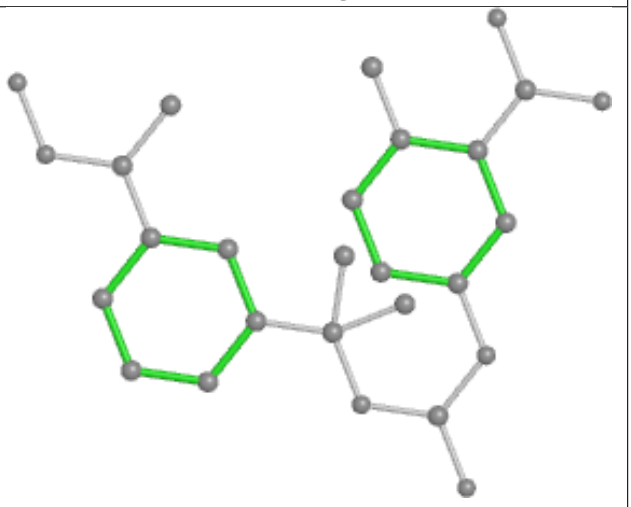
Bond lengths



Bond angles

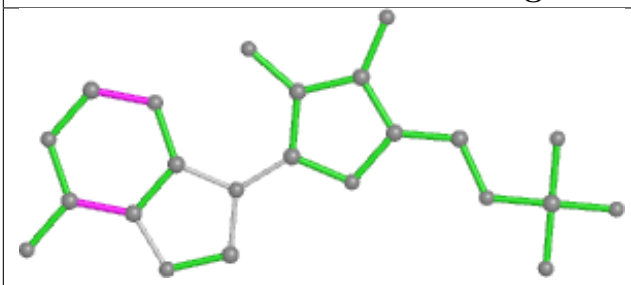


Torsions

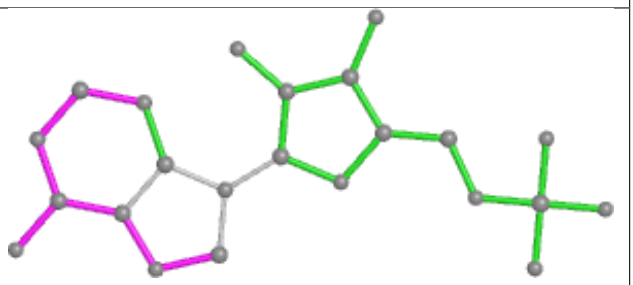


Rings

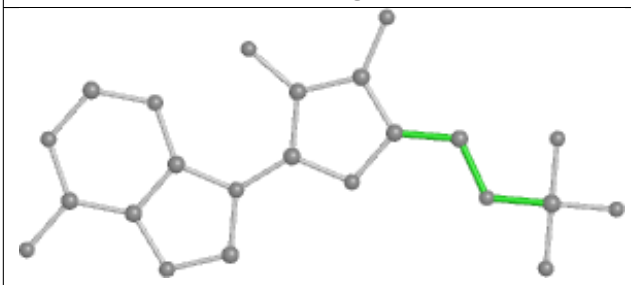
Ligand IMP H 504



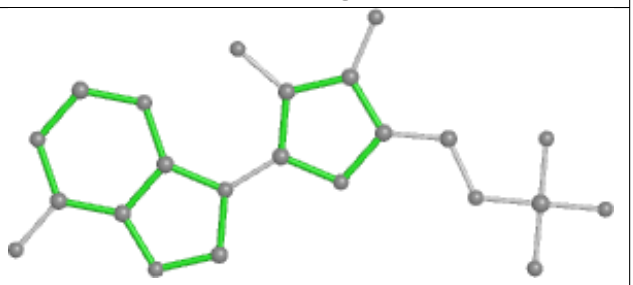
Bond lengths



Bond angles

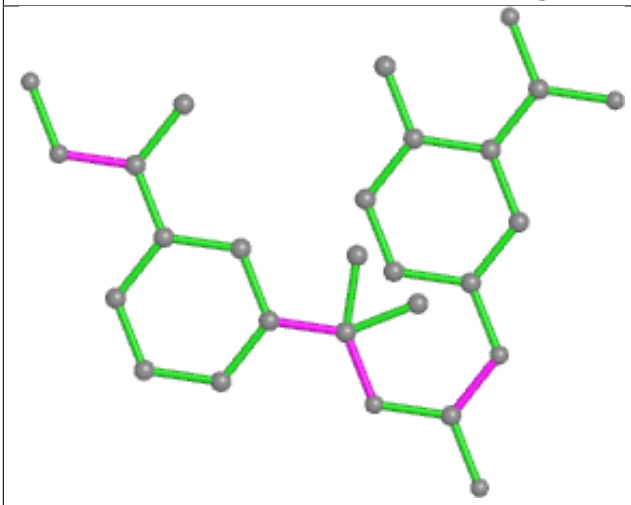


Torsions



Rings

Ligand 2F0 E 509



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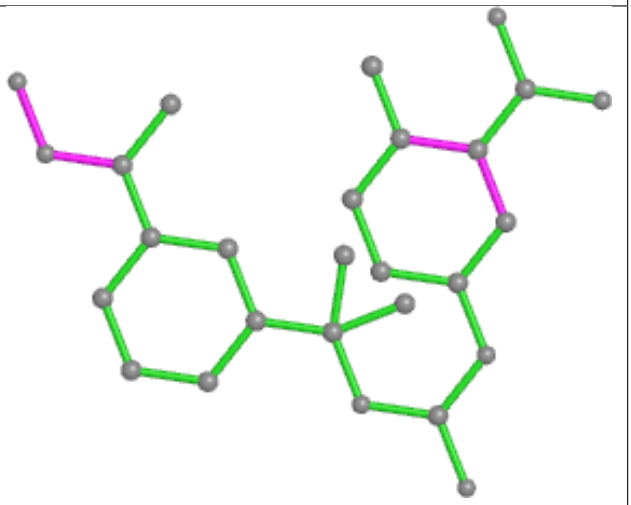
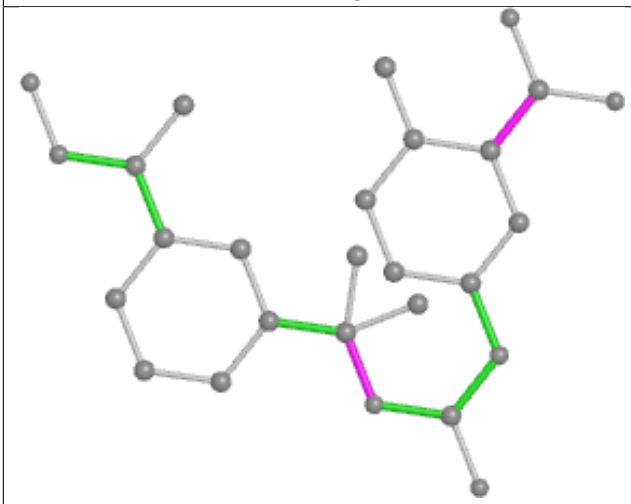
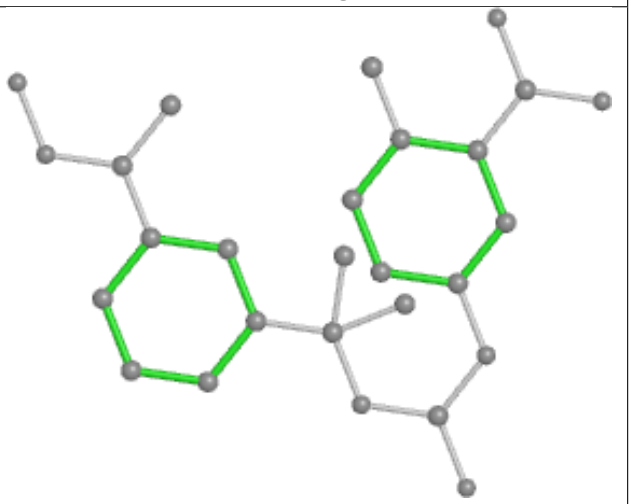


Bond angles

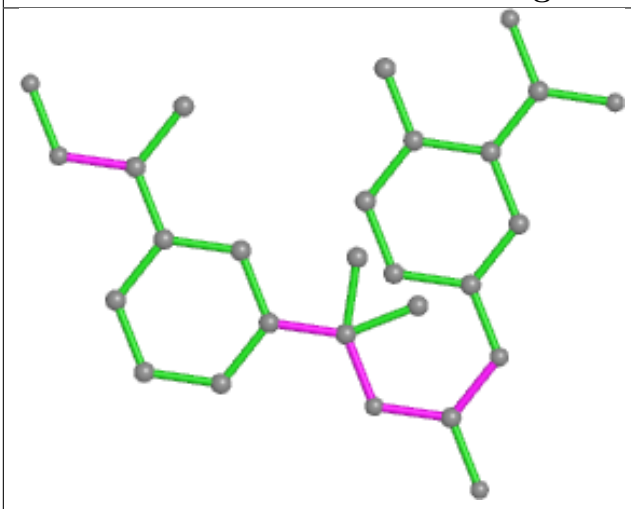


Torsions

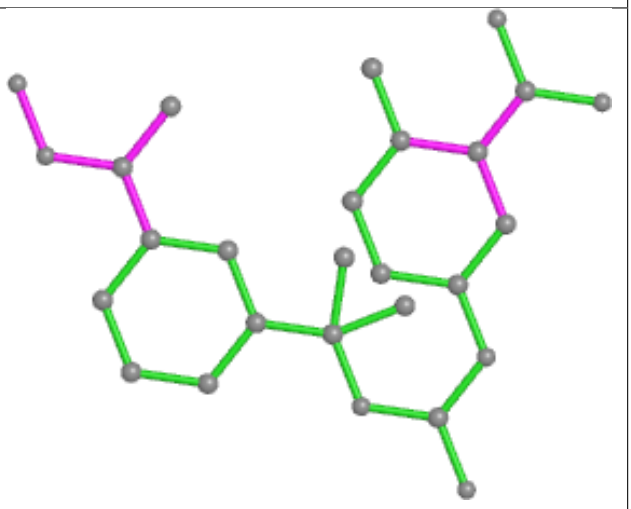


Rings

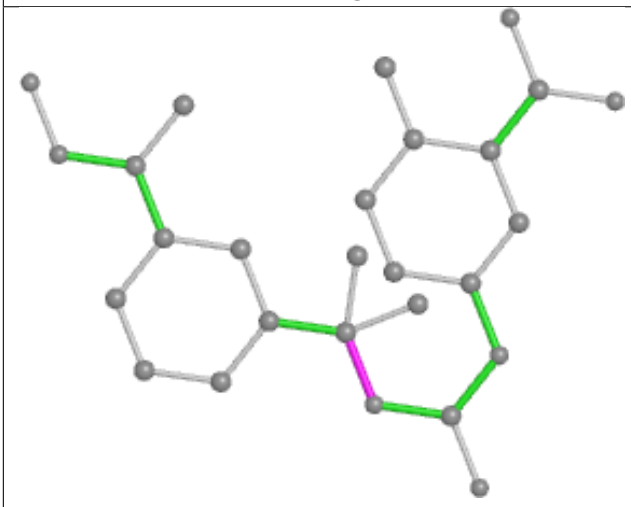
Ligand 2F0 E 502



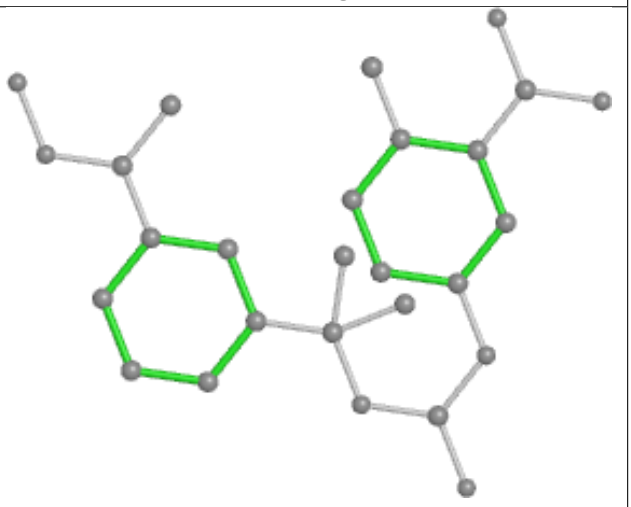
Bond lengths



Bond angles

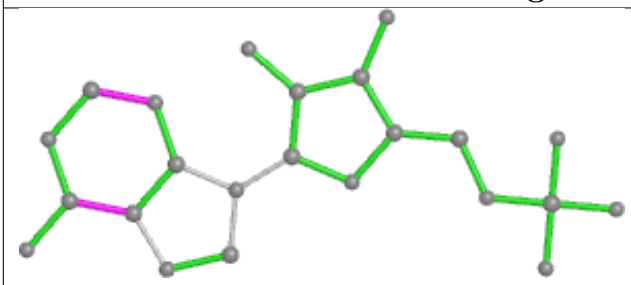


Torsions

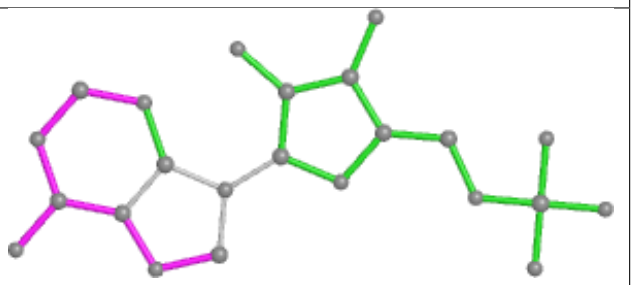


Rings

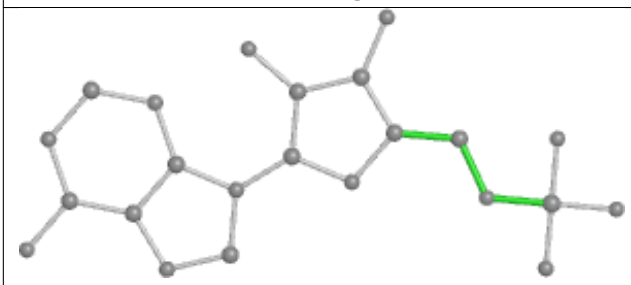
Ligand IMP F 501



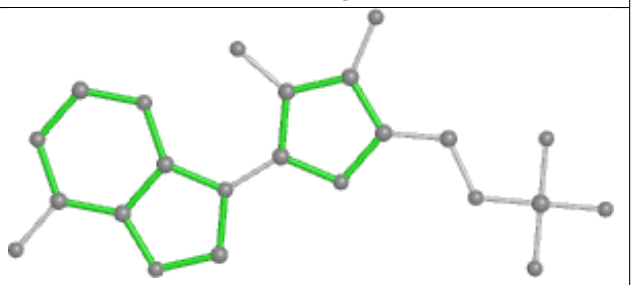
Bond lengths



Bond angles

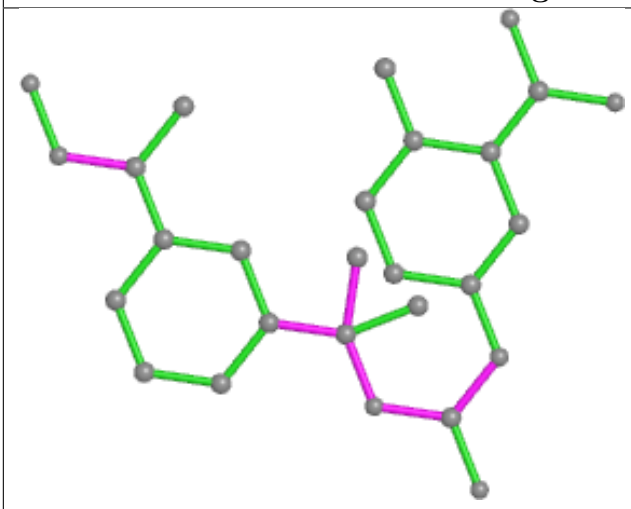


Torsions

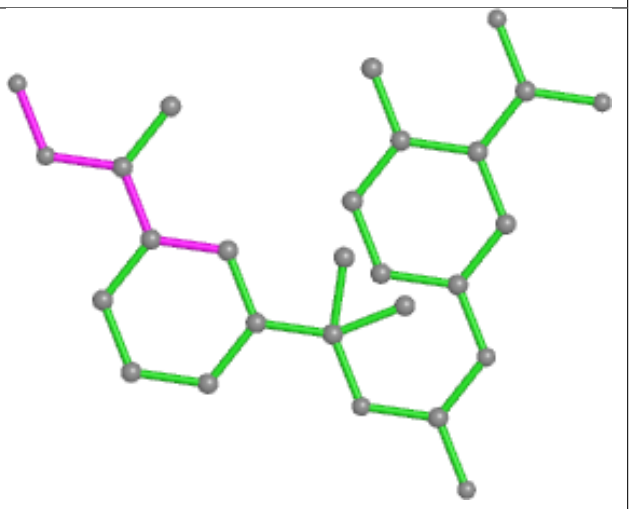


Rings

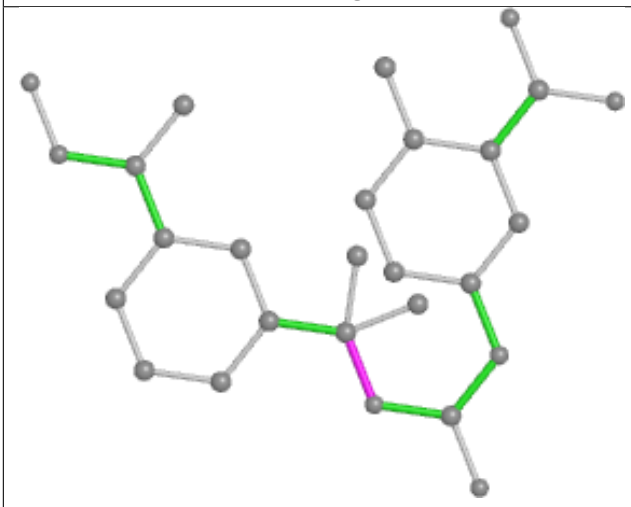
Ligand 2F0 A 502



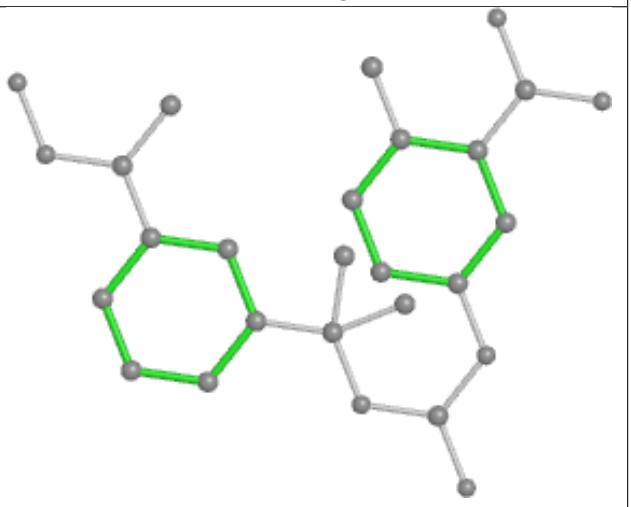
Bond lengths



Bond angles

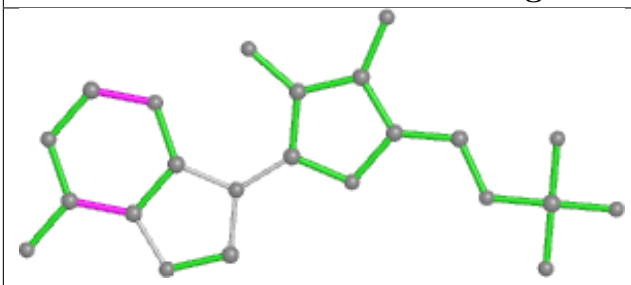


Torsions

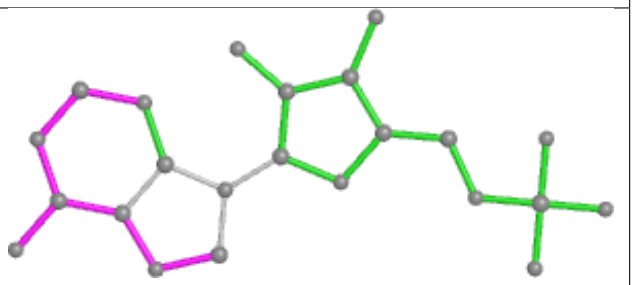


Rings

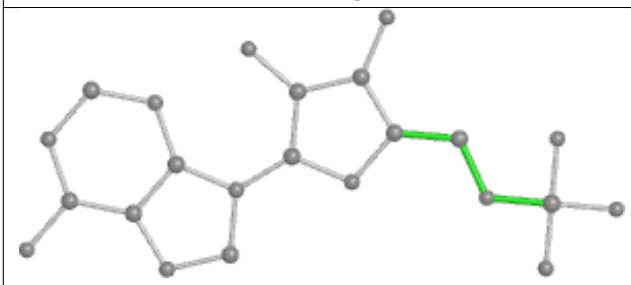
Ligand IMP A 501



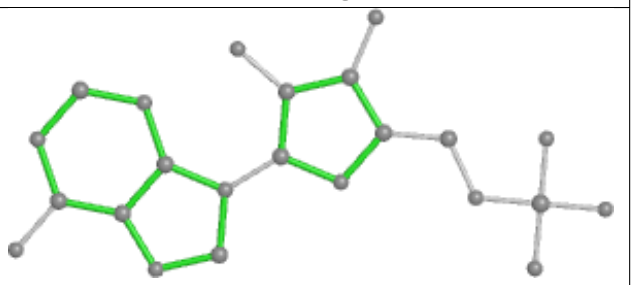
Bond lengths



Bond angles

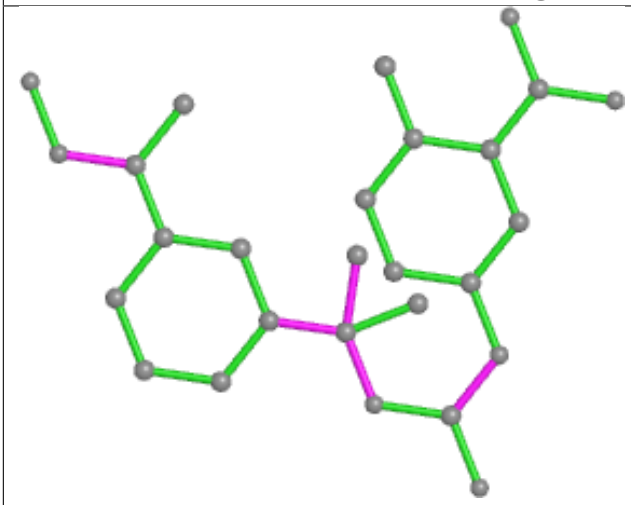


Torsions

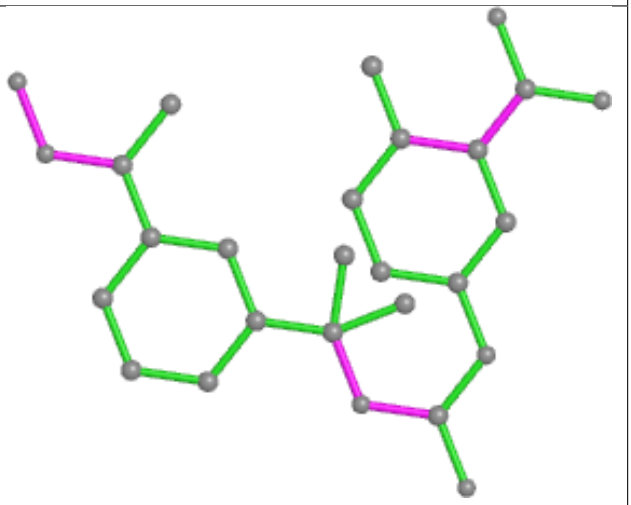


Rings

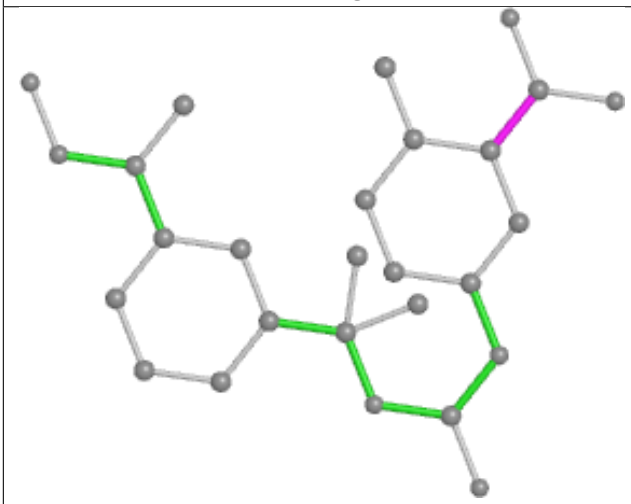
Ligand 2F0 C 503



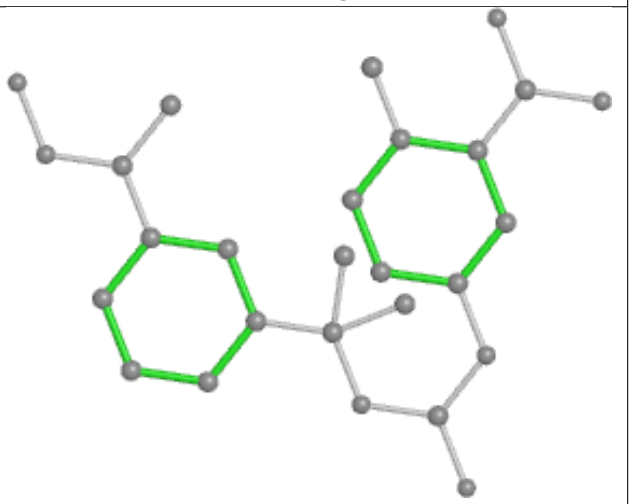
Bond lengths



Bond angles

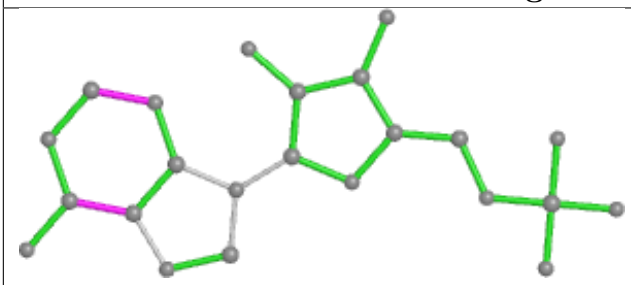


Torsions



Rings

Ligand IMP C 502



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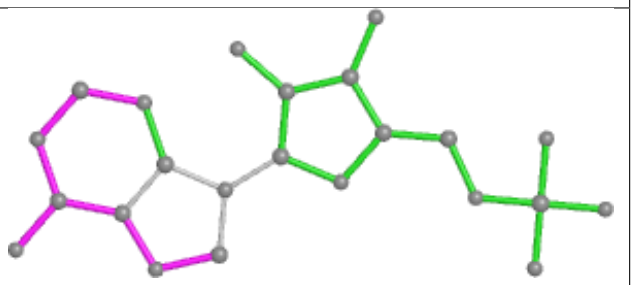
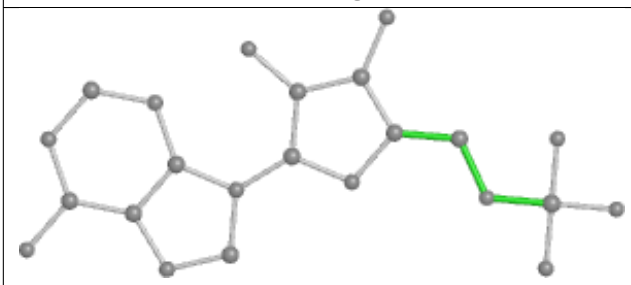
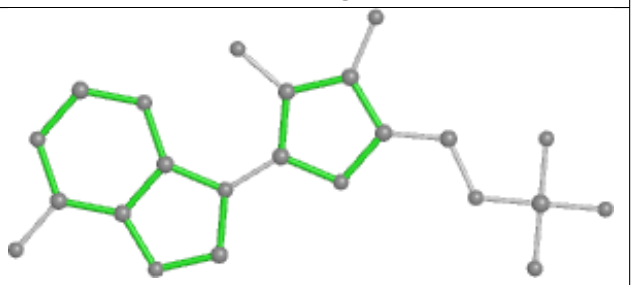


Bond angles

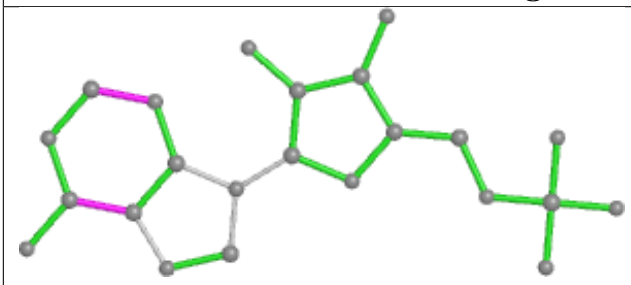


Torsions

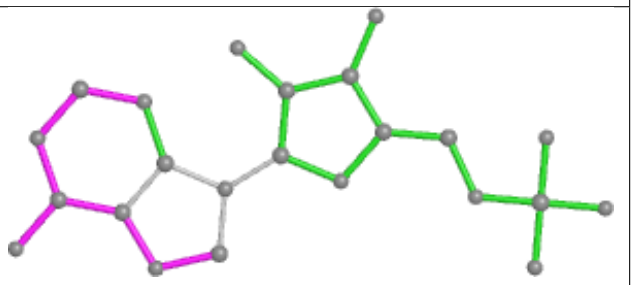


Rings

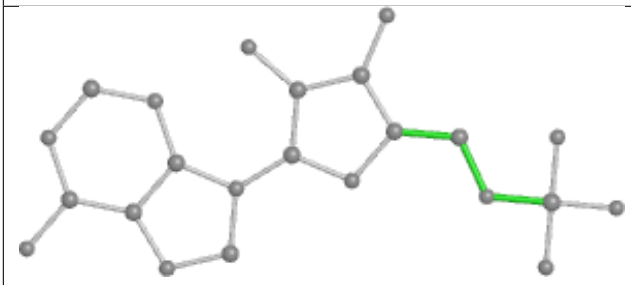
Ligand IMP G 501



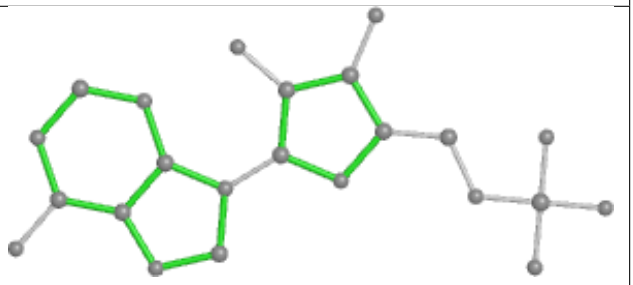
Bond lengths



Bond angles

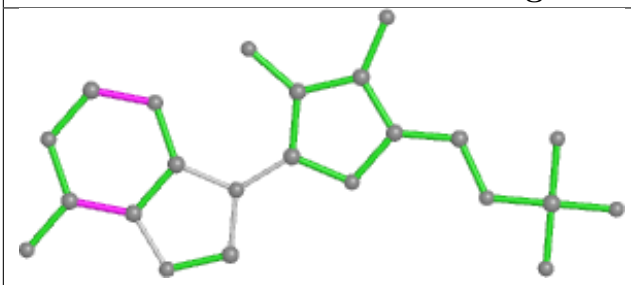


Torsions

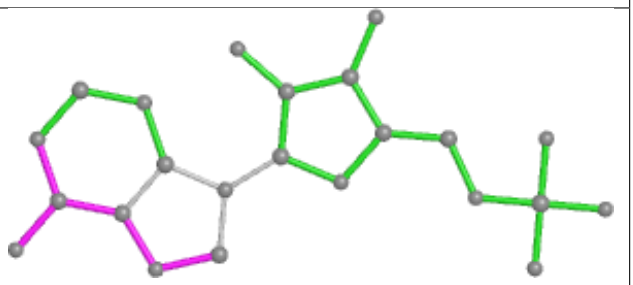


Rings

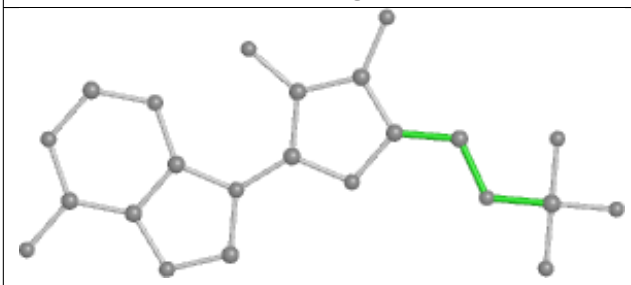
Ligand IMP B 500



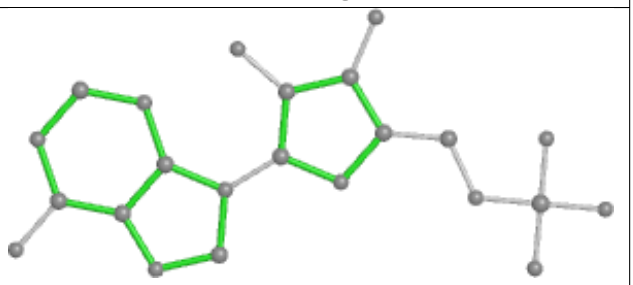
Bond lengths



Bond angles

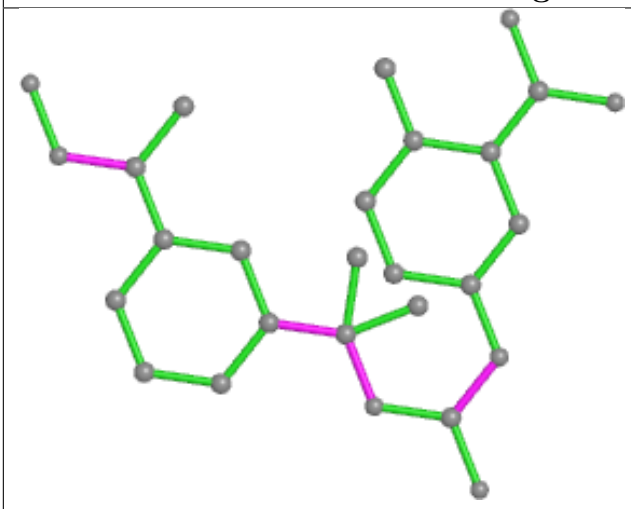


Torsions

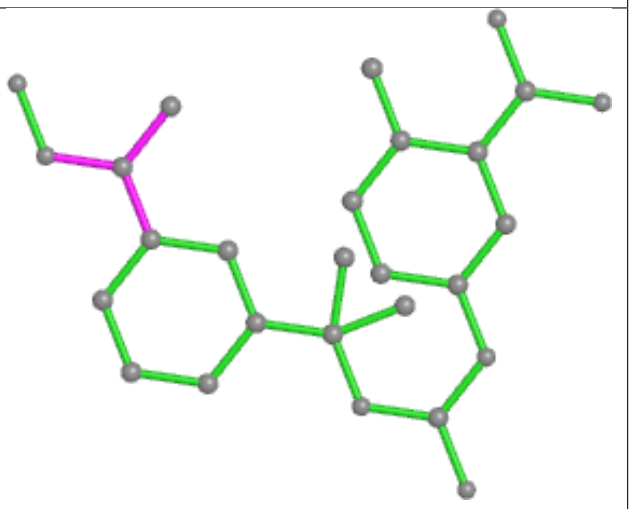


Rings

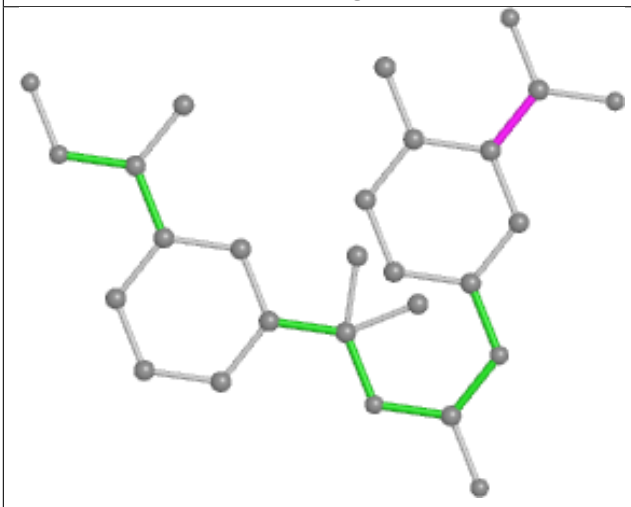
Ligand 2F0 B 501



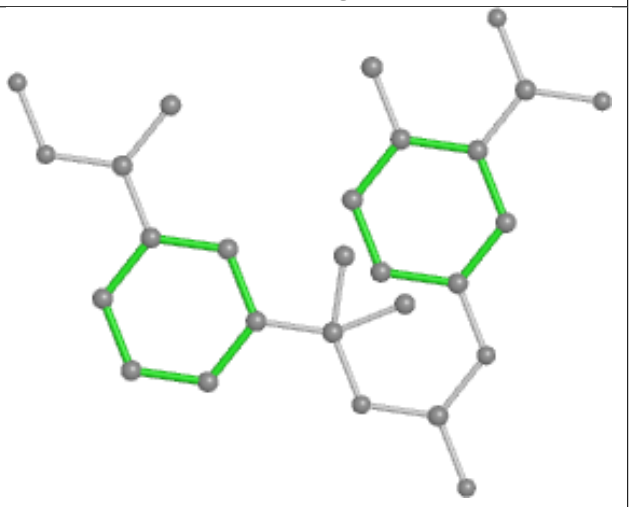
Bond lengths



Bond angles

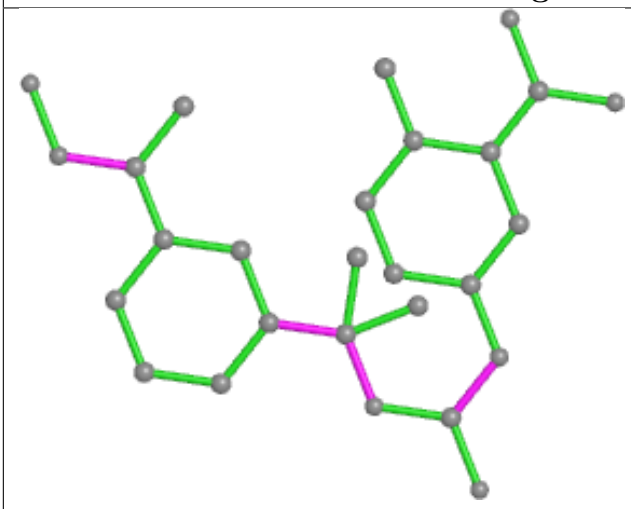


Torsions

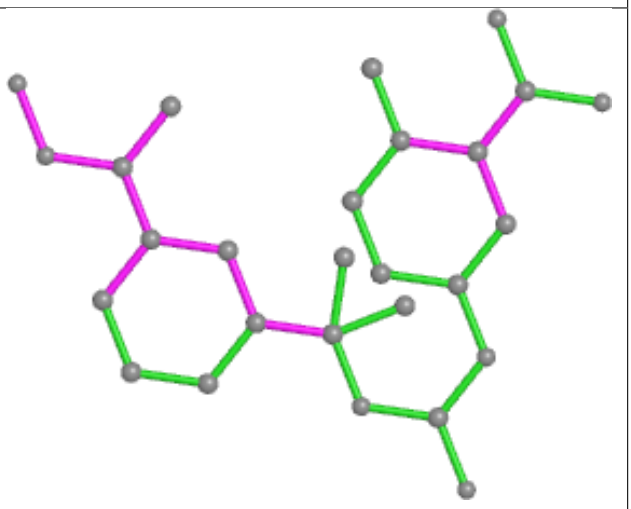


Rings

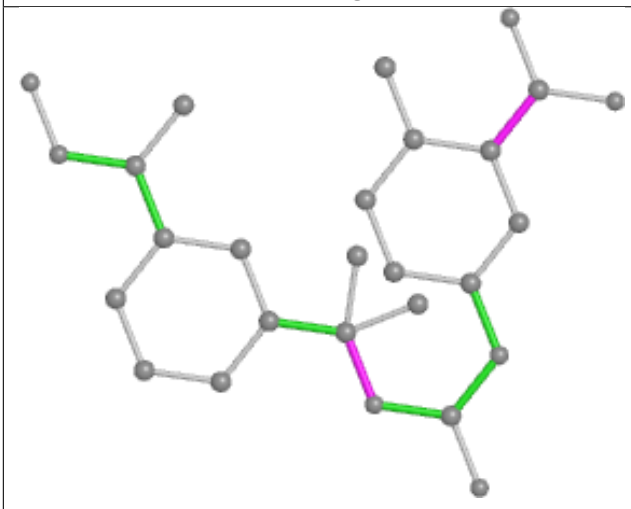
Ligand 2F0 D 501



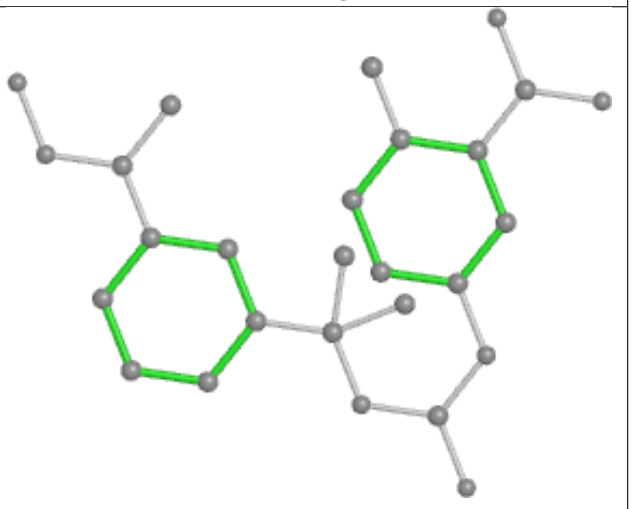
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	351/384 (91%)	0.49	32 (9%) 9 7	27, 47, 70, 84	1 (0%)
1	B	355/384 (92%)	0.35	9 (2%) 57 59	25, 45, 68, 102	2 (0%)
1	C	348/384 (90%)	0.27	6 (1%) 70 72	32, 45, 64, 74	0
1	D	352/384 (91%)	0.56	25 (7%) 16 14	30, 48, 68, 97	0
1	E	352/384 (91%)	0.46	22 (6%) 20 19	31, 46, 73, 89	1 (0%)
1	F	350/384 (91%)	0.59	29 (8%) 11 9	34, 50, 70, 85	1 (0%)
1	G	356/384 (92%)	0.50	22 (6%) 20 19	31, 49, 67, 87	1 (0%)
1	H	350/384 (91%)	0.57	25 (7%) 16 14	33, 51, 70, 80	1 (0%)
All	All	2814/3072 (91%)	0.47	170 (6%) 21 20	25, 48, 70, 102	7 (0%)

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	ALA	7.3
1	H	-2	SER	6.5
1	H	226	ALA	6.0
1	E	413	LEU	5.5
1	H	250	LEU	5.2
1	F	-2	SER	4.7
1	C	486	SER	4.6
1	F	229	VAL	4.5
1	H	271	TYR	4.5
1	D	249	VAL	4.5
1	D	227	VAL	4.4
1	A	225	ALA	4.3
1	H	228	GLY	4.3
1	H	249	VAL	4.3
1	F	395	GLY	4.1
1	A	224	GLY	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	244	SER	4.1
1	B	-4	PHE	4.0
1	E	382	GLY	3.9
1	D	248	ILE	3.9
1	G	278	ALA	3.8
1	A	477	GLN	3.8
1	H	246	ASP	3.8
1	F	248	ILE	3.8
1	F	482	ALA	3.7
1	F	251	ASP	3.7
1	D	241	VAL	3.7
1	D	246	ASP	3.7
1	A	223	VAL	3.6
1	D	228	GLY	3.6
1	H	243	ALA	3.6
1	A	251	ASP	3.5
1	A	413	LEU	3.5
1	G	36	LEU	3.4
1	A	298	VAL	3.4
1	H	227	VAL	3.4
1	G	250	LEU	3.4
1	F	394	VAL	3.3
1	G	251	ASP	3.3
1	F	230	THR	3.3
1	F	481	GLU	3.2
1	H	85	VAL	3.2
1	E	250	LEU	3.2
1	A	250	LEU	3.2
1	F	475	HIS	3.2
1	C	380	TYR	3.2
1	F	380	TYR	3.1
1	F	399	LYS	3.1
1	D	237	ILE	3.1
1	D	413	LEU	3.1
1	D	412	LYS	3.1
1	G	277	ILE	3.1
1	E	-3	GLN	3.1
1	B	412	LYS	3.0
1	H	241	VAL	3.0
1	B	251	ASP	3.0
1	G	245	VAL	3.0
1	H	316	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	271	TYR	3.0
1	A	280	ASN	2.9
1	E	255	GLY	2.9
1	F	223	VAL	2.9
1	E	0	ALA	2.9
1	A	357	GLY	2.9
1	G	-4	PHE	2.9
1	F	376	GLU	2.9
1	G	380	TYR	2.8
1	E	225	ALA	2.8
1	H	247	ALA	2.8
1	F	375	GLY	2.8
1	F	249	VAL	2.8
1	A	383	ARG	2.8
1	E	477	GLN	2.8
1	E	237	ILE	2.8
1	A	92	GLY	2.8
1	D	222	LEU	2.8
1	E	239	ALA	2.7
1	F	387	VAL	2.7
1	A	382	GLY	2.7
1	D	394	VAL	2.7
1	H	224	GLY	2.7
1	G	230	THR	2.7
1	G	292	GLU	2.7
1	A	40	LEU	2.7
1	B	413	LEU	2.7
1	F	388	TYR	2.7
1	D	277	ILE	2.7
1	D	431	THR	2.7
1	A	222	LEU	2.6
1	F	74	LYS	2.6
1	D	399	LYS	2.6
1	G	336	ILE	2.6
1	A	459	GLN	2.6
1	E	241	VAL	2.6
1	E	476	VAL	2.6
1	H	245	VAL	2.6
1	C	482	ALA	2.5
1	H	244	SER	2.5
1	G	354	LEU	2.5
1	F	84	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	486	SER	2.5
1	A	229	VAL	2.5
1	F	61	ILE	2.5
1	C	75	ASN	2.5
1	F	277	ILE	2.4
1	A	387	VAL	2.4
1	F	260	VAL	2.4
1	H	413	LEU	2.4
1	B	379	ILE	2.4
1	D	74	LYS	2.4
1	A	487	LEU	2.4
1	F	225	ALA	2.4
1	F	69	LEU	2.4
1	D	266	GLU	2.4
1	B	378	GLU	2.3
1	E	226	ALA	2.3
1	E	375	GLY	2.3
1	G	385	PHE	2.3
1	D	275	ASN	2.3
1	E	399	LYS	2.3
1	E	243	ALA	2.3
1	A	70	GLY	2.3
1	A	255	GLY	2.3
1	F	371	ALA	2.3
1	A	241	VAL	2.3
1	A	341	ASP	2.2
1	E	238	ASP	2.2
1	A	247	ALA	2.2
1	F	263	LYS	2.2
1	H	426	GLY	2.2
1	A	394	VAL	2.2
1	E	251	ASP	2.2
1	E	28	ARG	2.2
1	G	333	LYS	2.2
1	B	250	LEU	2.2
1	A	82	ALA	2.2
1	D	247	ALA	2.2
1	A	232	ASP	2.2
1	F	224	GLY	2.2
1	G	231	ALA	2.2
1	C	394	VAL	2.1
1	B	369	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	364	GLY	2.1
1	A	243	ALA	2.1
1	G	358	ALA	2.1
1	H	82	ALA	2.1
1	D	-2	SER	2.1
1	G	290	LEU	2.1
1	H	251	ASP	2.1
1	G	331	ALA	2.1
1	A	273	SER	2.1
1	H	86	ASP	2.1
1	D	46	LEU	2.1
1	E	229	VAL	2.1
1	E	376	GLU	2.1
1	D	225	ALA	2.1
1	G	274	LEU	2.1
1	A	2	TRP	2.1
1	F	294	GLY	2.1
1	G	302	ILE	2.1
1	H	248	ILE	2.1
1	H	360	VAL	2.1
1	H	89	LYS	2.1
1	A	239	ALA	2.1
1	D	389	ARG	2.1
1	G	225	ALA	2.0
1	B	252	THR	2.0
1	C	383	ARG	2.0
1	G	40	LEU	2.0
1	E	74	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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
7	EDO	F	504	4/4	0.62	0.39	66,67,69,69	0
4	FMT	F	507	3/3	0.66	0.37	69,69,70,70	0
8	SO4	G	502	5/5	0.66	0.53	127,128,128,128	0
5	GOL	A	505	6/6	0.67	0.30	48,51,51,52	0
5	GOL	E	506	6/6	0.70	0.30	50,52,53,54	0
6	MLI	A	506	7/7	0.70	0.40	87,88,91,91	0
7	EDO	D	502	4/4	0.71	0.25	59,60,60,60	0
7	EDO	D	503	4/4	0.72	0.30	51,53,55,56	0
8	SO4	G	503	5/5	0.73	0.34	144,144,145,145	0
4	FMT	D	507	3/3	0.77	0.28	62,62,63,64	0
4	FMT	H	502	3/3	0.79	0.31	68,68,68,68	0
4	FMT	E	504	3/3	0.80	0.19	53,53,53,53	0
7	EDO	F	505	4/4	0.81	0.13	56,58,59,59	0
7	EDO	C	506	4/4	0.81	0.38	54,56,58,59	0
4	FMT	H	506	3/3	0.81	0.24	65,65,65,65	0
4	FMT	B	503	3/3	0.82	0.35	46,46,47,49	0
4	FMT	D	506	3/3	0.83	0.14	43,43,46,47	0
4	FMT	E	503	3/3	0.84	0.24	74,74,74,75	0
7	EDO	C	504	4/4	0.85	0.19	53,54,54,54	0
4	FMT	H	501	3/3	0.85	0.19	62,62,63,63	0
4	FMT	A	504	3/3	0.86	0.37	62,62,63,64	0
4	FMT	H	503	3/3	0.86	0.16	66,66,67,67	0
7	EDO	D	505	4/4	0.86	0.24	55,56,57,57	0
7	EDO	E	505	4/4	0.86	0.14	41,43,45,46	0
6	MLI	E	508	7/7	0.88	0.25	64,65,67,68	0
8	SO4	C	505	5/5	0.88	0.24	119,119,119,119	0
7	EDO	B	502	4/4	0.89	0.38	71,71,71,72	0
3	2F0	F	502	27/27	0.89	0.24	42,49,54,67	0
3	2F0	H	505	27/27	0.90	0.24	47,53,59,63	0
4	FMT	A	503	3/3	0.91	0.31	48,48,48,49	0
3	2F0	E	509	27/27	0.91	0.26	39,51,55,57	0
3	2F0	B	501	27/27	0.91	0.30	41,50,56,61	0
3	2F0	D	501	27/27	0.91	0.22	34,42,57,61	0
3	2F0	A	502	27/27	0.92	0.29	37,45,50,58	0
3	2F0	E	502	27/27	0.92	0.23	38,43,52,54	0
2	IMP	E	501	23/23	0.92	0.19	31,35,43,44	0
3	2F0	C	503	27/27	0.92	0.25	43,50,54,56	0
4	FMT	C	501	3/3	0.92	0.33	69,69,70,71	0
4	FMT	F	503	3/3	0.93	0.16	42,42,43,44	0
2	IMP	F	501	23/23	0.94	0.20	37,44,47,48	0
2	IMP	G	501	23/23	0.95	0.16	36,39,41,42	0

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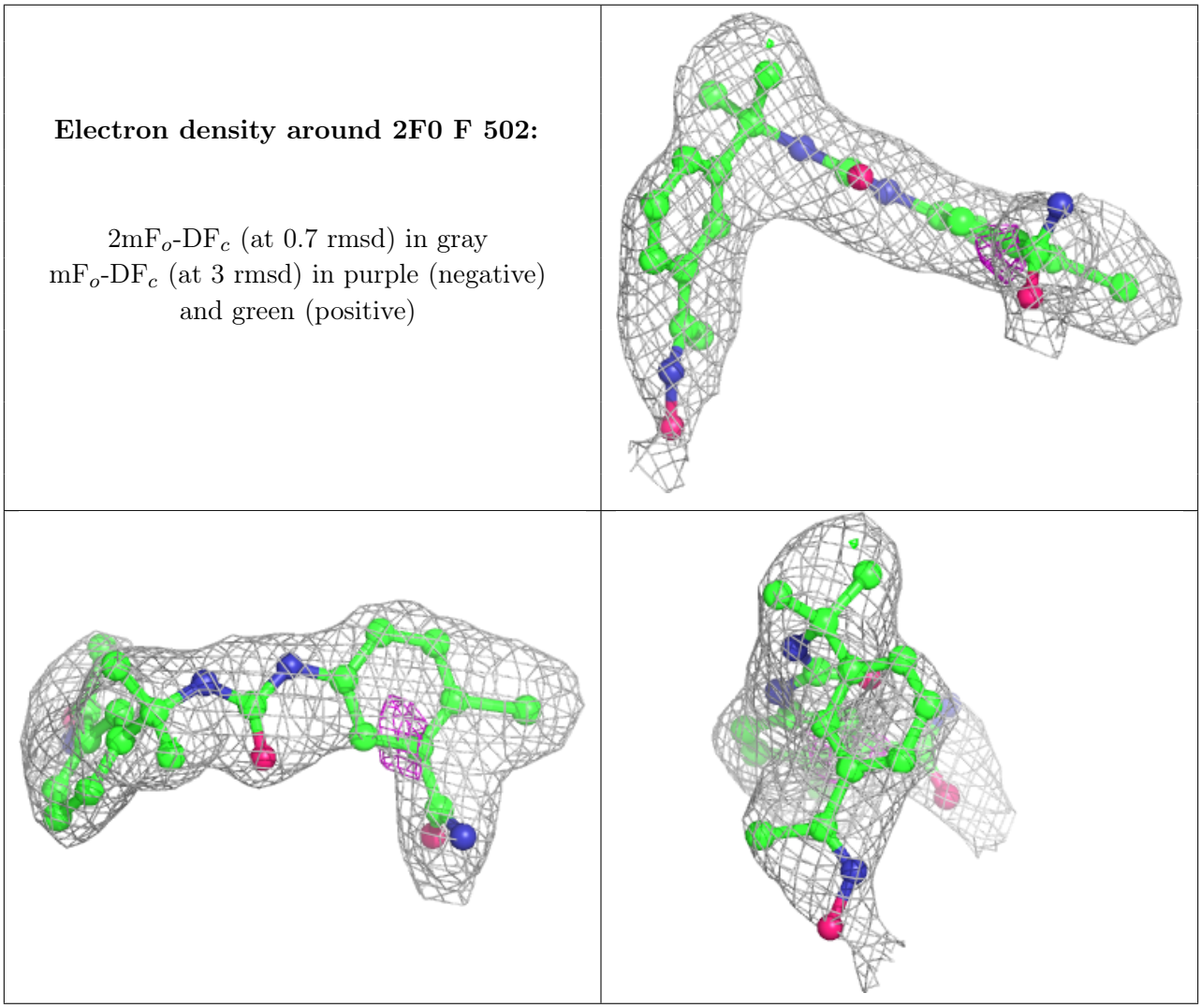
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IMP	H	504	23/23	0.95	0.18	37,41,47,48	0
7	EDO	F	506	4/4	0.95	0.20	39,39,39,40	0
4	FMT	E	507	3/3	0.95	0.17	37,37,37,37	0
2	IMP	A	501	23/23	0.95	0.15	35,40,44,45	0
2	IMP	D	504	23/23	0.95	0.24	36,41,45,49	0
2	IMP	C	502	23/23	0.96	0.17	32,41,44,46	0
2	IMP	B	500	23/23	0.96	0.16	33,36,38,39	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.

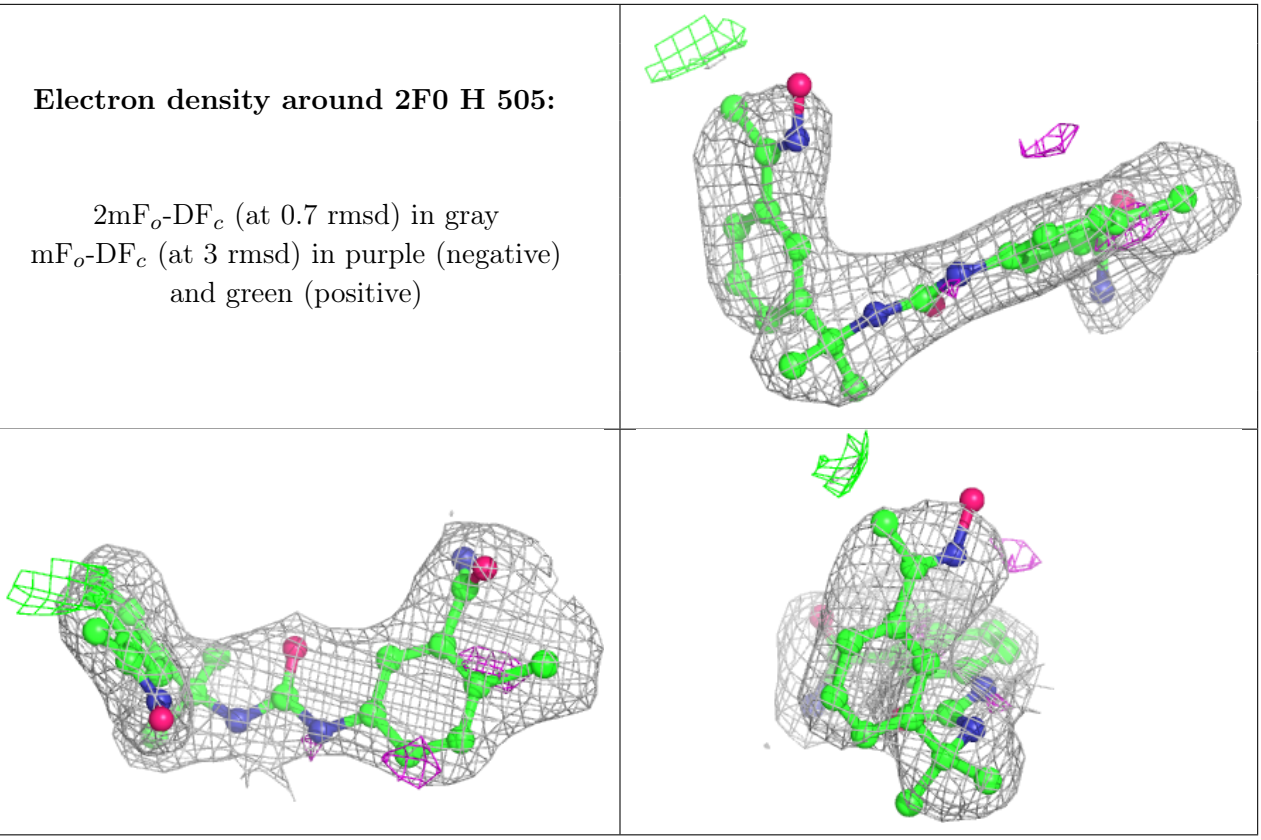
Electron density around 2F0 F 502:

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



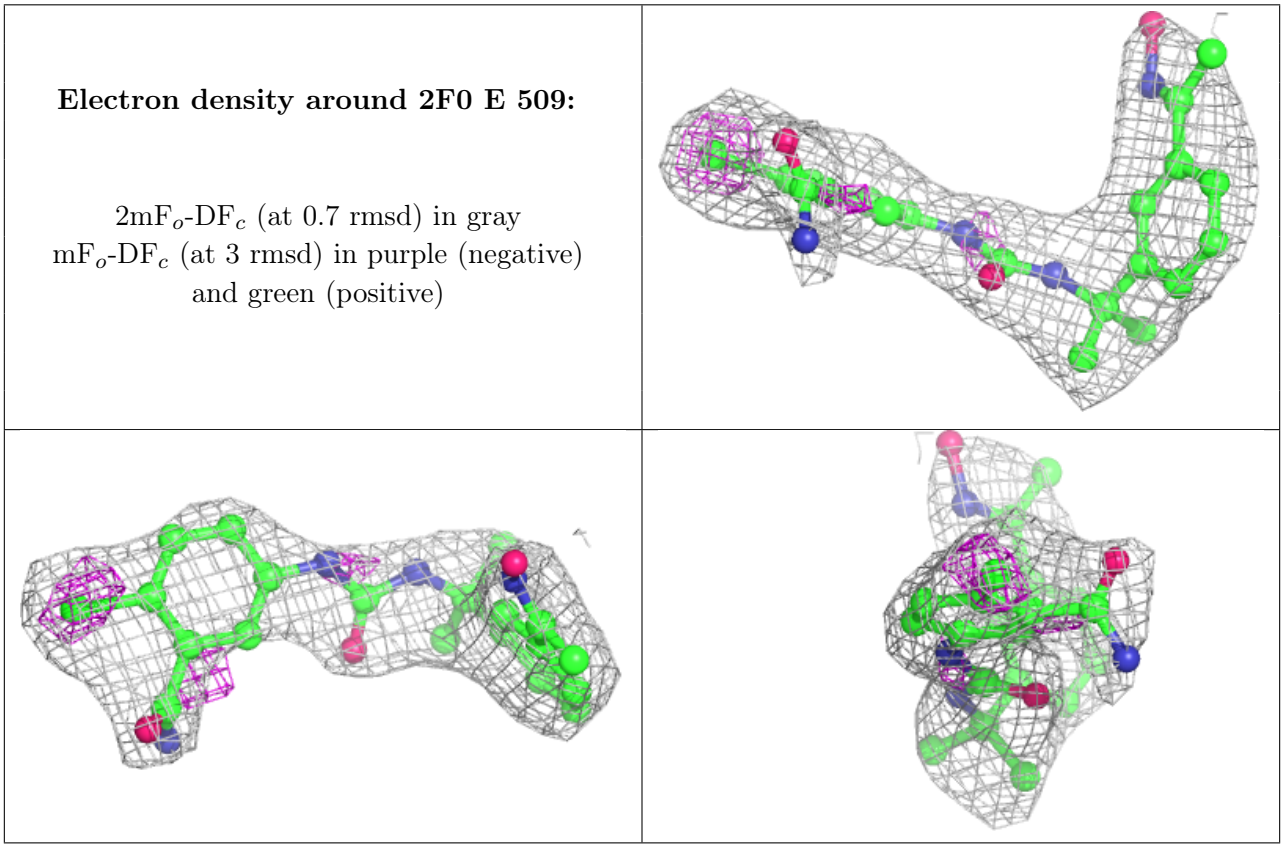
Electron density around 2F0 H 505:

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



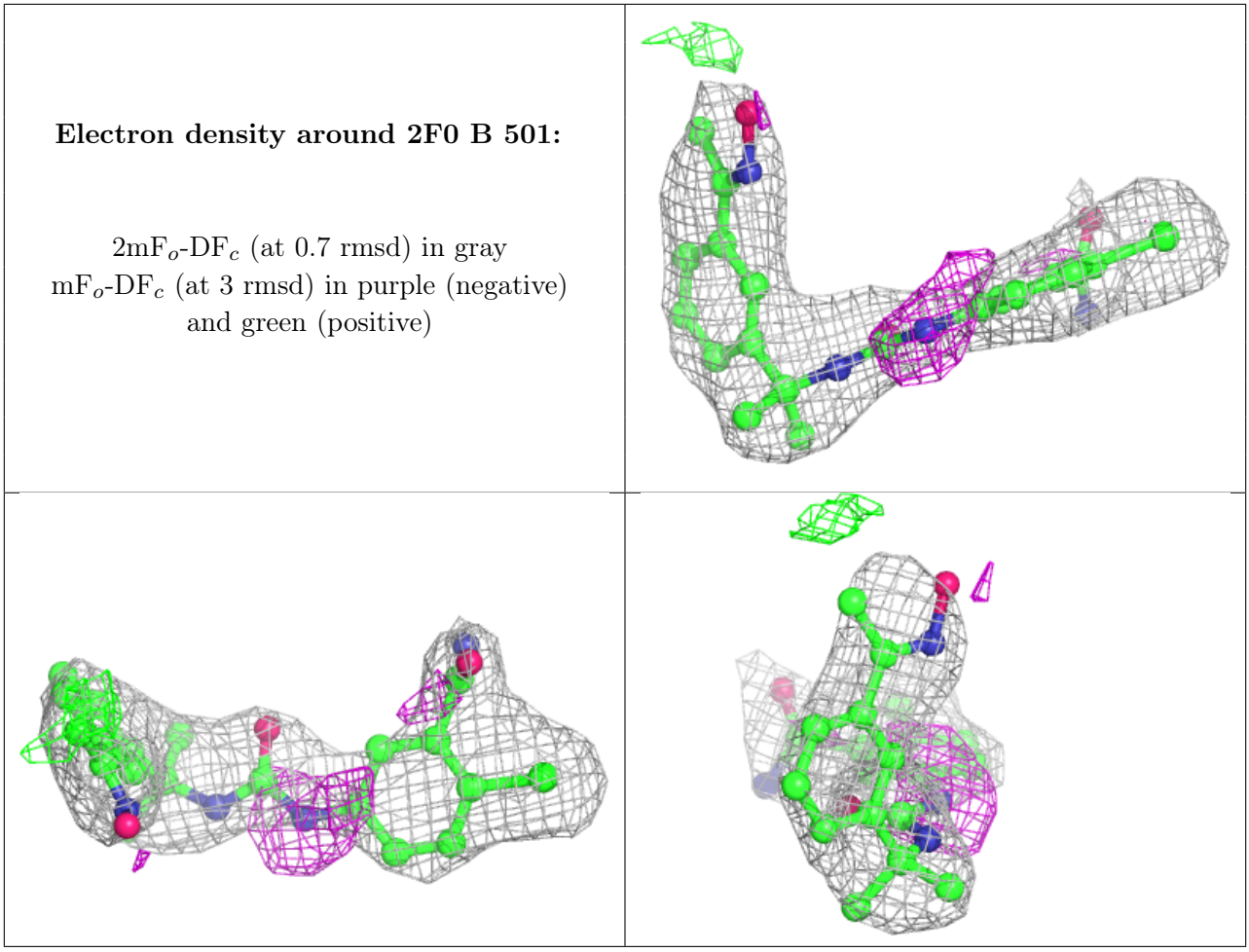
Electron density around 2F0 E 509:

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



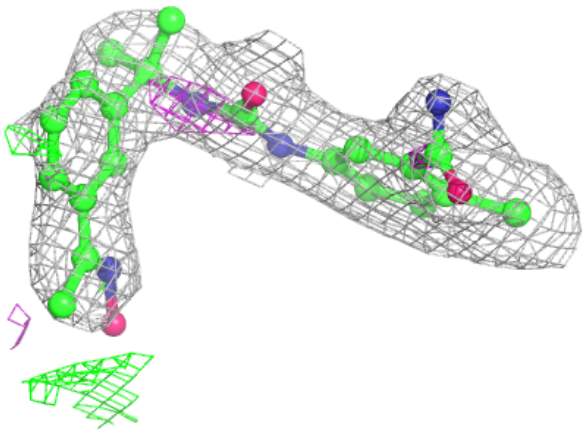
Electron density around 2F0 B 501:

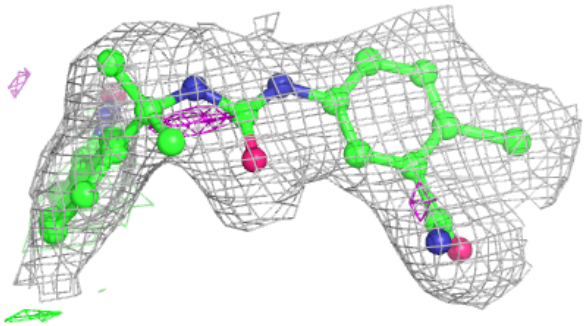
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

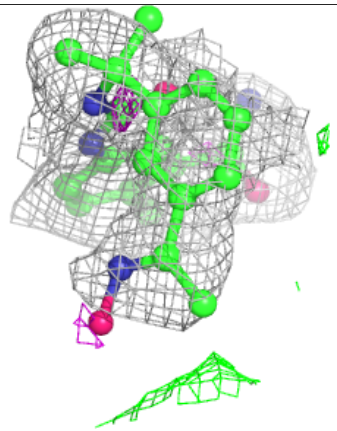


Electron density around 2F0 D 501:

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

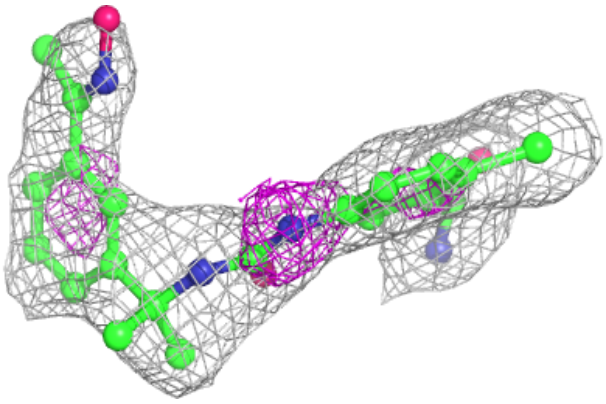


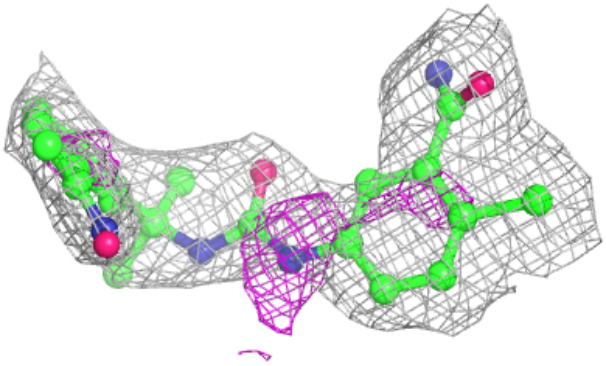


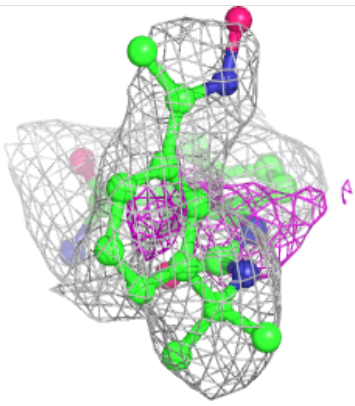


Electron density around 2F0 A 502:

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

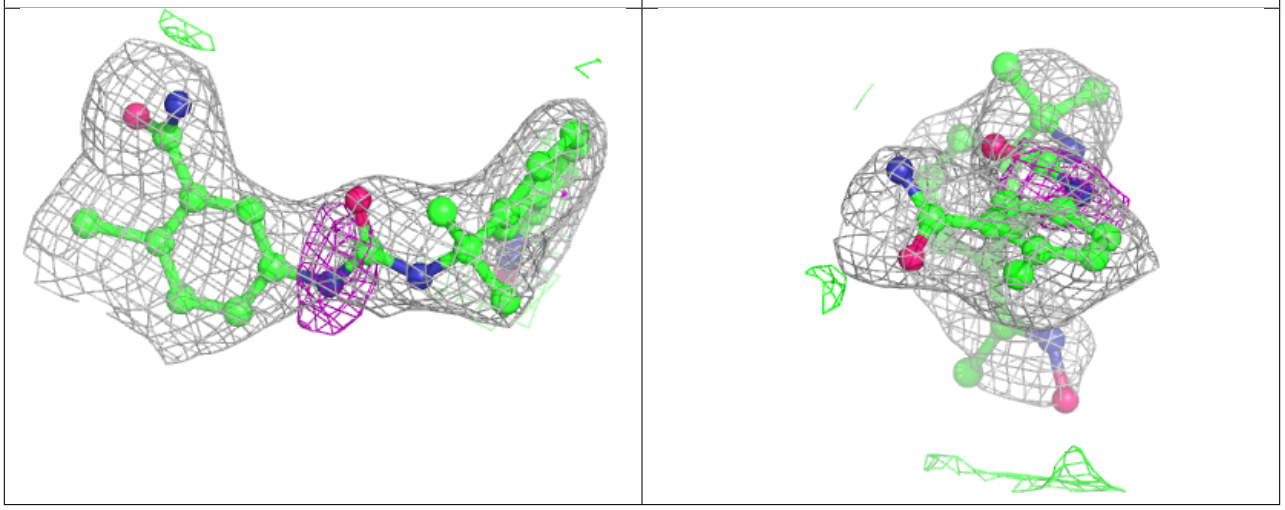






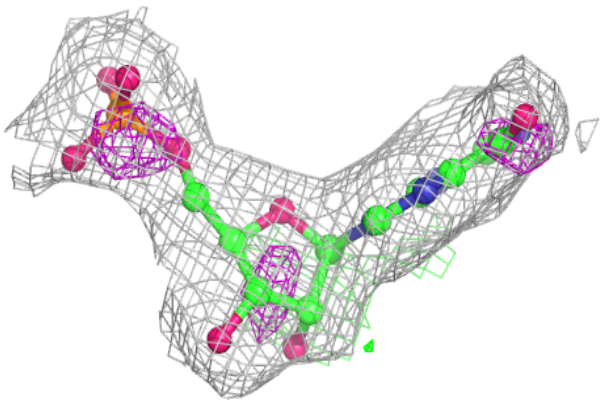
Electron density around 2F0 E 502:

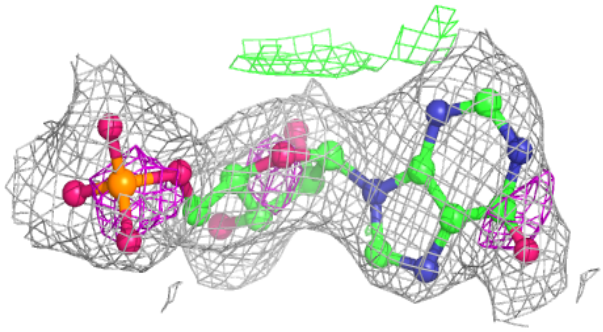
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

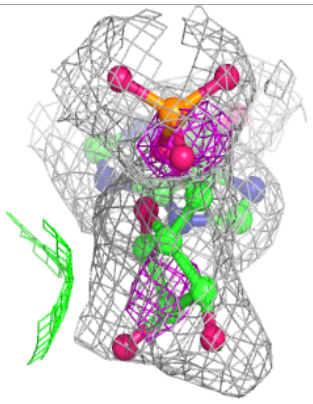


Electron density around IMP E 501:

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

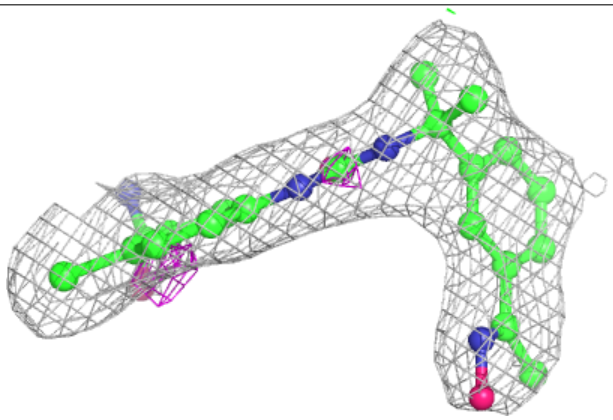


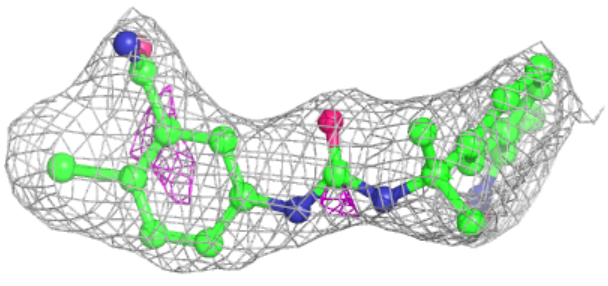


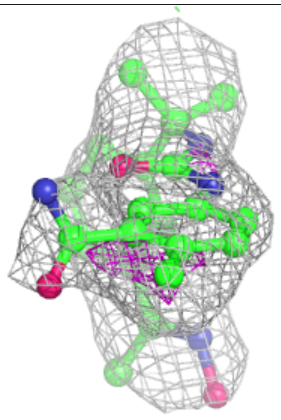


Electron density around 2F0 C 503:

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

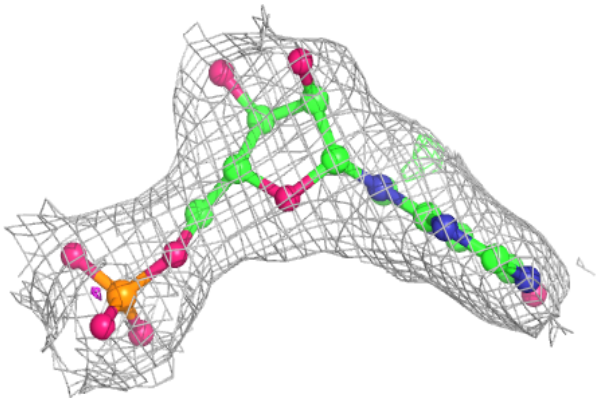


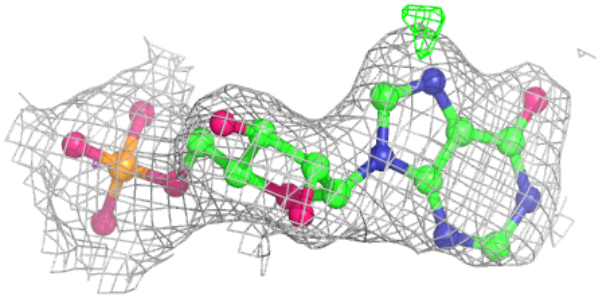


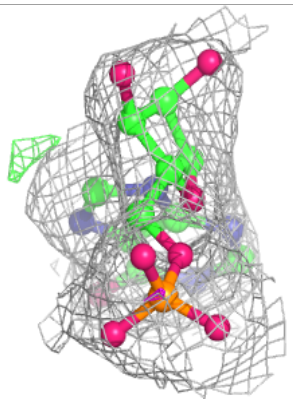


Electron density around IMP F 501:

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

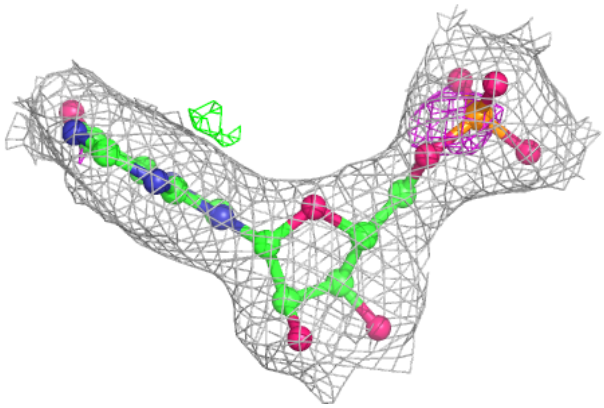


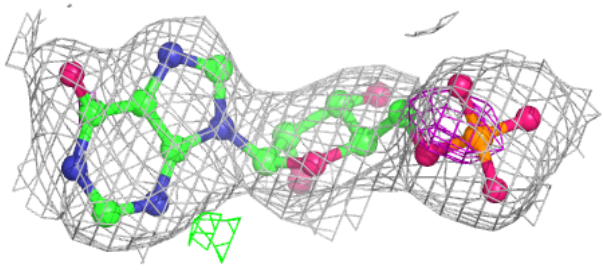


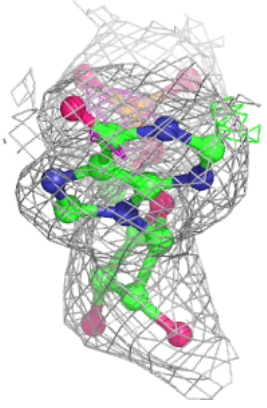


Electron density around IMP G 501:

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

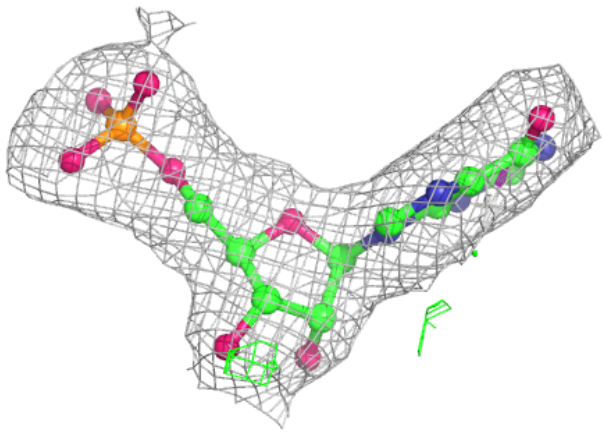


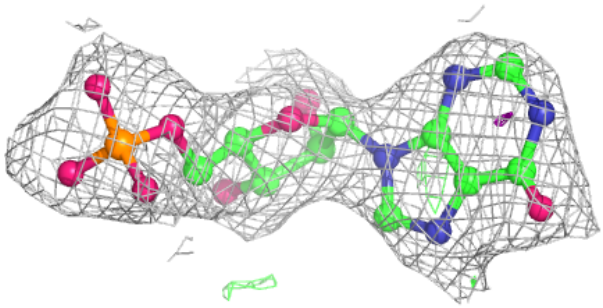


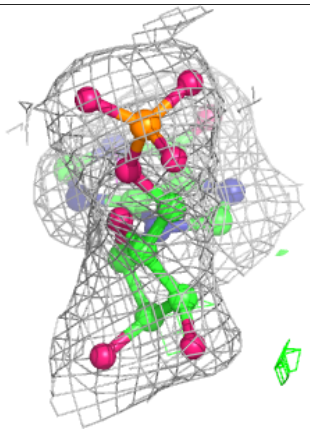


Electron density around IMP H 504:

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

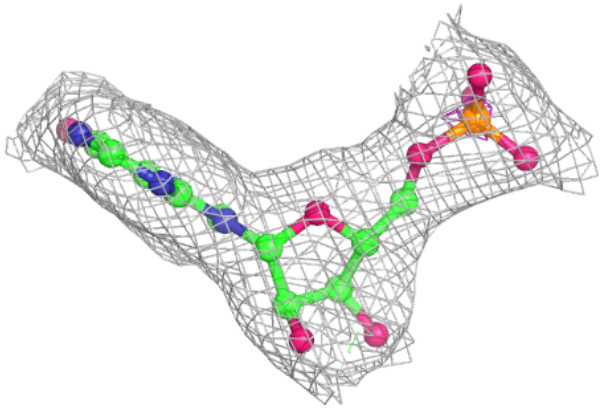


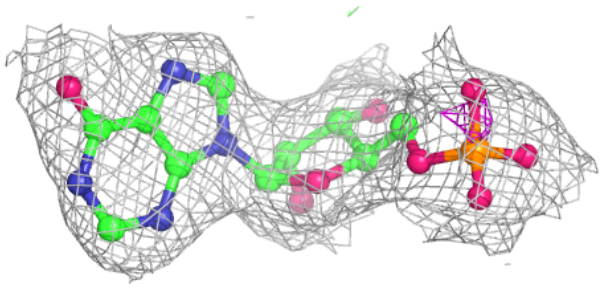


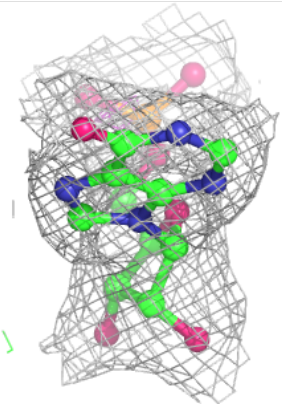


Electron density around IMP A 501:

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

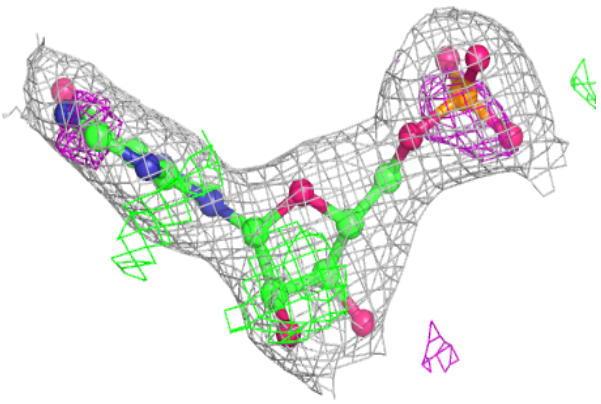


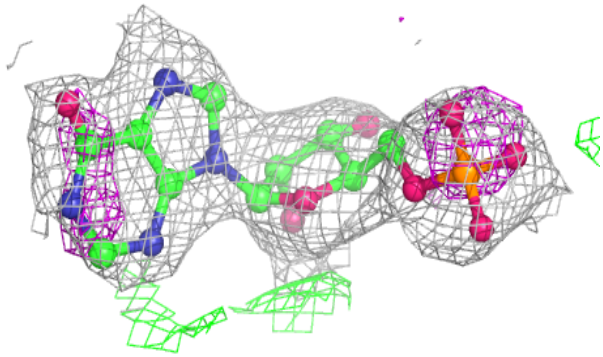


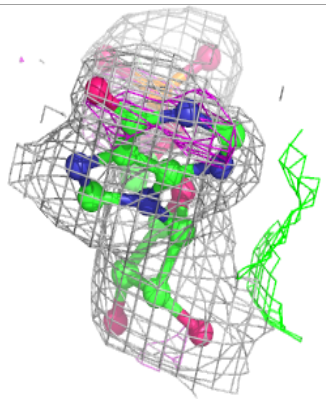


Electron density around IMP D 504:

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

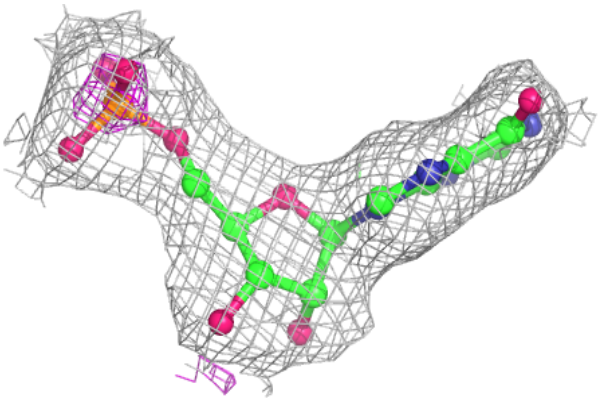


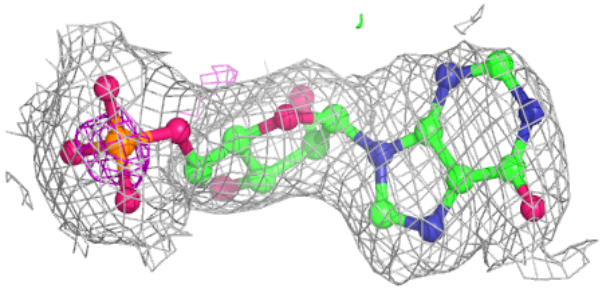


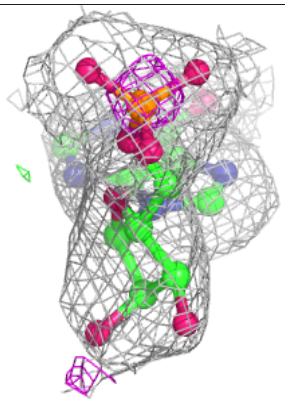


Electron density around IMP C 502:

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

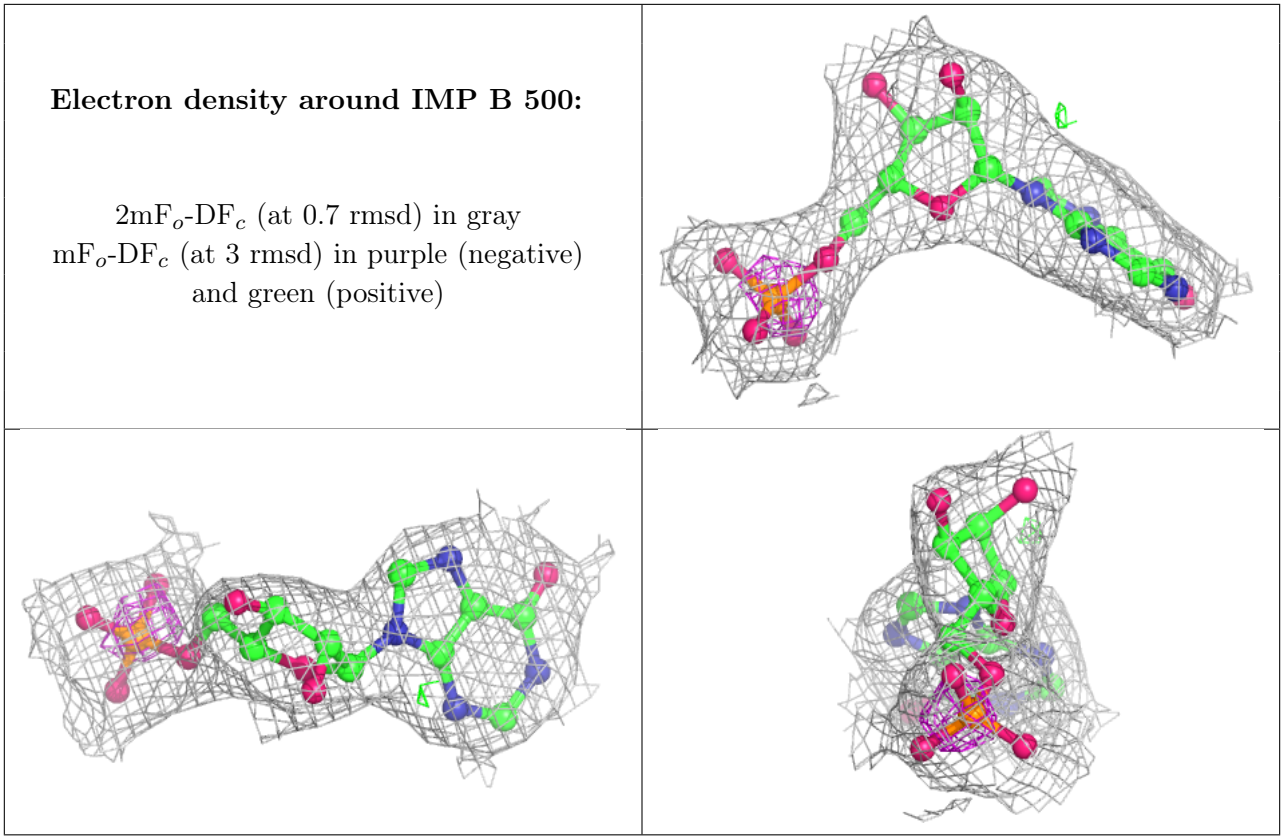






Electron density around IMP B 500:

$2mF_o$-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.