Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 07:27 PM EDT

PDB ID	:	5URS
Title	:	Crystal Structure of the Catalytic Domain of the Inosine Monophosphate Dehydrogenase from Bacillus anthracis in the complex with IMP and the inhibitor P178
Authors	:	Kim, Y.; Maltseva, N.; Makowska-Grzyska, M.; Gu, M.; Gollapalli, D.; Hedstrom, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2017-02-12
Resolution	:	2.39 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:

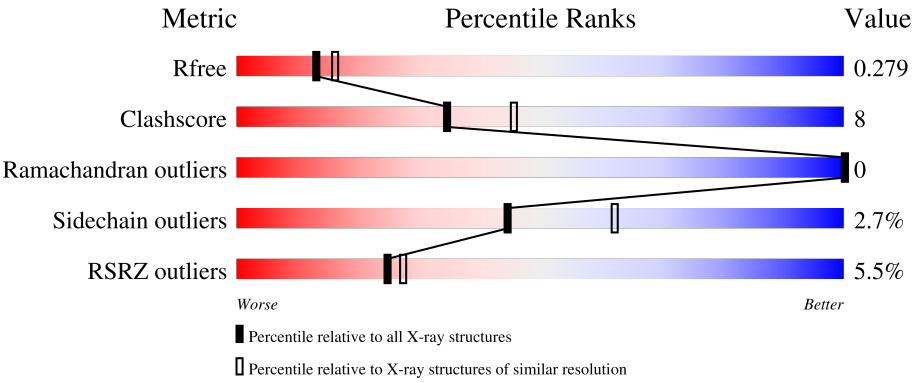
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.39 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	3% 74% 17% • 9%
1	B	384	3% 71% 19% • 9%
1	C	384	6% 76% 14% • 9%

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

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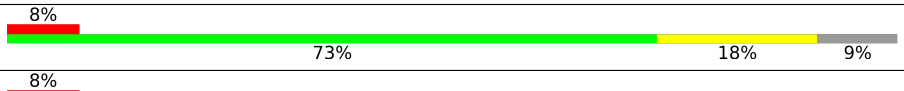
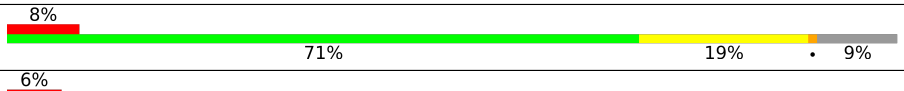
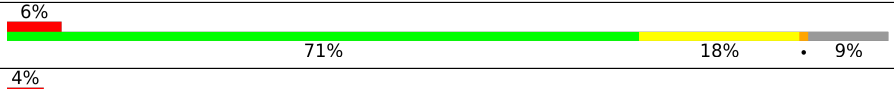
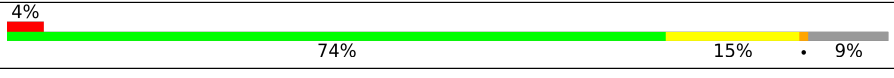
Mol	Chain	Length	Quality of chain
1	D	384	
1	E	384	
1	F	384	
1	G	384	
1	H	384	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 21357 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	2	0
			2593	1628	455	493	17			
1	B	350	Total	C	N	O	S	0	0	0
			2567	1612	450	489	16			
1	C	349	Total	C	N	O	S	0	0	0
			2558	1606	448	488	16			
1	D	350	Total	C	N	O	S	0	0	0
			2569	1614	449	490	16			
1	E	350	Total	C	N	O	S	0	0	0
			2570	1614	450	490	16			
1	F	351	Total	C	N	O	S	0	0	0
			2575	1618	451	490	16			
1	G	349	Total	C	N	O	S	0	0	0
			2558	1606	448	488	16			
1	H	348	Total	C	N	O	S	0	0	0
			2552	1603	447	486	16			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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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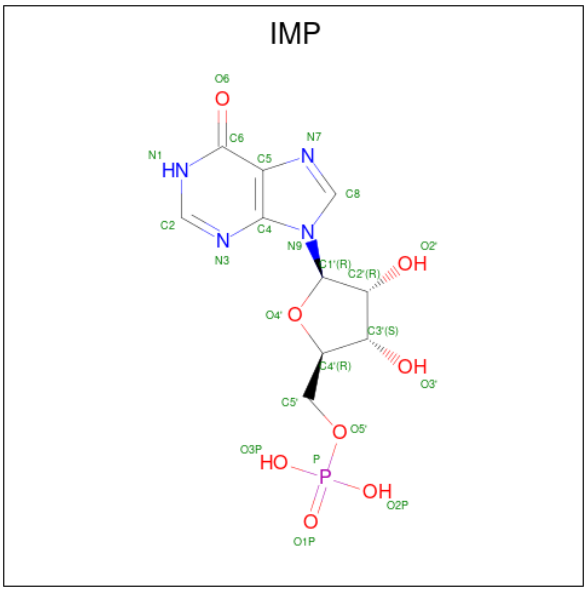
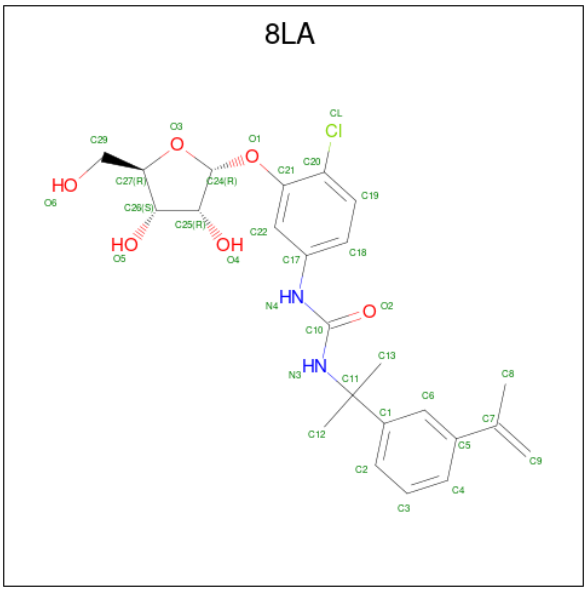
Chain	Residue	Modelled	Actual	Comment	Reference
G	220	GLY	-	linker	UNP Q81W29
H	-23	MET	-	initiating methionine	UNP Q81W29
H	-22	HIS	-	expression tag	UNP Q81W29
H	-21	HIS	-	expression tag	UNP Q81W29
H	-20	HIS	-	expression tag	UNP Q81W29
H	-19	HIS	-	expression tag	UNP Q81W29
H	-18	HIS	-	expression tag	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 N-[4-chloro-3-(alpha-D-ribofuranosyloxy)phenyl]-N'-{2-[3-(prop-1-en-2-yl)phenyl]propan-2-yl}urea (three-letter code: 8LA) (formula: $C_{24}H_{29}ClN_2O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Cl N O 33 24 1 2 6	0	0
3	B	1	Total C Cl N O 33 24 1 2 6	0	0
3	C	1	Total C Cl N O 33 24 1 2 6	0	0
3	D	1	Total C Cl N O 33 24 1 2 6	0	0
3	E	1	Total C Cl N O 33 24 1 2 6	0	0
3	F	1	Total C Cl N O 33 24 1 2 6	0	0
3	G	1	Total C Cl N O 33 24 1 2 6	0	0
3	H	1	Total C Cl N O 33 24 1 2 6	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total K 2 2	0	0
4	B	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	E	2	Total K 2 2	0	0

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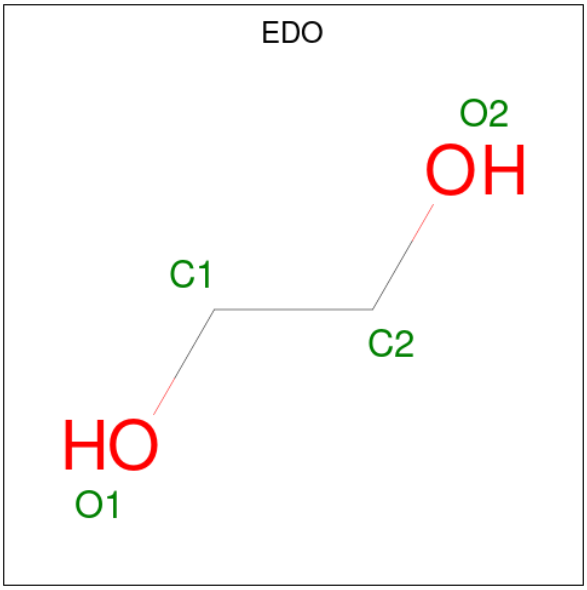
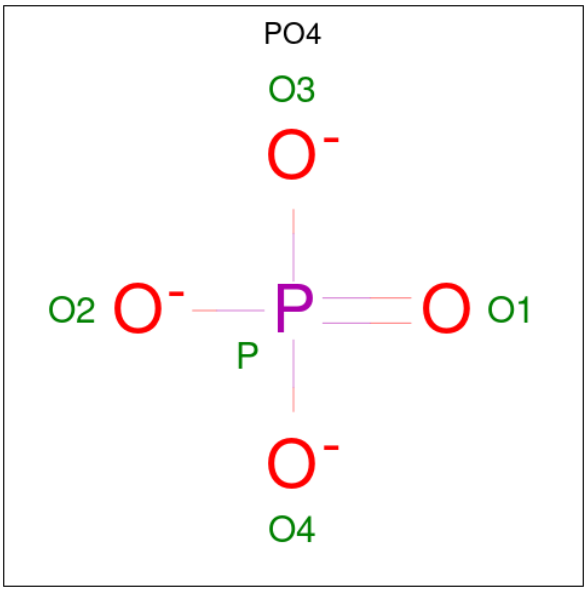
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total K 1 1	0	0
4	G	1	Total K 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



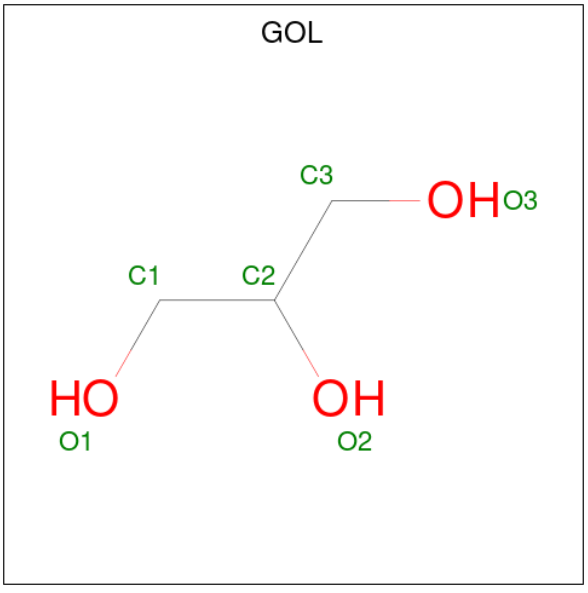
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



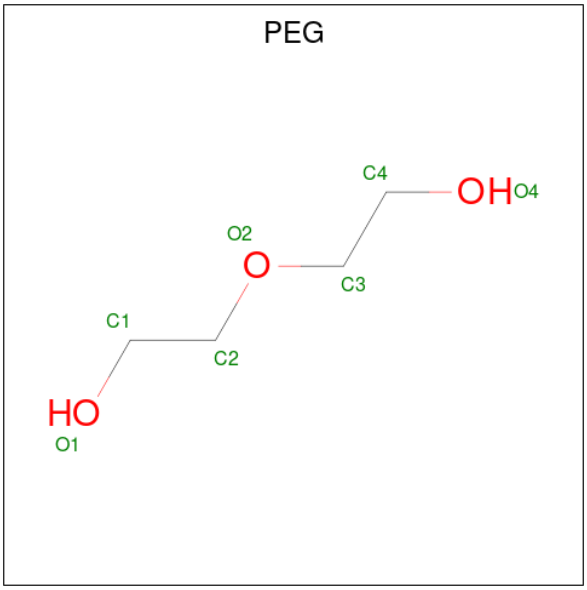
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	E	1	Total O P 5 4 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 6 3 3	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 9 is water.

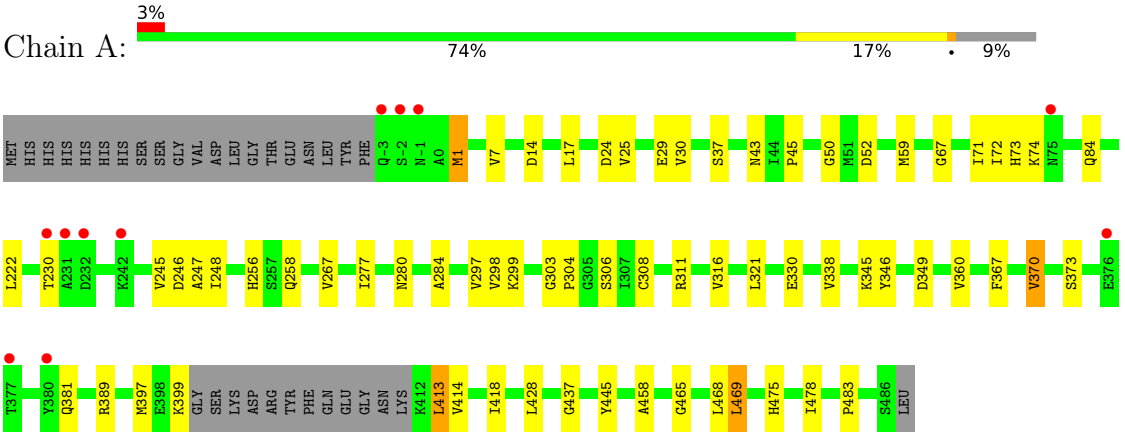
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	44	Total O 44 44	0	0
9	B	48	Total O 48 48	0	0
9	C	40	Total O 40 40	0	0
9	D	47	Total O 47 47	0	0
9	E	45	Total O 45 45	0	0
9	F	40	Total O 40 40	0	0
9	G	30	Total O 30 30	0	0
9	H	33	Total O 33 33	0	0

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.

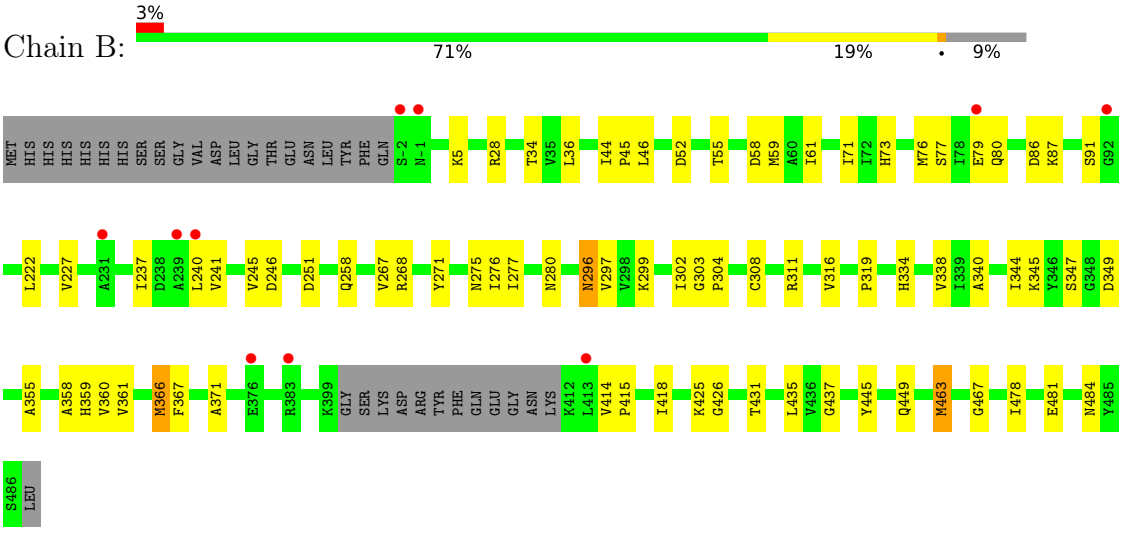
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain A:



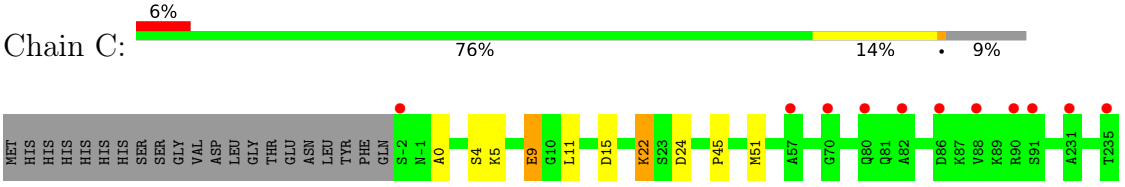
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

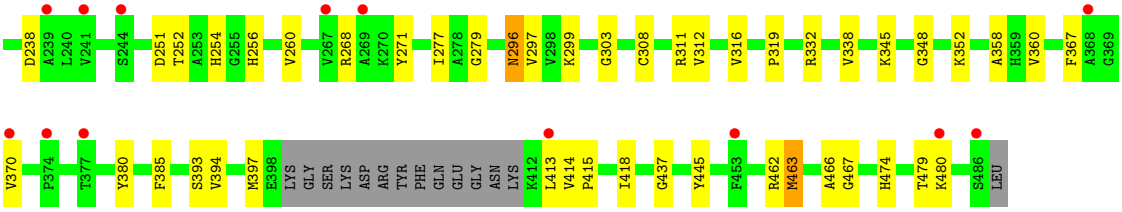
Chain B:



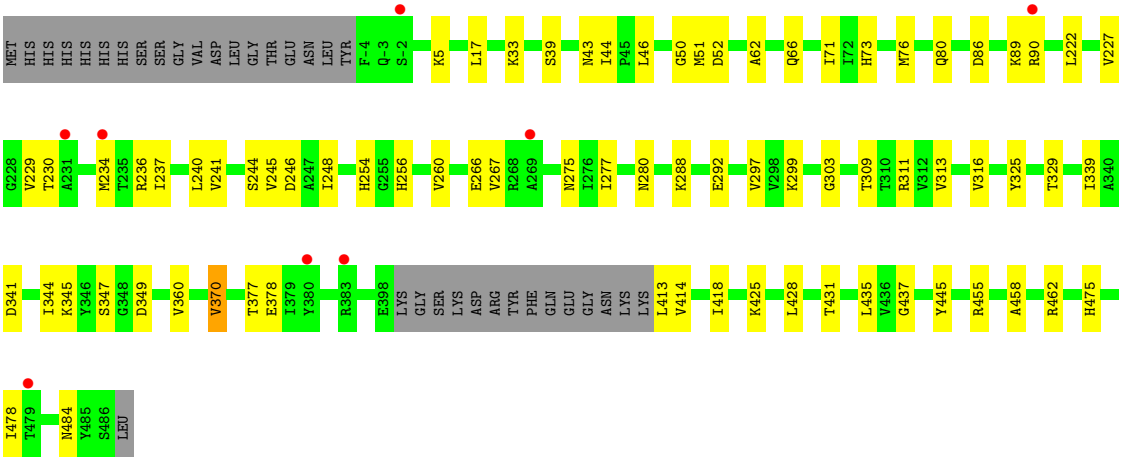
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain C:

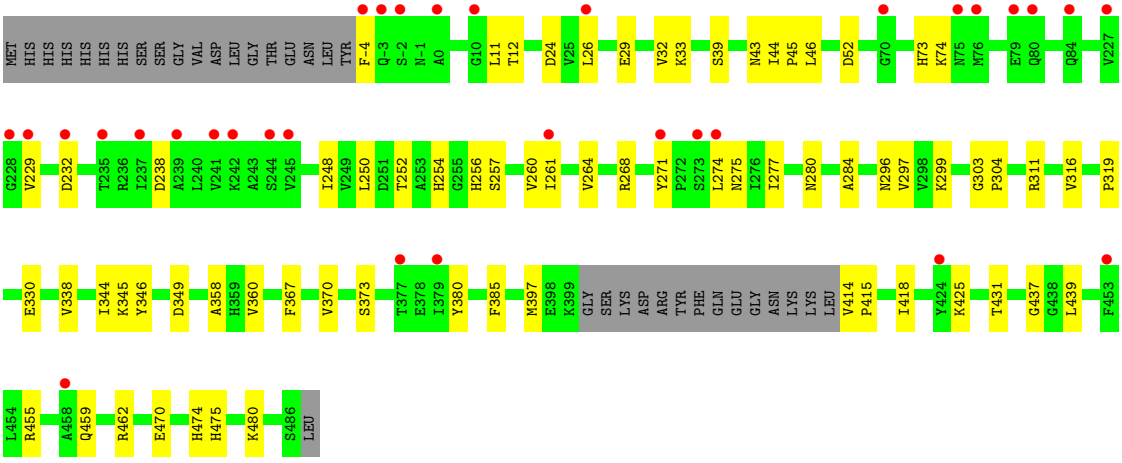




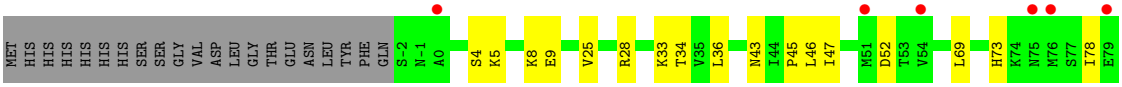
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

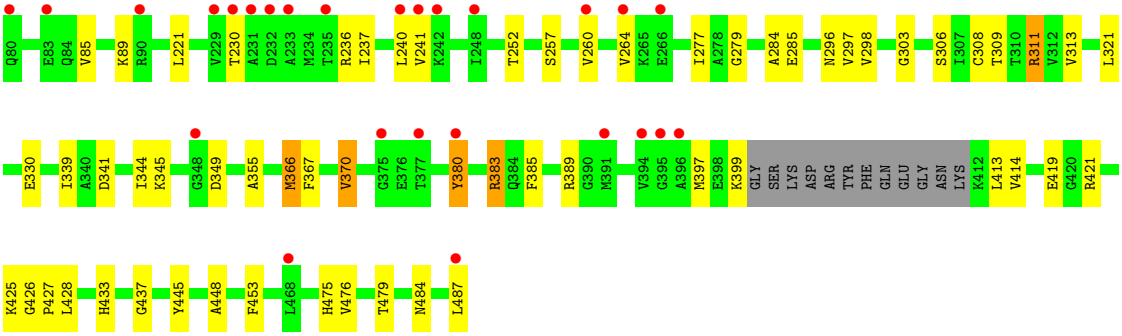


• Molecule 1: Inosine-5'-monophosphate dehydrogenase



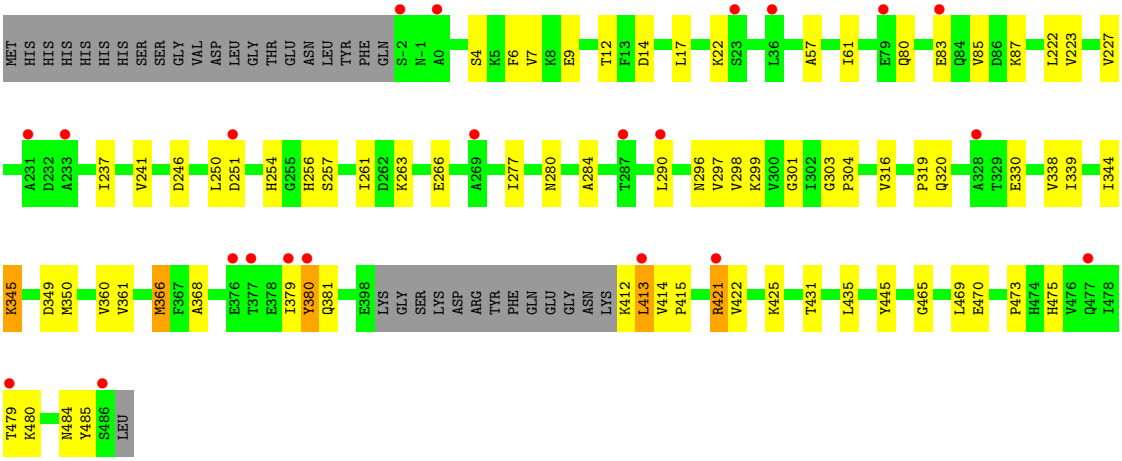
• Molecule 1: Inosine-5'-monophosphate dehydrogenase





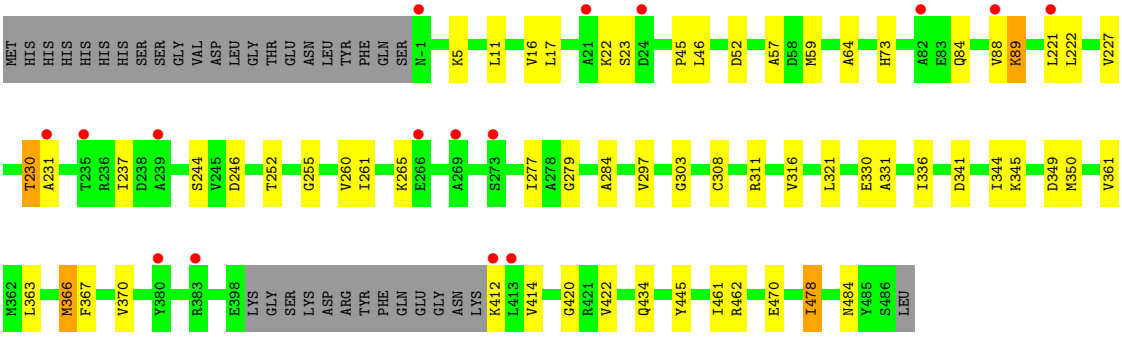
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

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	85.34Å 89.58Å 104.16Å 98.71° 89.82° 96.69°	Depositor
Resolution (Å)	42.86 – 2.39 44.29 – 2.39	Depositor EDS
% Data completeness (in resolution range)	95.6 (42.86-2.39) 95.6 (44.29-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.224 , 0.279 0.225 , 0.279	Depositor DCC
R_{free} test set	5762 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	21357	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.93% 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: K, IMP, PO4, EDO, PEG, GOL, 8LA

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	0.45	0/2629	0.64	0/3551
1	B	0.45	1/2603 (0.0%)	0.65	1/3518 (0.0%)
1	C	0.42	0/2594	0.65	0/3507
1	D	0.45	0/2606	0.66	0/3524
1	E	0.38	0/2607	0.61	0/3524
1	F	0.41	0/2611	0.64	0/3529
1	G	0.44	0/2594	0.63	1/3507 (0.0%)
1	H	0.43	0/2588	0.65	0/3499
All	All	0.43	1/20832 (0.0%)	0.64	2/28159 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	481	GLU	C-N	-5.29	1.21	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	28	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	G	421	ARG	NE-CZ-NH1	5.58	123.09	120.30

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	2593	0	2654	47	0
1	B	2567	0	2625	52	0
1	C	2558	0	2613	43	0
1	D	2569	0	2617	49	0
1	E	2570	0	2619	49	0
1	F	2575	0	2637	53	0
1	G	2558	0	2613	64	0
1	H	2552	0	2608	59	0
2	A	23	0	11	1	0
2	B	23	0	11	1	0
2	C	23	0	11	0	0
2	D	23	0	11	2	0
2	E	23	0	11	0	0
2	F	23	0	11	1	0
2	G	23	0	11	0	0
2	H	23	0	11	3	0
3	A	33	0	0	0	0
3	B	33	0	0	0	0
3	C	33	0	0	1	0
3	D	33	0	0	0	0
3	E	33	0	0	1	0
3	F	33	0	0	1	0
3	G	33	0	0	0	0
3	H	33	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	4	0	6	0	0
6	C	10	0	0	2	0
6	E	5	0	0	0	0
7	D	6	0	8	0	0
8	E	7	0	10	0	0
9	A	44	0	0	0	0
9	B	48	0	0	1	0
9	C	40	0	0	2	0
9	D	47	0	0	2	0
9	E	45	0	0	2	0
9	F	40	0	0	4	0
9	G	30	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	33	0	0	0	0
All	All	21357	0	21098	348	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 8.

All (348) 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:G:380:TYR:HD1	1:G:381:GLN:H	1.34	0.76
1:F:437:GLY:HA3	1:H:414:VAL:HG21	1.68	0.74
1:C:345:LYS:HD2	1:D:475:HIS:CE1	2.27	0.69
1:F:370:VAL:HG21	1:F:428:LEU:HA	1.74	0.69
1:F:252:THR:HG21	1:F:260:VAL:HG21	1.75	0.68
1:G:380:TYR:HD2	1:G:421:ARG:CZ	2.06	0.67
1:D:288:LYS:NZ	1:D:292:GLU:OE2	2.27	0.65
1:E:254:HIS:O	1:E:257:SER:OG	2.14	0.64
1:D:76:MET:HG2	1:D:80:GLN:HB3	1.80	0.64
1:A:414:VAL:HG21	1:C:437:GLY:HA3	1.79	0.63
1:H:52:ASP:HA	1:H:73:HIS:CD2	2.33	0.63
1:H:344:ILE:HG22	1:H:366:MET:HE1	1.80	0.62
1:G:14:ASP:OD1	1:G:345:LYS:NZ	2.30	0.62
1:H:308:CYS:SG	2:H:500:IMP:H2	2.40	0.61
1:C:15:ASP:OD1	9:C:601:HOH:O	2.16	0.61
1:E:261:ILE:HD12	1:G:22:LYS:HZ3	1.66	0.61
1:F:355:ALA:O	1:H:5:LYS:HE3	2.00	0.60
1:B:437:GLY:HA3	1:D:414:VAL:HG21	1.83	0.60
1:A:437:GLY:HA3	1:B:414:VAL:HG21	1.82	0.60
1:A:345:LYS:HG2	1:A:349:ASP:OD2	2.00	0.60
1:E:238:ASP:OD1	1:E:271:TYR:OH	2.14	0.60
1:C:252:THR:HG21	1:C:260:VAL:HG21	1.83	0.60
1:F:8:LYS:NZ	9:F:603:HOH:O	2.35	0.59
1:B:280:ASN:OD1	1:B:299:LYS:HE3	2.01	0.59
1:D:455:ARG:NH2	9:D:602:HOH:O	2.33	0.59
1:E:252:THR:HG21	1:E:260:VAL:HG21	1.85	0.59
1:G:425:LYS:HE2	1:G:431:THR:OG1	2.02	0.58
1:B:344:ILE:HG23	1:B:349:ASP:HB2	1.85	0.58
1:F:277:ILE:HG12	1:F:297:VAL:HB	1.86	0.58
1:C:380:TYR:HB3	1:C:385:PHE:CD2	2.39	0.58
1:F:427:PRO:O	9:F:601:HOH:O	2.17	0.58
1:G:316:VAL:HG11	1:H:445:TYR:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ASP:HA	1:B:73:HIS:CD2	2.38	0.58
1:A:222:LEU:HA	1:A:246:ASP:OD2	2.04	0.58
1:E:44:ILE:HD12	1:E:46:LEU:HD12	1.84	0.58
1:G:380:TYR:HD1	1:G:381:GLN:N	1.98	0.58
1:E:252:THR:OG1	3:E:502:8LA:O4	2.22	0.58
1:H:230:THR:HG22	1:H:231:ALA:H	1.69	0.57
1:B:268:ARG:NH1	1:B:296:ASN:OD1	2.36	0.57
1:H:311:ARG:HG2	1:H:316:VAL:O	2.04	0.57
1:C:332:ARG:HD2	6:C:503:PO4:O1	2.03	0.57
1:G:4:SER:O	1:G:7:VAL:HG12	2.04	0.57
1:A:475:HIS:CE1	1:B:345:LYS:HD2	2.40	0.57
1:B:338:VAL:HG23	1:B:358:ALA:HA	1.85	0.57
1:E:475:HIS:CE1	1:F:345:LYS:HD2	2.39	0.57
1:F:366:MET:O	1:F:425:LYS:NZ	2.36	0.57
1:A:280:ASN:OD1	1:A:299:LYS:HE3	2.05	0.57
1:F:309:THR:O	1:F:313:VAL:HG22	2.05	0.56
1:H:222:LEU:HA	1:H:246:ASP:OD2	2.06	0.56
1:H:363:LEU:HD13	1:H:366:MET:HE3	1.88	0.56
1:H:341:ASP:OD1	2:H:500:IMP:O3'	2.16	0.56
1:F:285:GLU:HG2	9:F:618:HOH:O	2.06	0.56
1:D:227:VAL:HG13	1:D:236:ARG:HD2	1.87	0.55
1:F:475:HIS:NE2	1:H:345:LYS:HD2	2.21	0.55
1:B:222:LEU:HA	1:B:246:ASP:OD2	2.05	0.55
1:H:344:ILE:HG23	1:H:349:ASP:HB2	1.88	0.55
1:B:58:ASP:O	1:B:61:ILE:HG13	2.06	0.55
1:A:413:LEU:HD12	1:A:414:VAL:N	2.21	0.55
1:C:414:VAL:HG21	1:D:437:GLY:HA3	1.87	0.55
1:E:256:HIS:NE2	1:G:22:LYS:HB2	2.22	0.55
1:E:338:VAL:HG23	1:E:358:ALA:HA	1.87	0.55
1:B:45:PRO:HA	1:B:360:VAL:HG22	1.89	0.55
1:G:366:MET:O	1:G:425:LYS:NZ	2.38	0.55
1:A:24:ASP:OD1	1:B:258:GLN:HB2	2.06	0.54
1:G:339:ILE:HG23	1:G:360:VAL:HG13	1.88	0.54
1:C:418:ILE:HD13	1:D:478:ILE:HG12	1.89	0.54
1:H:350:MET:HG3	1:H:361:VAL:HG11	1.90	0.54
1:E:248:ILE:HG12	1:E:274:LEU:HD21	1.89	0.54
1:F:89:LYS:HE2	1:F:221:LEU:O	2.07	0.54
1:C:312:VAL:HA	6:C:504:PO4:O4	2.07	0.54
1:G:277:ILE:HG12	1:G:297:VAL:HB	1.88	0.54
1:G:280:ASN:OD1	1:G:299:LYS:HE3	2.08	0.54
1:G:414:VAL:HG13	1:H:484:ASN:HD22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:ASP:OD1	1:C:299:LYS:NZ	2.31	0.54
1:B:77:SER:OG	1:B:80:GLN:HG2	2.08	0.54
1:D:303:GLY:HA3	1:D:311:ARG:HE	1.74	0.53
1:C:394:VAL:HG22	1:C:413:LEU:CD1	2.39	0.53
1:D:425:LYS:HE2	1:D:431:THR:OG1	2.08	0.53
1:F:383:ARG:HG3	1:F:385:PHE:CE2	2.44	0.53
1:G:80:GLN:HA	1:G:83:GLU:OE1	2.08	0.53
1:B:61:ILE:HD11	9:B:646:HOH:O	2.08	0.53
1:H:277:ILE:HG12	1:H:297:VAL:HB	1.89	0.53
1:E:470:GLU:OE1	1:F:311:ARG:NH1	2.38	0.53
1:F:78:ILE:HG12	1:F:236:ARG:HB2	1.89	0.53
1:G:298:VAL:HB	1:G:338:VAL:HG12	1.90	0.53
1:E:280:ASN:OD1	1:E:299:LYS:HE3	2.09	0.53
1:G:261:ILE:HD12	1:H:22:LYS:NZ	2.24	0.53
1:D:52:ASP:HA	1:D:73:HIS:CD2	2.44	0.53
1:G:412:LYS:HE3	1:H:434:GLN:HE21	1.74	0.53
1:A:345:LYS:HG3	1:A:346:TYR:CD2	2.45	0.52
1:A:478:ILE:HG12	1:B:418:ILE:HD13	1.89	0.52
1:C:277:ILE:HG12	1:C:297:VAL:HB	1.91	0.52
1:C:9:GLU:OE2	1:D:462:ARG:NH2	2.43	0.52
1:D:339:ILE:HG12	1:D:360:VAL:HG23	1.91	0.52
1:E:345:LYS:HD2	1:G:475:HIS:CE1	2.45	0.52
1:C:252:THR:OG1	3:C:502:8LA:O4	2.25	0.52
1:F:479:THR:HG23	1:H:420:GLY:HA2	1.90	0.52
1:D:309:THR:O	1:D:313:VAL:HG22	2.10	0.52
1:E:319:PRO:HD3	1:G:17:LEU:HD12	1.91	0.52
1:A:256:HIS:CE1	1:C:22:LYS:HG2	2.45	0.51
1:A:483:PRO:HD2	1:B:415:PRO:HG3	1.91	0.51
1:B:240:LEU:HB3	1:B:245:VAL:HG11	1.92	0.51
1:G:465:GLY:O	1:G:469:LEU:HD13	2.11	0.51
1:E:11:LEU:HD11	1:E:462:ARG:HD3	1.93	0.51
1:E:316:VAL:HG11	1:G:445:TYR:HB3	1.92	0.51
1:B:340:ALA:HB3	1:B:361:VAL:HG12	1.92	0.51
1:D:89:LYS:HE3	1:D:244:SER:O	2.11	0.51
1:A:52:ASP:HA	1:A:73:HIS:CD2	2.46	0.51
1:B:87:LYS:O	1:B:91:SER:HB2	2.11	0.51
1:F:397:MET:HE3	1:F:413:LEU:HD13	1.93	0.51
1:H:252:THR:HG21	1:H:260:VAL:HG21	1.93	0.51
1:B:425:LYS:HE2	1:B:431:THR:OG1	2.11	0.50
1:A:370:VAL:HG21	1:A:428:LEU:HA	1.92	0.50
1:E:303:GLY:HA3	1:E:311:ARG:NE	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:319:PRO:HD3	1:H:17:LEU:HD12	1.92	0.50
1:F:344:ILE:HG23	1:F:349:ASP:HB2	1.94	0.50
1:A:458:ALA:O	1:B:5:LYS:HG2	2.12	0.50
1:D:39:SER:OG	1:D:275:ASN:ND2	2.44	0.50
1:D:237:ILE:O	1:D:241:VAL:HG23	2.11	0.50
1:D:246:ASP:O	1:D:275:ASN:HB2	2.12	0.50
1:D:413:LEU:HA	9:D:624:HOH:O	2.10	0.50
1:E:437:GLY:HA3	1:F:414:VAL:HG21	1.93	0.50
1:F:85:VAL:HG21	1:F:240:LEU:HD22	1.93	0.50
1:F:475:HIS:CD2	1:H:345:LYS:HD2	2.47	0.50
1:A:45:PRO:C	1:A:360:VAL:HG23	2.32	0.50
1:A:465:GLY:O	1:A:469:LEU:HD12	2.11	0.50
1:B:241:VAL:HG11	1:B:271:TYR:CE1	2.47	0.50
1:C:238:ASP:OD1	1:C:271:TYR:OH	2.24	0.50
1:E:439:LEU:C	1:E:439:LEU:HD23	2.33	0.50
1:C:463:MET:HE2	1:C:467:GLY:HA3	1.94	0.49
1:D:248:ILE:HD11	1:D:267:VAL:HG11	1.94	0.49
1:H:261:ILE:HG22	1:H:265:LYS:HE2	1.94	0.49
1:C:394:VAL:HG22	1:C:413:LEU:HD11	1.93	0.49
1:D:51:MET:SD	2:D:501:IMP:H8	2.52	0.49
1:E:284:ALA:HB1	1:E:330:GLU:HB2	1.93	0.49
1:B:478:ILE:HG12	1:D:418:ILE:HD12	1.94	0.49
1:G:413:LEU:HD13	1:G:413:LEU:H	1.76	0.49
1:C:303:GLY:HA2	1:C:308:CYS:SG	2.52	0.49
1:D:277:ILE:HG12	1:D:297:VAL:HB	1.94	0.49
1:G:473:PRO:HD2	1:G:485:TYR:OH	2.13	0.49
1:D:44:ILE:HD12	1:D:46:LEU:HD12	1.94	0.49
1:G:380:TYR:HD2	1:G:421:ARG:NH1	2.10	0.48
1:A:308:CYS:SG	2:A:501:IMP:H2	2.53	0.48
1:E:367:PHE:O	1:E:370:VAL:HG22	2.13	0.48
1:F:284:ALA:HB1	1:F:330:GLU:HB2	1.95	0.48
1:A:306:SER:HB2	1:C:474:HIS:O	2.13	0.48
1:A:25:VAL:HG23	1:A:29:GLU:HG3	1.96	0.48
1:F:257:SER:OG	1:F:260:VAL:HG23	2.13	0.48
1:D:33:LYS:HG2	1:D:43:ASN:HA	1.96	0.48
1:A:258:GLN:HB2	1:C:24:ASP:OD1	2.14	0.48
1:E:474:HIS:O	1:F:306:SER:HB2	2.14	0.48
1:F:46:LEU:HD23	1:F:367:PHE:HZ	1.78	0.48
1:H:227:VAL:HG11	1:H:237:ILE:HG13	1.94	0.48
1:E:303:GLY:HA3	1:E:311:ARG:HE	1.79	0.48
1:B:359:HIS:O	1:B:360:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:THR:HG22	1:C:279:GLY:O	2.14	0.47
1:A:59:MET:CE	1:A:367:PHE:HB3	2.45	0.47
1:B:76:MET:HB2	1:B:80:GLN:HG3	1.96	0.47
1:D:339:ILE:HG12	1:D:360:VAL:CG2	2.44	0.47
1:E:455:ARG:O	1:F:5:LYS:NZ	2.40	0.47
1:G:9:GLU:OE2	1:H:462:ARG:NH2	2.48	0.47
1:A:311:ARG:HG2	1:A:316:VAL:O	2.14	0.47
1:E:33:LYS:HG2	1:E:43:ASN:HA	1.95	0.47
1:F:383:ARG:HG3	1:F:385:PHE:HE2	1.79	0.47
1:A:303:GLY:HA2	1:A:308:CYS:SG	2.55	0.47
1:B:79:GLU:HG3	1:B:80:GLN:N	2.29	0.47
1:F:252:THR:OG1	3:F:501:8LA:O4	2.30	0.47
1:F:445:TYR:HB3	1:H:316:VAL:HG11	1.96	0.47
1:F:380:TYR:HD2	1:F:421:ARG:NH2	2.14	0.47
1:A:17:LEU:HD12	1:B:319:PRO:HD3	1.97	0.46
1:E:52:ASP:HA	1:E:73:HIS:CD2	2.50	0.46
1:F:476:VAL:HG22	1:H:422:VAL:CG1	2.45	0.46
1:G:87:LYS:HE3	1:G:87:LYS:HB2	1.73	0.46
1:B:277:ILE:HG12	1:B:297:VAL:HB	1.96	0.46
1:B:303:GLY:HA3	1:B:311:ARG:HG3	1.97	0.46
1:G:257:SER:HA	1:H:23:SER:O	2.14	0.46
1:A:397:MET:HE3	1:A:413:LEU:HD11	1.97	0.46
1:F:33:LYS:HG2	1:F:43:ASN:HA	1.97	0.46
1:D:370:VAL:HG11	1:D:428:LEU:HB2	1.98	0.46
1:A:389:ARG:HH22	1:A:399:LYS:HE3	1.81	0.46
1:G:85:VAL:HG13	1:G:223:VAL:HG11	1.96	0.46
1:A:245:VAL:HG22	1:A:247:ALA:H	1.81	0.46
1:A:445:TYR:HB3	1:B:316:VAL:HG11	1.98	0.46
1:B:267:VAL:HG12	1:B:276:ILE:HD11	1.97	0.46
1:G:380:TYR:CD1	1:G:381:GLN:N	2.81	0.46
1:G:301:GLY:HA2	1:G:320:GLN:OE1	2.16	0.46
1:D:280:ASN:OD1	1:D:299:LYS:HE3	2.16	0.46
1:G:413:LEU:HB2	9:G:618:HOH:O	2.14	0.46
1:G:380:TYR:CD2	1:G:421:ARG:CZ	2.92	0.46
1:A:413:LEU:HD12	1:A:414:VAL:H	1.80	0.46
1:B:445:TYR:HB3	1:D:316:VAL:HG11	1.98	0.46
1:A:72:ILE:HD13	1:A:84:GLN:HB3	1.98	0.45
1:B:371:ALA:N	1:B:426:GLY:O	2.42	0.45
1:C:345:LYS:HD2	1:D:475:HIS:ND1	2.31	0.45
1:C:380:TYR:HB3	1:C:385:PHE:CE2	2.51	0.45
1:D:222:LEU:HA	1:D:246:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:PRO:C	1:E:360:VAL:HG23	2.36	0.45
1:G:480:LYS:NZ	9:G:602:HOH:O	2.41	0.45
1:B:366:MET:O	1:B:425:LYS:NZ	2.37	0.45
1:G:250:LEU:HD23	1:G:250:LEU:HA	1.83	0.45
1:C:5:LYS:HG2	1:D:458:ALA:O	2.15	0.45
1:D:344:ILE:HG23	1:D:349:ASP:HB2	1.99	0.45
1:E:380:TYR:HB3	1:E:385:PHE:CD1	2.51	0.45
1:F:303:GLY:N	9:F:606:HOH:O	2.43	0.45
1:A:14:ASP:HB2	1:C:466:ALA:HB1	1.98	0.45
1:C:311:ARG:HG2	1:C:316:VAL:O	2.16	0.45
1:D:341:ASP:OD2	2:D:501:IMP:O2'	2.33	0.45
1:E:311:ARG:HG2	1:E:316:VAL:O	2.17	0.45
1:C:415:PRO:HD2	1:D:484:ASN:ND2	2.32	0.45
1:D:234:MET:HE1	1:D:266:GLU:HB3	1.99	0.45
1:A:1:MET:HE2	1:A:1:MET:HB3	1.85	0.45
1:E:344:ILE:HG23	1:E:349:ASP:HB2	1.99	0.45
1:H:331:ALA:HB1	1:H:336:ILE:O	2.16	0.45
1:C:268:ARG:NH2	1:C:296:ASN:HD21	2.15	0.45
1:E:425:LYS:HE2	1:E:431:THR:OG1	2.17	0.45
1:D:254:HIS:CE1	1:D:256:HIS:HB3	2.52	0.45
1:D:347:SER:HB3	1:D:435:LEU:HD23	1.99	0.44
1:F:252:THR:HG22	1:F:279:GLY:O	2.17	0.44
1:F:321:LEU:HD12	1:F:321:LEU:HA	1.82	0.44
1:G:57:ALA:O	1:G:61:ILE:HG13	2.17	0.44
1:B:227:VAL:HG11	1:B:237:ILE:HD11	1.99	0.44
1:B:303:GLY:N	1:B:304:PRO:CD	2.80	0.44
1:G:479:THR:HG22	1:G:480:LYS:HG3	2.00	0.44
1:H:255:GLY:HA2	1:H:260:VAL:HG21	1.98	0.44
1:G:414:VAL:HG13	1:H:484:ASN:ND2	2.33	0.44
1:H:89:LYS:HE3	1:H:221:LEU:O	2.16	0.44
1:B:355:ALA:O	1:D:5:LYS:HE3	2.18	0.44
1:H:252:THR:HG21	1:H:260:VAL:CG2	2.48	0.44
1:B:308:CYS:SG	2:B:500:IMP:H2	2.58	0.44
1:B:311:ARG:HG2	1:B:316:VAL:O	2.17	0.44
1:G:473:PRO:HG2	1:G:485:TYR:CE1	2.52	0.44
1:A:316:VAL:HG11	1:C:445:TYR:HB3	1.99	0.43
1:C:45:PRO:C	1:C:360:VAL:HG23	2.38	0.43
1:C:393:SER:O	1:C:397:MET:HE2	2.17	0.43
1:E:277:ILE:HG12	1:E:297:VAL:HB	1.99	0.43
1:G:6:PHE:O	1:H:462:ARG:NH1	2.46	0.43
1:H:303:GLY:HA2	1:H:308:CYS:SG	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HG12	1:A:297:VAL:HB	1.99	0.43
1:C:11:LEU:HD11	1:C:462:ARG:HE	1.83	0.43
1:E:415:PRO:HD2	1:G:484:ASN:ND2	2.33	0.43
1:F:52:ASP:HA	1:F:73:HIS:CD2	2.53	0.43
1:F:303:GLY:HA2	1:F:308:CYS:SG	2.59	0.43
1:C:0:ALA:O	1:C:4:SER:OG	2.30	0.43
1:C:348:GLY:O	1:C:352:LYS:HG3	2.19	0.43
1:E:268:ARG:NH2	1:E:296:ASN:OD1	2.52	0.43
1:F:341:ASP:OD2	2:F:500:IMP:O2'	2.29	0.43
1:G:344:ILE:HG23	1:G:349:ASP:HB2	2.00	0.43
1:B:463:MET:HE2	1:B:467:GLY:HA3	2.01	0.43
1:E:414:VAL:HA	1:E:415:PRO:HD3	1.83	0.43
1:H:59:MET:CE	1:H:367:PHE:HB3	2.48	0.43
1:A:14:ASP:HB3	1:A:468:LEU:HD22	2.01	0.43
1:C:319:PRO:HD3	1:D:17:LEU:HD12	2.01	0.43
1:F:476:VAL:HG22	1:H:422:VAL:HG12	2.00	0.43
1:G:415:PRO:HD2	1:H:484:ASN:ND2	2.33	0.43
1:H:45:PRO:O	1:H:361:VAL:HG22	2.19	0.43
1:H:462:ARG:HH11	1:H:462:ARG:HD3	1.72	0.43
1:B:275:ASN:HA	1:B:296:ASN:HD21	1.83	0.43
1:D:240:LEU:O	1:D:245:VAL:HG12	2.18	0.43
1:F:370:VAL:HG22	1:F:426:GLY:O	2.19	0.43
1:G:12:THR:OG1	1:H:470:GLU:OE1	2.35	0.43
1:H:46:LEU:HD23	1:H:367:PHE:HZ	1.83	0.43
1:C:338:VAL:HG22	9:C:607:HOH:O	2.19	0.43
1:D:62:ALA:O	1:D:66:GLN:HG2	2.19	0.43
1:F:445:TYR:HB2	1:H:316:VAL:HG21	2.01	0.43
1:B:44:ILE:HD12	1:B:46:LEU:HD12	2.01	0.43
1:D:50:GLY:HA2	1:D:71:ILE:O	2.19	0.43
1:H:45:PRO:C	1:H:46:LEU:HD12	2.40	0.43
1:E:26:LEU:HB2	1:E:29:GLU:HG2	2.01	0.42
1:F:433:HIS:NE2	1:H:412:LYS:HA	2.34	0.42
1:G:237:ILE:O	1:G:241:VAL:HG13	2.18	0.42
1:A:475:HIS:ND1	1:B:345:LYS:HD2	2.35	0.42
1:B:34:THR:HG21	1:B:360:VAL:CG2	2.48	0.42
1:F:448:ALA:HA	1:F:453:PHE:CD1	2.54	0.42
1:G:303:GLY:N	1:G:304:PRO:CD	2.82	0.42
1:H:478:ILE:H	1:H:478:ILE:HG13	1.51	0.42
1:C:367:PHE:O	1:C:370:VAL:HG22	2.19	0.42
1:E:32:VAL:HG23	1:E:43:ASN:O	2.19	0.42
1:G:256:HIS:NE2	1:H:22:LYS:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:THR:HG22	1:H:279:GLY:O	2.20	0.42
1:A:50:GLY:HA2	1:A:71:ILE:O	2.20	0.42
1:A:59:MET:HE1	1:A:367:PHE:HB3	2.01	0.42
1:E:39:SER:HB2	1:E:275:ASN:HD21	1.84	0.42
1:E:459:GLN:OE1	1:F:4:SER:OG	2.28	0.42
1:F:47:ILE:HG12	1:F:69:LEU:HB3	2.01	0.42
1:G:251:ASP:OD1	1:G:299:LYS:NZ	2.49	0.42
1:G:319:PRO:HD2	1:H:461:ILE:HD13	2.01	0.42
1:H:11:LEU:HD11	1:H:462:ARG:HD2	2.02	0.42
1:E:303:GLY:N	1:E:304:PRO:CD	2.83	0.42
1:E:462:ARG:NH1	1:F:9:GLU:HG3	2.34	0.42
1:F:298:VAL:O	1:F:339:ILE:N	2.40	0.42
1:B:55:THR:HA	1:B:59:MET:HB3	2.01	0.42
1:C:252:THR:HG21	1:C:260:VAL:CG2	2.50	0.42
1:E:24:ASP:OD2	9:E:602:HOH:O	2.21	0.42
1:F:389:ARG:HH22	1:F:399:LYS:NZ	2.18	0.42
1:H:367:PHE:O	1:H:370:VAL:HG22	2.20	0.42
1:B:302:ILE:HD13	1:B:302:ILE:HA	1.84	0.42
1:G:350:MET:HG3	1:G:361:VAL:HG21	2.02	0.42
1:E:229:VAL:HG21	1:E:260:VAL:HG22	2.02	0.42
1:F:45:PRO:C	1:F:46:LEU:HD12	2.41	0.42
1:G:263:LYS:HA	1:G:266:GLU:HG2	2.01	0.42
1:A:298:VAL:O	1:A:338:VAL:HA	2.20	0.42
1:A:303:GLY:N	1:A:304:PRO:CD	2.83	0.42
1:B:45:PRO:CA	1:B:360:VAL:HG22	2.50	0.42
1:D:325:TYR:O	1:D:329:THR:OG1	2.28	0.42
1:E:303:GLY:HA3	1:E:311:ARG:HG3	2.01	0.42
1:B:418:ILE:H	1:B:418:ILE:HG13	1.78	0.41
1:C:316:VAL:HG11	1:D:445:TYR:HB3	2.02	0.41
1:C:338:VAL:HG23	1:C:358:ALA:HA	2.02	0.41
1:D:229:VAL:HG21	1:D:260:VAL:HG22	2.03	0.41
1:B:334:HIS:HB3	1:G:379:ILE:HG22	2.03	0.41
1:H:64:ALA:HB1	1:H:221:LEU:HB3	2.01	0.41
1:H:89:LYS:HD3	1:H:244:SER:O	2.21	0.41
1:H:308:CYS:SG	2:H:500:IMP:C2	3.08	0.41
1:A:248:ILE:HD11	1:A:267:VAL:HG11	2.02	0.41
1:B:59:MET:CE	1:B:367:PHE:HB3	2.50	0.41
1:B:347:SER:HB3	1:B:435:LEU:HD23	2.03	0.41
1:C:479:THR:HG22	1:C:480:LYS:HG3	2.03	0.41
1:G:254:HIS:CE1	1:G:256:HIS:HB3	2.56	0.41
1:G:284:ALA:HB1	1:G:330:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:350:MET:HE1	1:G:435:LEU:O	2.21	0.41
1:H:84:GLN:O	1:H:88:VAL:HG23	2.21	0.41
1:A:284:ALA:HB1	1:A:330:GLU:HB2	2.02	0.41
1:E:345:LYS:HG3	1:E:346:TYR:CD2	2.55	0.41
1:F:260:VAL:O	1:F:264:VAL:HG23	2.21	0.41
1:H:57:ALA:N	1:H:84:GLN:OE1	2.53	0.41
1:E:250:LEU:HD12	1:E:264:VAL:HG22	2.02	0.41
1:A:43:ASN:HB2	1:A:67:GLY:HA3	2.03	0.41
1:C:254:HIS:CE1	1:C:256:HIS:HB3	2.55	0.41
1:D:89:LYS:HD3	1:D:89:LYS:HA	1.87	0.41
1:E:12:THR:OG1	1:G:470:GLU:OE1	2.34	0.41
1:G:413:LEU:C	1:G:413:LEU:HD22	2.41	0.41
1:A:321:LEU:HA	1:A:321:LEU:HD12	1.81	0.41
1:G:222:LEU:HA	1:G:246:ASP:OD2	2.20	0.41
1:G:227:VAL:HG11	1:G:237:ILE:HG13	2.03	0.41
1:A:303:GLY:HA3	1:A:311:ARG:HG3	2.02	0.40
1:D:311:ARG:HG2	1:D:316:VAL:O	2.21	0.40
1:E:74:LYS:HG2	9:E:605:HOH:O	2.21	0.40
1:D:86:ASP:OD2	1:D:90:ARG:NE	2.40	0.40
1:E:480:LYS:HD2	1:F:419:GLU:OE1	2.21	0.40
1:G:261:ILE:HD12	1:H:22:LYS:HZ3	1.86	0.40
1:G:339:ILE:HG12	1:G:360:VAL:CG1	2.51	0.40
1:G:368:ALA:HB3	1:G:422:VAL:HG21	2.03	0.40
1:H:284:ALA:HB1	1:H:330:GLU:HB2	2.04	0.40
1:A:25:VAL:HG21	1:A:30:VAL:HG12	2.04	0.40
1:B:55:THR:HB	1:B:71:ILE:O	2.21	0.40
1:F:237:ILE:O	1:F:241:VAL:HG23	2.22	0.40
1:G:413:LEU:CD1	1:G:413:LEU:N	2.84	0.40
1:H:16:VAL:HG21	1:H:321:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/384 (91%)	340 (97%)	9 (3%)	0	100	100
1	B	346/384 (90%)	336 (97%)	10 (3%)	0	100	100
1	C	345/384 (90%)	338 (98%)	7 (2%)	0	100	100
1	D	346/384 (90%)	339 (98%)	7 (2%)	0	100	100
1	E	346/384 (90%)	338 (98%)	8 (2%)	0	100	100
1	F	347/384 (90%)	337 (97%)	10 (3%)	0	100	100
1	G	345/384 (90%)	336 (97%)	9 (3%)	0	100	100
1	H	344/384 (90%)	336 (98%)	8 (2%)	0	100	100
All	All	2768/3072 (90%)	2700 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	271/298 (91%)	259 (96%)	12 (4%)	28	42
1	B	268/298 (90%)	260 (97%)	8 (3%)	41	59
1	C	267/298 (90%)	262 (98%)	5 (2%)	57	73
1	D	268/298 (90%)	263 (98%)	5 (2%)	57	73
1	E	268/298 (90%)	263 (98%)	5 (2%)	57	73
1	F	269/298 (90%)	256 (95%)	13 (5%)	25	39
1	G	267/298 (90%)	261 (98%)	6 (2%)	52	69
1	H	266/298 (89%)	262 (98%)	4 (2%)	65	79
All	All	2144/2384 (90%)	2086 (97%)	58 (3%)	44	62

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	VAL

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Mol	Chain	Res	Type
1	A	37	SER
1	A	74[A]	LYS
1	A	74[B]	LYS
1	A	230	THR
1	A	370	VAL
1	A	373	SER
1	A	381	GLN
1	A	413	LEU
1	A	418	ILE
1	A	469	LEU
1	B	36	LEU
1	B	86	ASP
1	B	251	ASP
1	B	296	ASN
1	B	366	MET
1	B	449	GLN
1	B	463	MET
1	B	484	ASN
1	C	9	GLU
1	C	22	LYS
1	C	51	MET
1	C	296	ASN
1	C	463	MET
1	D	230	THR
1	D	345	LYS
1	D	370	VAL
1	D	377	THR
1	D	378	GLU
1	E	-4	PHE
1	E	232	ASP
1	E	373	SER
1	E	397	MET
1	E	418	ILE
1	F	25	VAL
1	F	28	ARG
1	F	34	THR
1	F	36	LEU
1	F	230	THR
1	F	296	ASN
1	F	311	ARG
1	F	366	MET
1	F	370	VAL

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Mol	Chain	Res	Type
1	F	380	TYR
1	F	383	ARG
1	F	484	ASN
1	F	487	LEU
1	G	290	LEU
1	G	296	ASN
1	G	345	LYS
1	G	366	MET
1	G	380	TYR
1	G	413	LEU
1	H	89	LYS
1	H	230	THR
1	H	366	MET
1	H	478	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	434	GLN
1	B	484	ASN
1	G	475	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 for Mogul analysis.

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	IMP	F	500	-	21,25,25	1.40	2 (9%)	24,38,38	1.58	5 (20%)
3	8LA	E	502	-	35,35,35	1.46	4 (11%)	50,51,51	1.71	6 (12%)
2	IMP	H	500	-	21,25,25	1.45	3 (14%)	24,38,38	1.72	6 (25%)
3	8LA	C	502	-	35,35,35	1.33	4 (11%)	50,51,51	1.75	9 (18%)
3	8LA	G	501	-	35,35,35	1.51	5 (14%)	50,51,51	1.83	9 (18%)
3	8LA	A	502	-	35,35,35	1.34	5 (14%)	50,51,51	1.29	2 (4%)
2	IMP	G	500	-	21,25,25	1.50	3 (14%)	24,38,38	1.28	3 (12%)
5	EDO	A	504	-	3,3,3	0.47	0	2,2,2	0.47	0
8	PEG	E	504	-	6,6,6	0.53	0	5,5,5	0.43	0
3	8LA	F	501	-	35,35,35	1.46	4 (11%)	50,51,51	1.96	5 (10%)
3	8LA	H	501	-	35,35,35	1.32	3 (8%)	50,51,51	1.47	6 (12%)
2	IMP	A	501	-	21,25,25	1.39	2 (9%)	24,38,38	1.21	4 (16%)
3	8LA	B	501	-	35,35,35	1.46	5 (14%)	50,51,51	1.28	4 (8%)
2	IMP	B	500	-	21,25,25	1.44	2 (9%)	24,38,38	1.21	2 (8%)
3	8LA	D	502	-	35,35,35	1.69	7 (20%)	50,51,51	1.94	9 (18%)
6	PO4	E	505	-	4,4,4	0.90	0	6,6,6	0.61	0
2	IMP	C	501	-	21,25,25	1.44	3 (14%)	24,38,38	1.38	3 (12%)
6	PO4	C	504	-	4,4,4	0.98	0	6,6,6	0.67	0
2	IMP	E	501	-	21,25,25	1.45	2 (9%)	24,38,38	1.45	5 (20%)
2	IMP	D	501	-	21,25,25	1.42	2 (9%)	24,38,38	1.30	3 (12%)
6	PO4	C	503	-	4,4,4	0.81	0	6,6,6	0.60	0
7	GOL	D	503	-	5,5,5	0.62	0	5,5,5	0.36	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	F	500	-	-	0/6/26/26	0/3/3/3
3	8LA	E	502	-	-	5/24/41/41	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	H	500	-	-	0/6/26/26	0/3/3/3
3	8LA	C	502	-	-	6/24/41/41	0/3/3/3
3	8LA	G	501	-	-	5/24/41/41	0/3/3/3
3	8LA	A	502	-	-	4/24/41/41	0/3/3/3
2	IMP	G	500	-	-	1/6/26/26	0/3/3/3
5	EDO	A	504	-	-	0/1/1/1	-
8	PEG	E	504	-	-	2/4/4/4	-
3	8LA	F	501	-	-	7/24/41/41	0/3/3/3
3	8LA	H	501	-	-	5/24/41/41	0/3/3/3
2	IMP	A	501	-	-	0/6/26/26	0/3/3/3
3	8LA	B	501	-	-	5/24/41/41	0/3/3/3
2	IMP	B	500	-	-	2/6/26/26	0/3/3/3
3	8LA	D	502	-	-	8/24/41/41	0/3/3/3
2	IMP	C	501	-	-	3/6/26/26	0/3/3/3
2	IMP	E	501	-	-	0/6/26/26	0/3/3/3
2	IMP	D	501	-	-	0/6/26/26	0/3/3/3
7	GOL	D	503	-	-	2/4/4/4	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	8LA	C21-C20	6.19	1.50	1.39
3	F	501	8LA	C21-C20	5.93	1.50	1.39
3	G	501	8LA	C21-C20	5.90	1.49	1.39
3	B	501	8LA	C21-C20	5.47	1.49	1.39
3	C	502	8LA	C21-C20	5.40	1.49	1.39
3	H	501	8LA	C21-C20	5.23	1.48	1.39
3	A	502	8LA	C21-C20	5.08	1.48	1.39
2	G	500	IMP	C2-N3	4.93	1.38	1.29
2	D	501	IMP	C2-N3	4.89	1.38	1.29
2	A	501	IMP	C2-N3	4.85	1.38	1.29
2	F	500	IMP	C2-N3	4.60	1.38	1.29
2	H	500	IMP	C2-N3	4.54	1.38	1.29
2	B	500	IMP	C2-N3	4.42	1.37	1.29
2	E	501	IMP	C2-N3	4.42	1.37	1.29
2	C	501	IMP	C2-N3	4.17	1.37	1.29
2	C	501	IMP	C5-C6	-4.12	1.39	1.47
2	E	501	IMP	C5-C6	-4.05	1.39	1.47
3	D	502	8LA	C21-C20	3.98	1.46	1.39
2	B	500	IMP	C5-C6	-3.77	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	IMP	C5-C6	-3.60	1.40	1.47
3	D	502	8LA	C11-C1	-3.44	1.49	1.53
2	H	500	IMP	C5-C6	-3.29	1.40	1.47
3	D	502	8LA	C8-C7	-3.20	1.30	1.46
3	D	502	8LA	C17-N4	-3.19	1.35	1.41
2	F	500	IMP	C5-C6	-3.11	1.41	1.47
3	G	501	8LA	C11-C1	-3.11	1.49	1.53
2	D	501	IMP	C5-C6	-3.02	1.41	1.47
3	E	502	8LA	C20-CL	3.00	1.80	1.73
2	A	501	IMP	C5-C6	-2.92	1.41	1.47
3	H	501	8LA	C8-C7	-2.90	1.32	1.46
3	C	502	8LA	C20-CL	2.89	1.80	1.73
3	B	501	8LA	C8-C7	-2.88	1.32	1.46
3	F	501	8LA	C8-C7	-2.88	1.32	1.46
3	A	502	8LA	C8-C7	-2.84	1.32	1.46
3	F	501	8LA	C17-N4	-2.76	1.36	1.41
3	F	501	8LA	C20-CL	2.75	1.80	1.73
3	E	502	8LA	C8-C7	-2.75	1.33	1.46
3	C	502	8LA	C8-C7	-2.74	1.33	1.46
3	D	502	8LA	C10-N4	-2.69	1.31	1.37
3	G	501	8LA	C8-C7	-2.67	1.33	1.46
3	B	501	8LA	C17-N4	-2.66	1.36	1.41
3	G	501	8LA	C20-CL	2.64	1.79	1.73
3	A	502	8LA	C11-C1	-2.51	1.50	1.53
3	H	501	8LA	C20-CL	2.43	1.79	1.73
3	D	502	8LA	O2-C10	-2.43	1.18	1.23
3	B	501	8LA	C11-N3	-2.42	1.44	1.47
3	B	501	8LA	C20-CL	2.37	1.79	1.73
3	A	502	8LA	C17-N4	-2.30	1.37	1.41
3	G	501	8LA	C17-N4	-2.28	1.37	1.41
3	C	502	8LA	C11-C1	-2.25	1.51	1.53
3	D	502	8LA	C24-C25	-2.15	1.50	1.52
2	C	501	IMP	C5-C4	-2.10	1.37	1.43
2	G	500	IMP	C2-N1	2.07	1.39	1.35
3	E	502	8LA	C17-N4	-2.06	1.37	1.41
2	H	500	IMP	P-O3P	-2.05	1.46	1.54
3	A	502	8LA	C20-CL	2.03	1.78	1.73

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	501	8LA	O1-C21-C20	10.81	125.64	116.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	502	8LA	O1-C21-C20	9.48	124.47	116.13
3	G	501	8LA	O1-C21-C20	9.04	124.08	116.13
3	C	502	8LA	O1-C21-C20	8.72	123.80	116.13
3	E	502	8LA	O1-C21-C20	7.99	123.16	116.13
3	H	501	8LA	O1-C21-C20	5.73	121.17	116.13
3	A	502	8LA	O1-C21-C20	5.12	120.63	116.13
3	B	501	8LA	O1-C21-C20	5.10	120.61	116.13
2	H	500	IMP	O6-C6-N1	-4.72	114.59	120.32
2	F	500	IMP	O6-C6-N1	-4.56	114.78	120.32
3	F	501	8LA	C21-C20-CL	4.02	124.14	119.43
3	D	502	8LA	O1-C24-C25	3.94	113.44	106.78
3	F	501	8LA	C21-O1-C24	3.79	125.33	118.09
3	E	502	8LA	C21-C20-CL	3.76	123.85	119.43
2	C	501	IMP	C8-N7-C5	3.58	109.80	102.99
3	A	502	8LA	C21-O1-C24	3.57	124.91	118.09
3	C	502	8LA	C21-O1-C24	3.51	124.80	118.09
3	H	501	8LA	O1-C24-C25	3.48	112.67	106.78
2	H	500	IMP	C8-N7-C5	3.42	109.51	102.99
3	F	501	8LA	O1-C21-C22	-3.39	116.13	123.79
2	B	500	IMP	C8-N7-C5	3.36	109.40	102.99
3	D	502	8LA	C11-N3-C10	3.34	131.25	124.17
3	H	501	8LA	C21-O1-C24	3.31	124.42	118.09
2	E	501	IMP	C8-N7-C5	3.27	109.22	102.99
3	D	502	8LA	C21-O1-C24	3.24	124.29	118.09
3	E	502	8LA	C21-O1-C24	3.21	124.23	118.09
3	G	501	8LA	C21-O1-C24	3.21	124.22	118.09
2	F	500	IMP	C8-N7-C5	3.10	108.90	102.99
2	F	500	IMP	O6-C6-C5	-2.93	118.65	124.37
3	G	501	8LA	C21-C20-CL	2.90	122.83	119.43
2	E	501	IMP	C5-C6-N1	2.85	118.98	113.95
2	G	500	IMP	C5-C6-N1	2.84	118.97	113.95
2	D	501	IMP	C8-N7-C5	2.81	108.34	102.99
2	G	500	IMP	C8-N7-C5	2.75	108.23	102.99
3	B	501	8LA	C13-C11-C12	-2.71	106.30	109.55
2	H	500	IMP	O6-C6-C5	-2.70	119.10	124.37
2	D	501	IMP	O5'-P-O1P	-2.69	98.94	106.47
3	E	502	8LA	O1-C21-C22	-2.67	117.76	123.79
3	D	502	8LA	C17-C22-C21	2.66	123.04	119.45
2	G	500	IMP	O6-C6-C5	-2.65	119.19	124.37
2	C	501	IMP	O3P-P-O2P	2.65	117.75	107.64
2	C	501	IMP	C5-C6-N1	2.64	118.61	113.95
3	C	502	8LA	O1-C21-C22	-2.61	117.88	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	IMP	C5-C6-N1	2.56	118.48	113.95
2	A	501	IMP	C5-C6-N1	2.56	118.47	113.95
2	A	501	IMP	C8-N7-C5	2.52	107.80	102.99
3	B	501	8LA	C21-O1-C24	2.52	122.90	118.09
3	F	501	8LA	C13-C11-C12	-2.52	106.53	109.55
3	D	502	8LA	C1-C11-N3	2.49	114.45	110.82
2	H	500	IMP	O3P-P-O5'	-2.42	100.29	106.73
3	C	502	8LA	C29-C27-C26	-2.40	109.30	115.09
3	G	501	8LA	C3-C2-C1	-2.38	118.26	120.76
3	C	502	8LA	O3-C24-O1	-2.37	104.42	109.39
2	D	501	IMP	C5-C6-N1	2.37	118.14	113.95
2	F	500	IMP	C5-C6-N1	2.37	118.13	113.95
3	C	502	8LA	C13-C11-C12	-2.35	106.73	109.55
2	F	500	IMP	O3P-P-O2P	2.33	116.56	107.64
3	H	501	8LA	C24-C25-C26	2.27	105.18	102.30
3	H	501	8LA	C11-N3-C10	2.26	128.96	124.17
3	D	502	8LA	C6-C1-C11	-2.24	117.12	120.70
2	A	501	IMP	O6-C6-N1	-2.24	117.60	120.32
2	E	501	IMP	O6-C6-N1	-2.23	117.61	120.32
3	G	501	8LA	C24-C25-C26	-2.18	99.54	102.30
3	C	502	8LA	C17-C22-C21	2.17	122.38	119.45
3	G	501	8LA	C13-C11-C12	-2.15	106.97	109.55
3	C	502	8LA	C12-C11-N3	2.15	113.66	107.89
3	G	501	8LA	C11-N3-C10	2.14	128.71	124.17
3	B	501	8LA	C11-N3-C10	2.14	128.70	124.17
3	C	502	8LA	O2-C10-N3	-2.14	119.95	123.84
2	A	501	IMP	O6-C6-C5	-2.09	120.28	124.37
3	E	502	8LA	C13-C11-C12	-2.09	107.04	109.55
2	E	501	IMP	O3P-P-O2P	2.07	115.54	107.64
3	D	502	8LA	C22-C21-C20	-2.07	116.40	119.26
3	D	502	8LA	O1-C21-C22	-2.06	119.13	123.79
2	H	500	IMP	C5-C6-N1	2.06	117.59	113.95
2	H	500	IMP	O2P-P-O1P	2.04	118.66	110.68
3	G	501	8LA	C22-C21-C20	-2.03	116.45	119.26
3	H	501	8LA	C13-C11-C12	-2.03	107.11	109.55
3	E	502	8LA	C12-C11-N3	2.03	113.35	107.89
3	G	501	8LA	C2-C1-C6	2.02	121.65	117.76
2	E	501	IMP	O6-C6-C5	-2.02	120.44	124.37

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	IMP	O4'-C4'-C5'-O5'
2	C	501	IMP	C5'-O5'-P-O2P
3	A	502	8LA	C20-C21-O1-C24
3	B	501	8LA	C20-C21-O1-C24
3	C	502	8LA	C20-C21-O1-C24
3	D	502	8LA	C20-C21-O1-C24
3	E	502	8LA	C20-C21-O1-C24
3	F	501	8LA	C20-C21-O1-C24
3	F	501	8LA	C22-C21-O1-C24
3	F	501	8LA	C26-C27-C29-O6
3	F	501	8LA	O3-C27-C29-O6
3	G	501	8LA	C20-C21-O1-C24
3	H	501	8LA	C20-C21-O1-C24
2	B	500	IMP	C3'-C4'-C5'-O5'
7	D	503	GOL	C1-C2-C3-O3
3	D	502	8LA	O3-C27-C29-O6
3	B	501	8LA	C22-C21-O1-C24
3	C	502	8LA	C22-C21-O1-C24
3	E	502	8LA	C22-C21-O1-C24
3	G	501	8LA	C22-C21-O1-C24
3	F	501	8LA	O3-C24-O1-C21
3	D	502	8LA	C12-C11-N3-C10
3	D	502	8LA	C13-C11-N3-C10
7	D	503	GOL	O2-C2-C3-O3
3	A	502	8LA	C22-C21-O1-C24
3	D	502	8LA	C22-C21-O1-C24
3	H	501	8LA	C22-C21-O1-C24
8	E	504	PEG	C1-C2-O2-C3
3	G	501	8LA	O3-C24-O1-C21
3	D	502	8LA	C4-C5-C7-C8
3	F	501	8LA	C4-C5-C7-C8
3	H	501	8LA	C4-C5-C7-C8
3	D	502	8LA	C1-C11-N3-C10
3	E	502	8LA	C4-C5-C7-C8
2	C	501	IMP	C5'-O5'-P-O1P
3	B	501	8LA	O3-C24-O1-C21
3	C	502	8LA	O3-C24-O1-C21
3	E	502	8LA	O3-C24-O1-C21
3	A	502	8LA	C4-C5-C7-C8
3	C	502	8LA	C4-C5-C7-C8
3	F	501	8LA	C6-C5-C7-C8
3	H	501	8LA	C6-C5-C7-C8
8	E	504	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	D	502	8LA	C6-C5-C7-C8
2	C	501	IMP	C5'-O5'-P-O3P
2	G	500	IMP	C5'-O5'-P-O3P
3	G	501	8LA	C4-C5-C7-C8
3	A	502	8LA	C6-C5-C7-C8
3	B	501	8LA	C4-C5-C7-C8
3	C	502	8LA	C6-C5-C7-C8
3	E	502	8LA	C6-C5-C7-C8
3	B	501	8LA	C6-C5-C7-C8
3	G	501	8LA	C6-C5-C7-C8
3	H	501	8LA	C26-C27-C29-O6
3	C	502	8LA	C26-C27-C29-O6

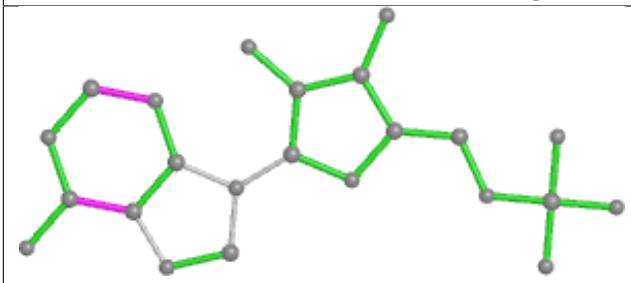
There are no ring outliers.

10 monomers are involved in 13 short contacts:

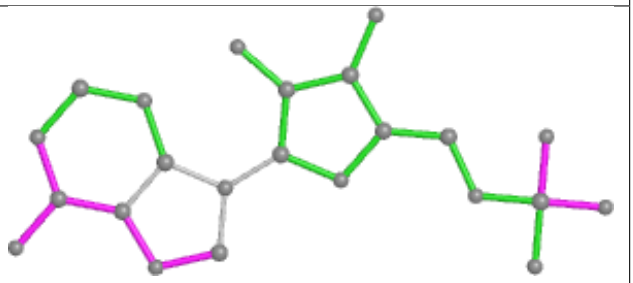
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	500	IMP	1	0
3	E	502	8LA	1	0
2	H	500	IMP	3	0
3	C	502	8LA	1	0
3	F	501	8LA	1	0
2	A	501	IMP	1	0
2	B	500	IMP	1	0
6	C	504	PO4	1	0
2	D	501	IMP	2	0
6	C	503	PO4	1	0

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.

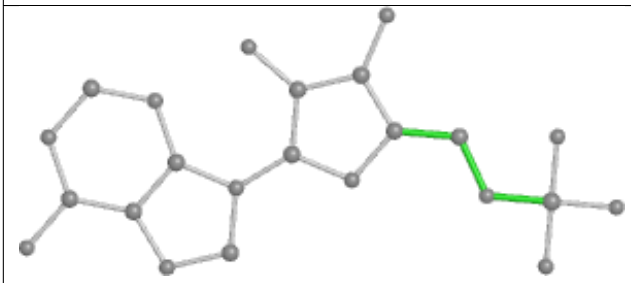
Ligand IMP F 500



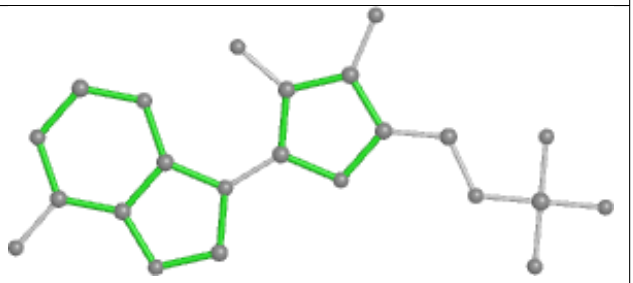
Bond lengths



Bond angles

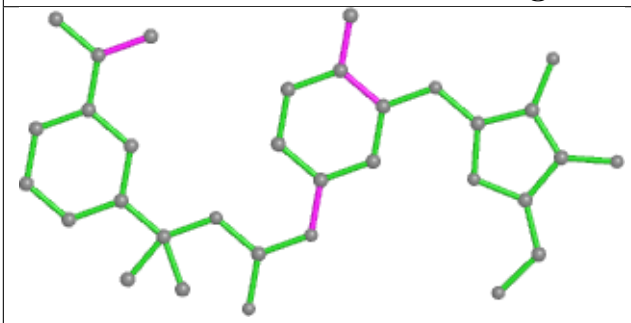


Torsions

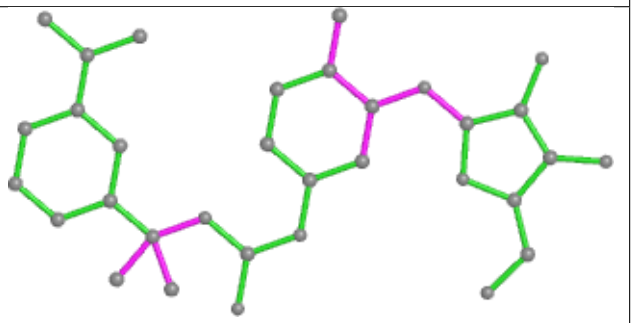


Rings

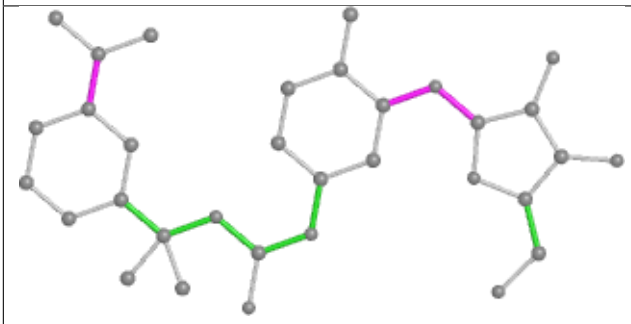
Ligand 8LA E 502



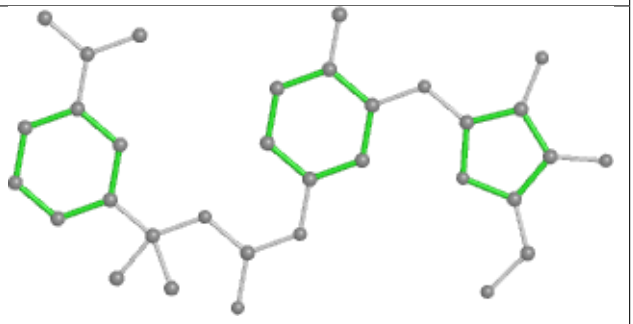
Bond lengths



Bond angles

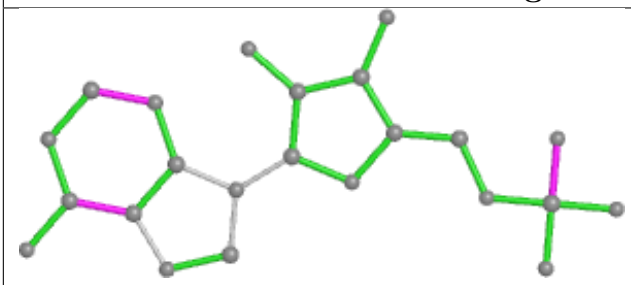


Torsions

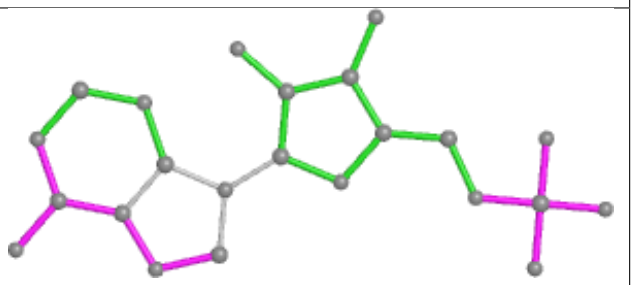


Rings

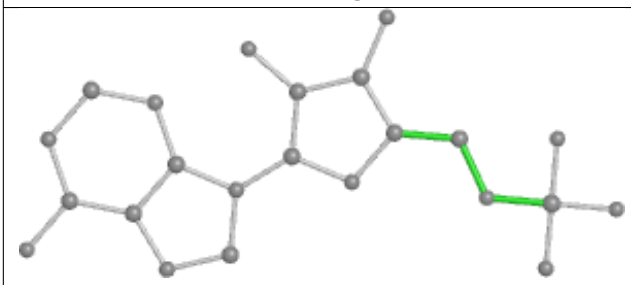
Ligand IMP H 500



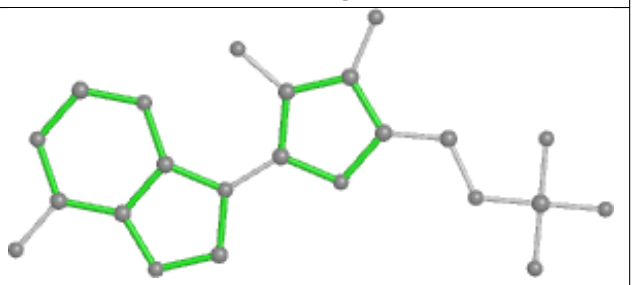
Bond lengths



Bond angles

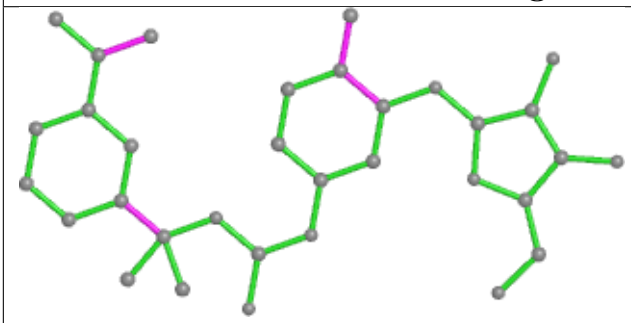


Torsions

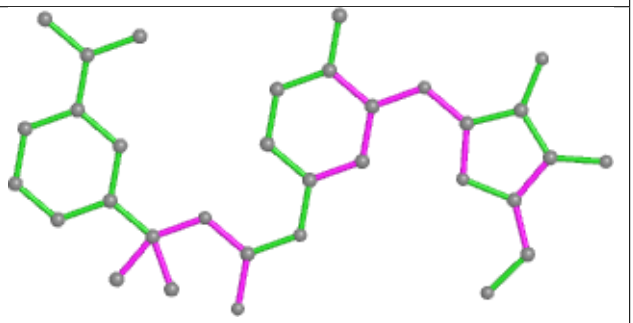


Rings

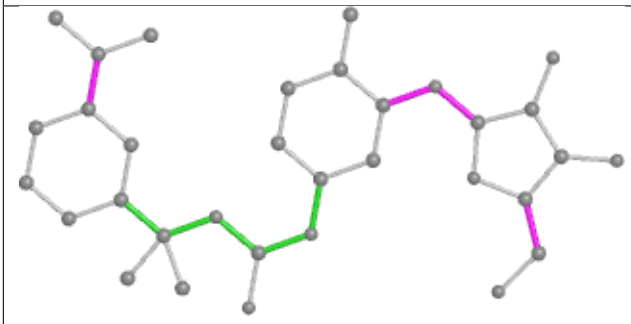
Ligand 8LA C 502



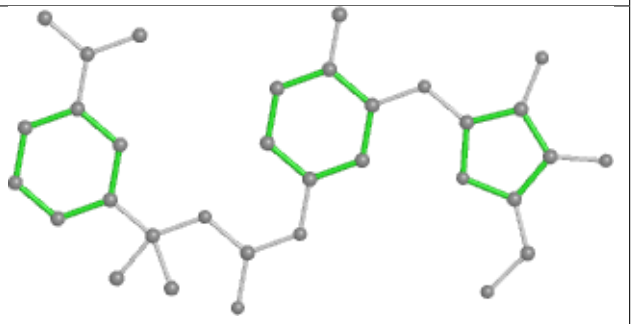
Bond lengths



Bond angles

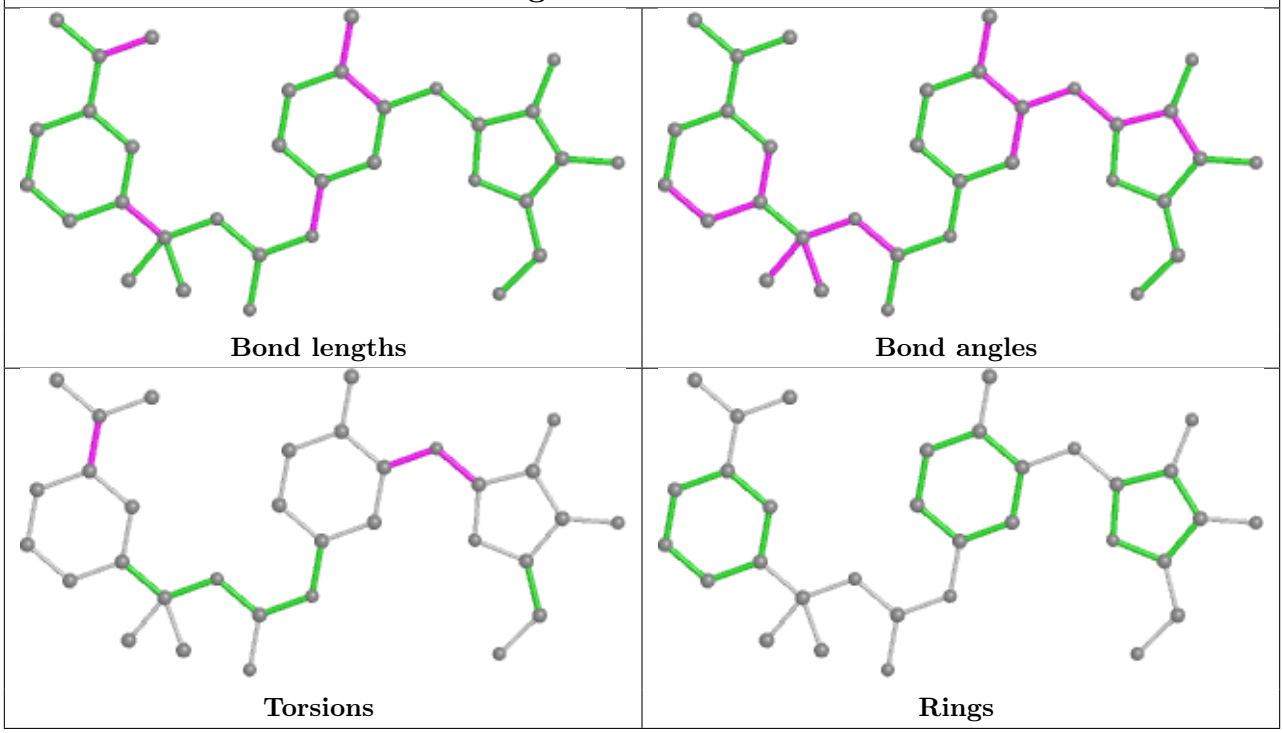


Torsions

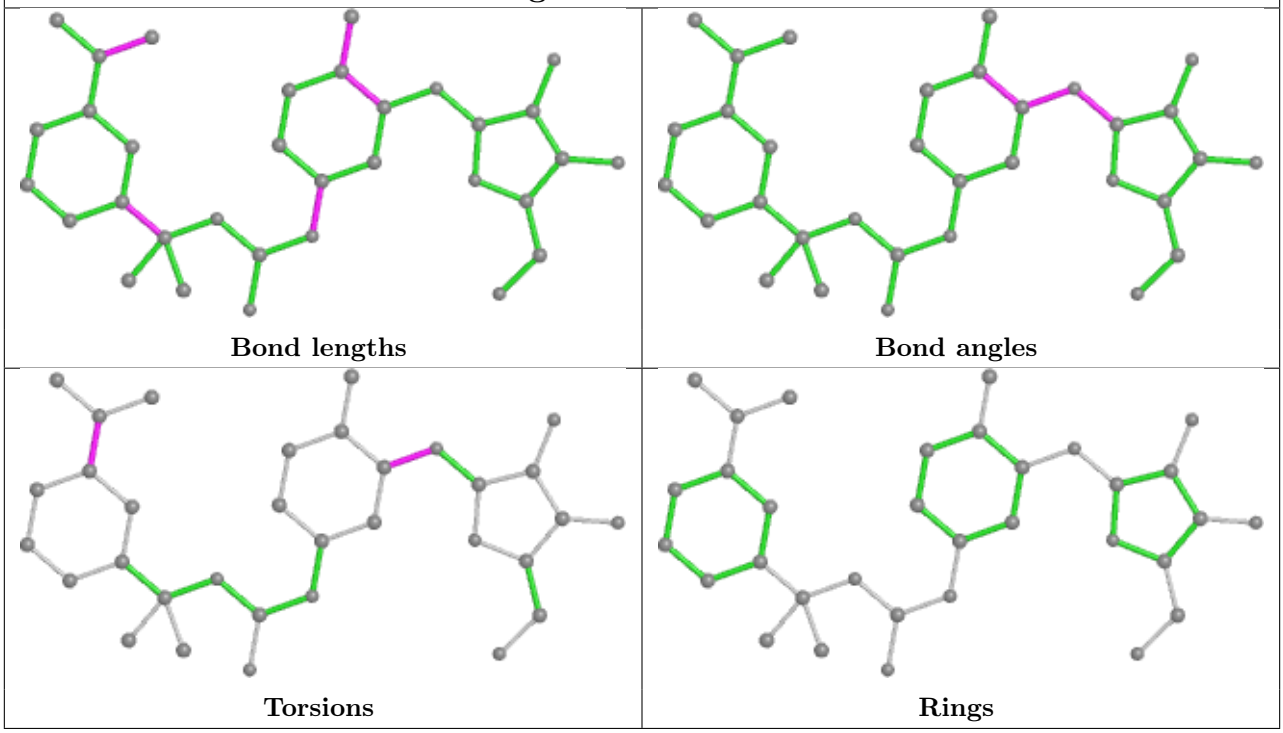


Rings

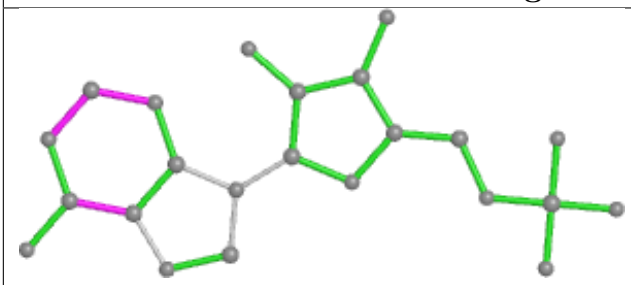
Ligand 8LA G 501



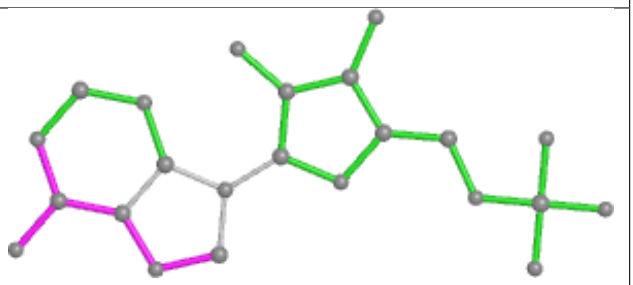
Ligand 8LA A 502



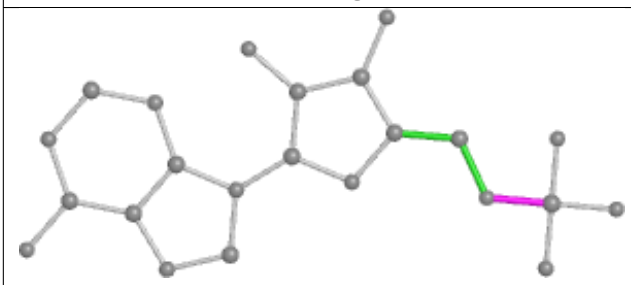
Ligand IMP G 500



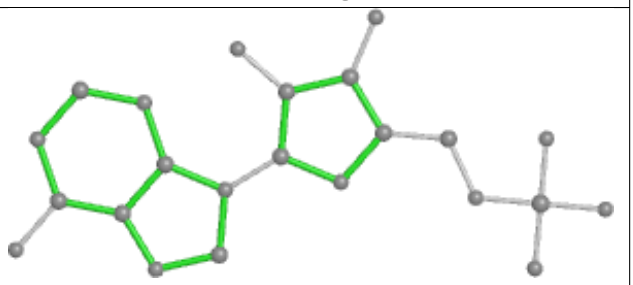
Bond lengths



Bond angles

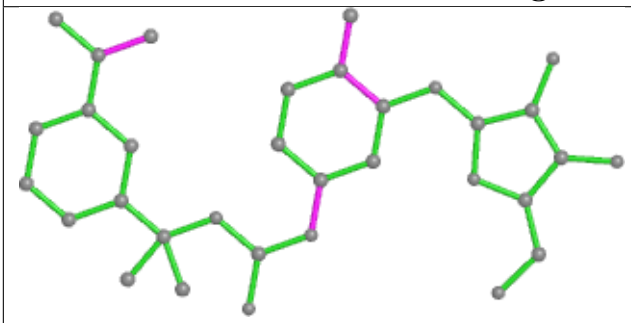


Torsions

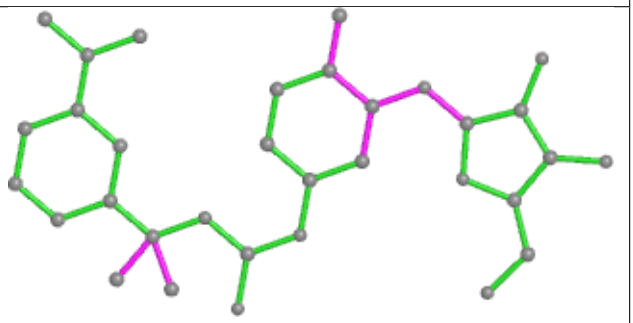


Rings

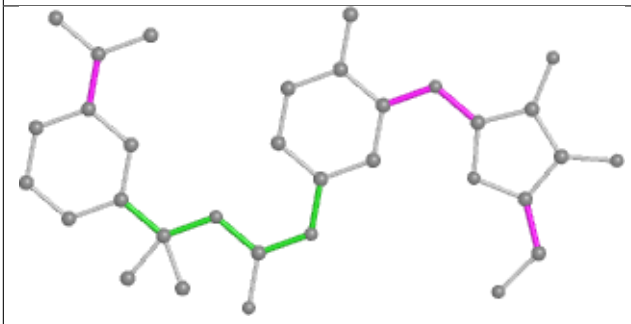
Ligand 8LA F 501



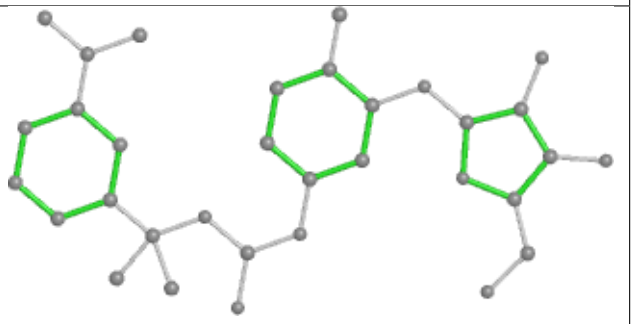
Bond lengths



Bond angles

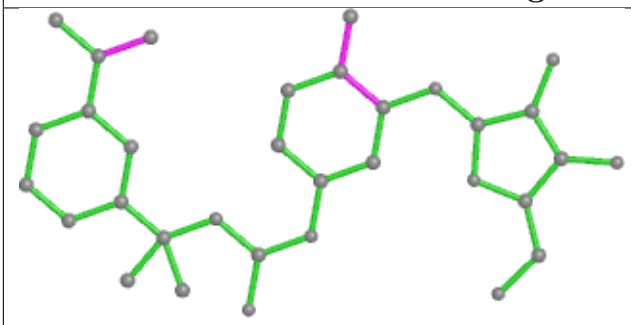


Torsions

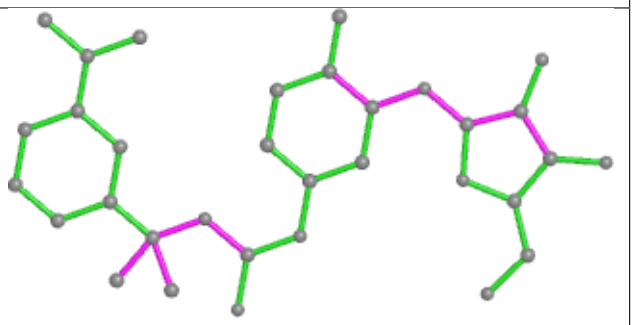


Rings

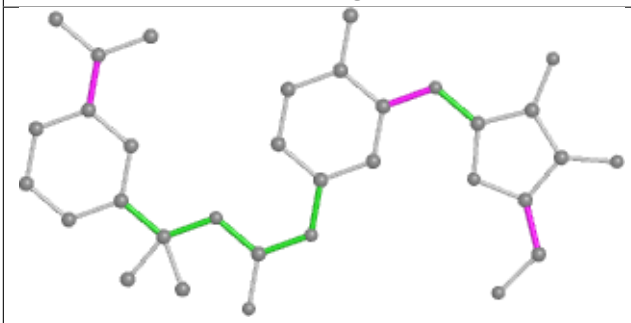
Ligand 8LA H 501



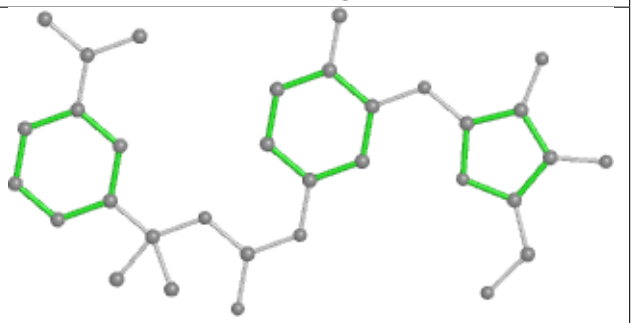
Bond lengths



Bond angles

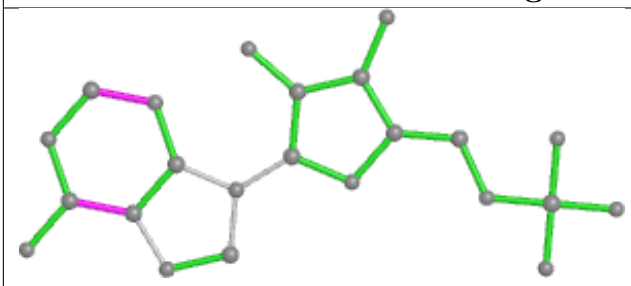


Torsions

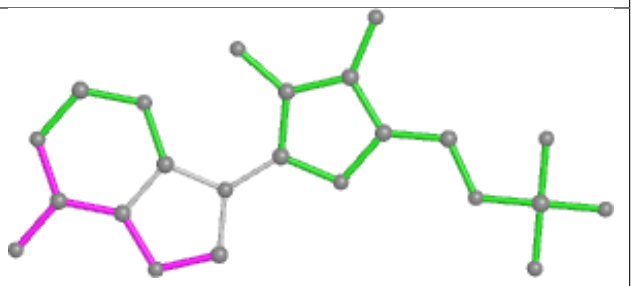


Rings

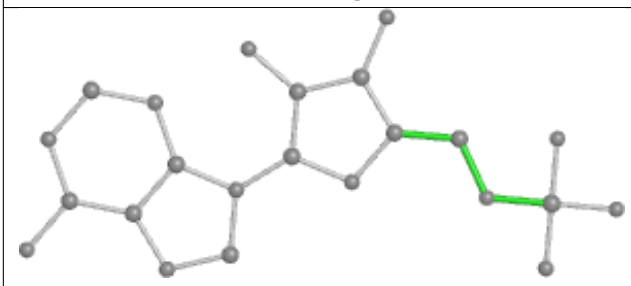
Ligand IMP A 501



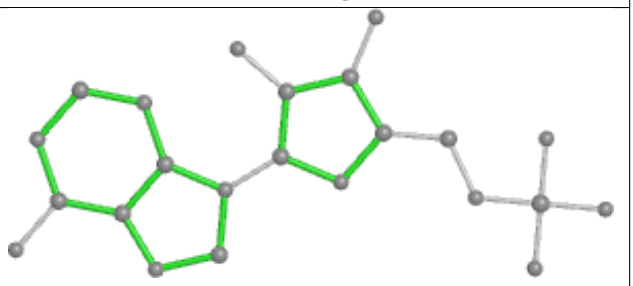
Bond lengths



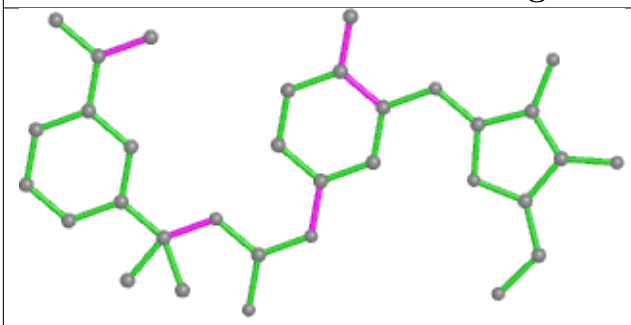
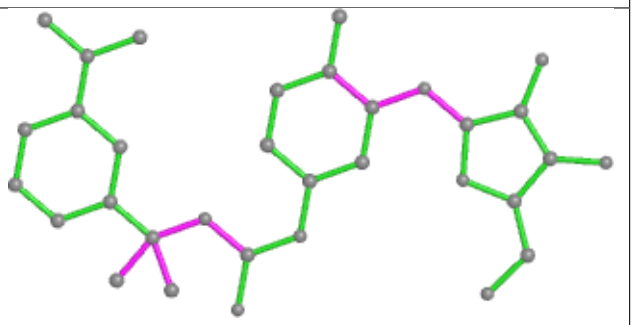
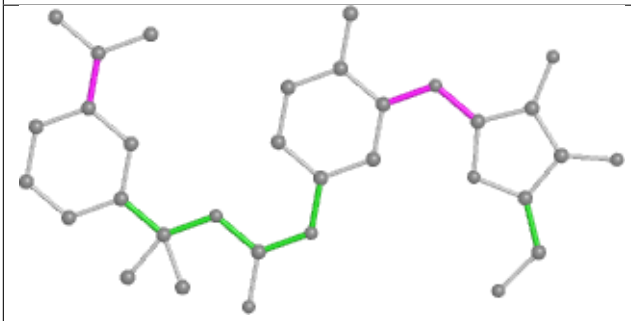
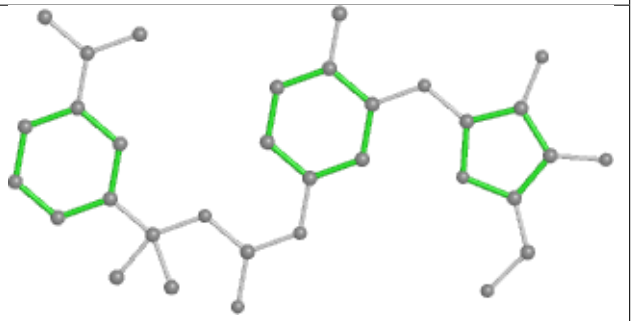
Bond angles

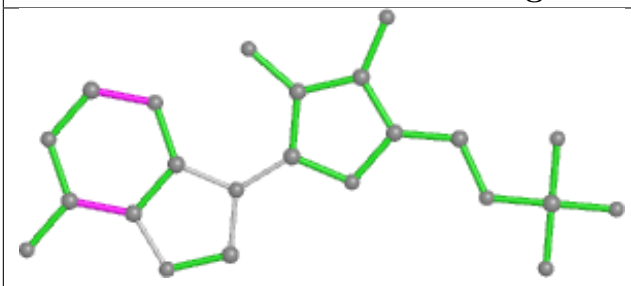
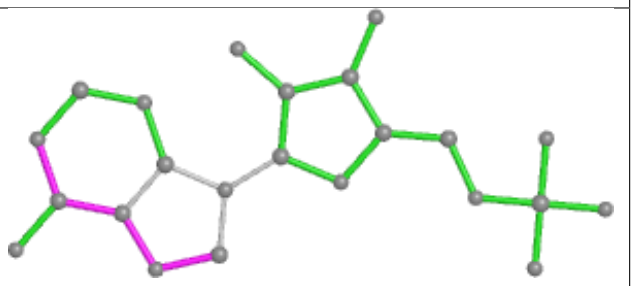
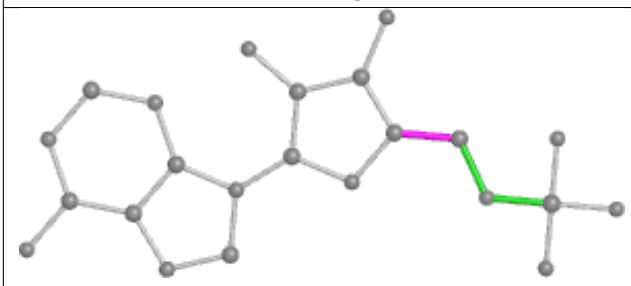
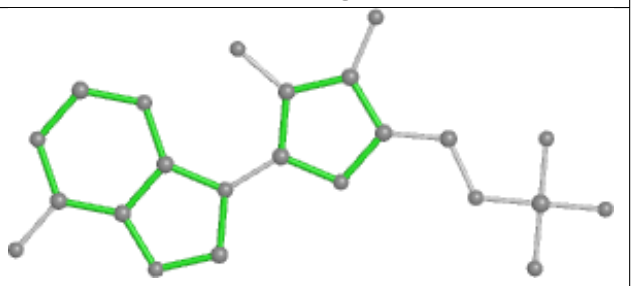


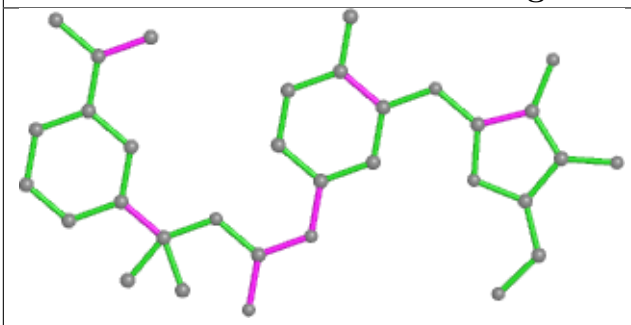
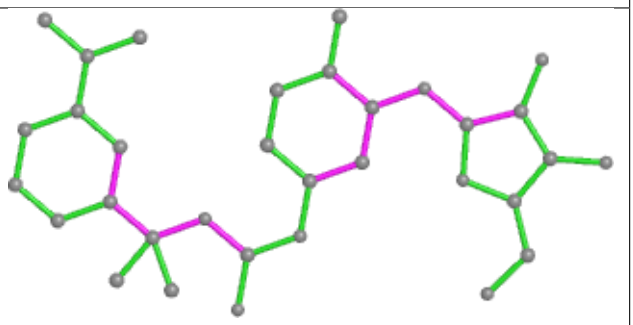
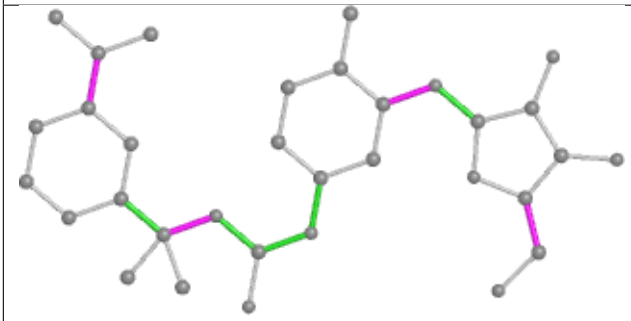
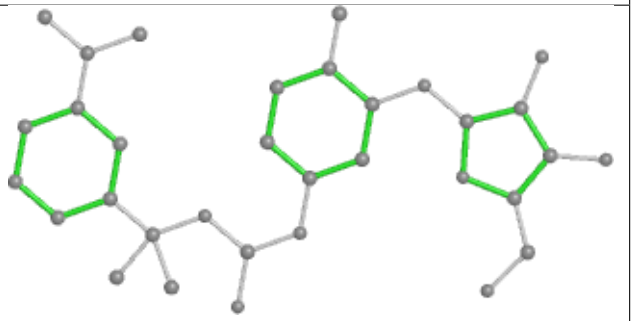
Torsions

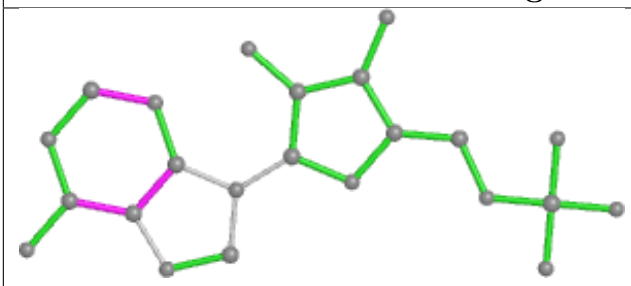
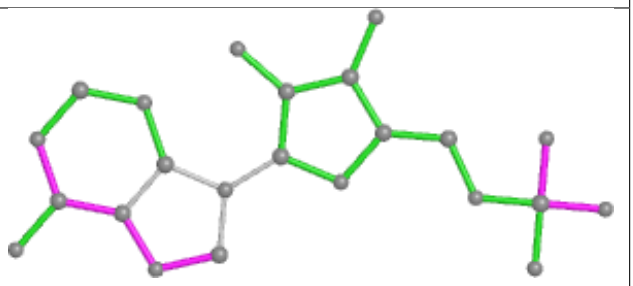
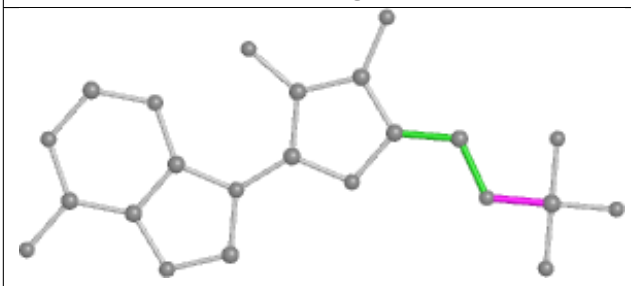
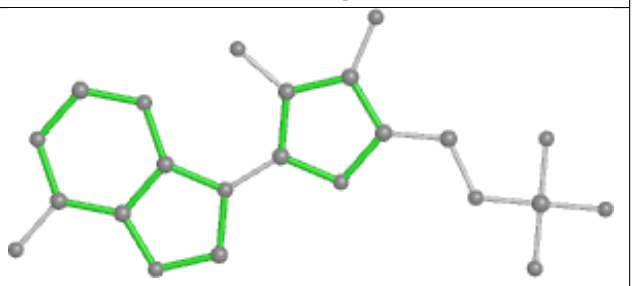


Rings

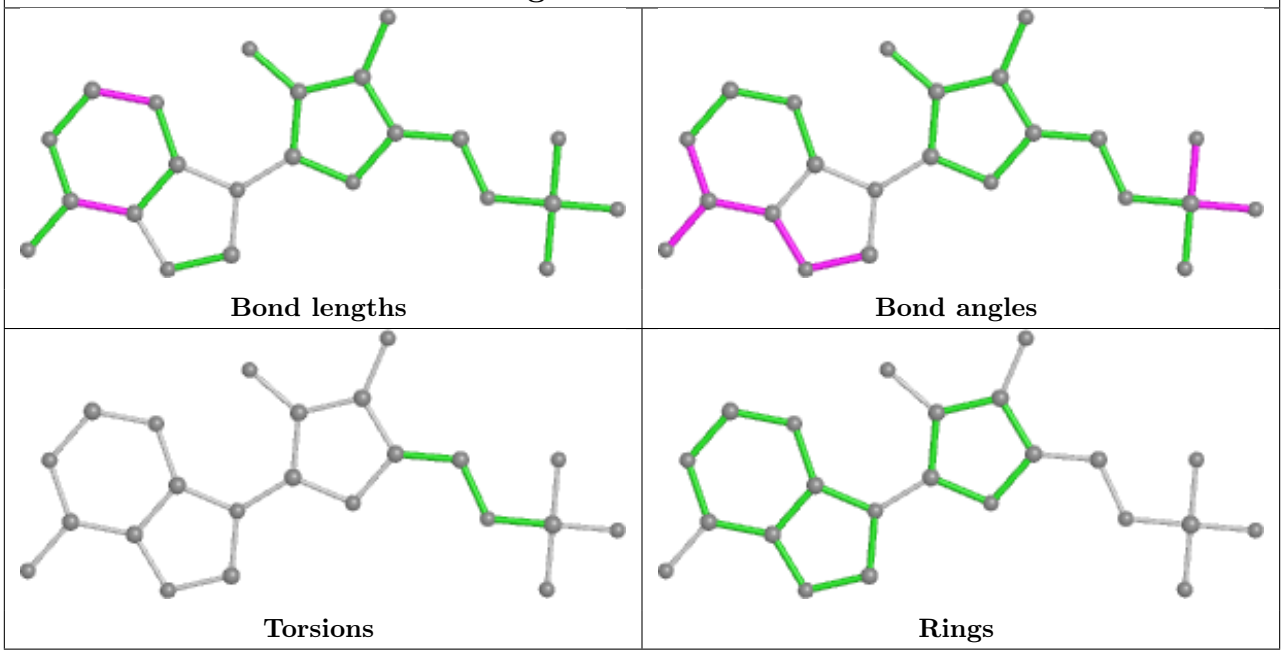
Ligand 8LA B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand IMP B 500	
 Bond lengths	 Bond angles
 Torsions	 Rings

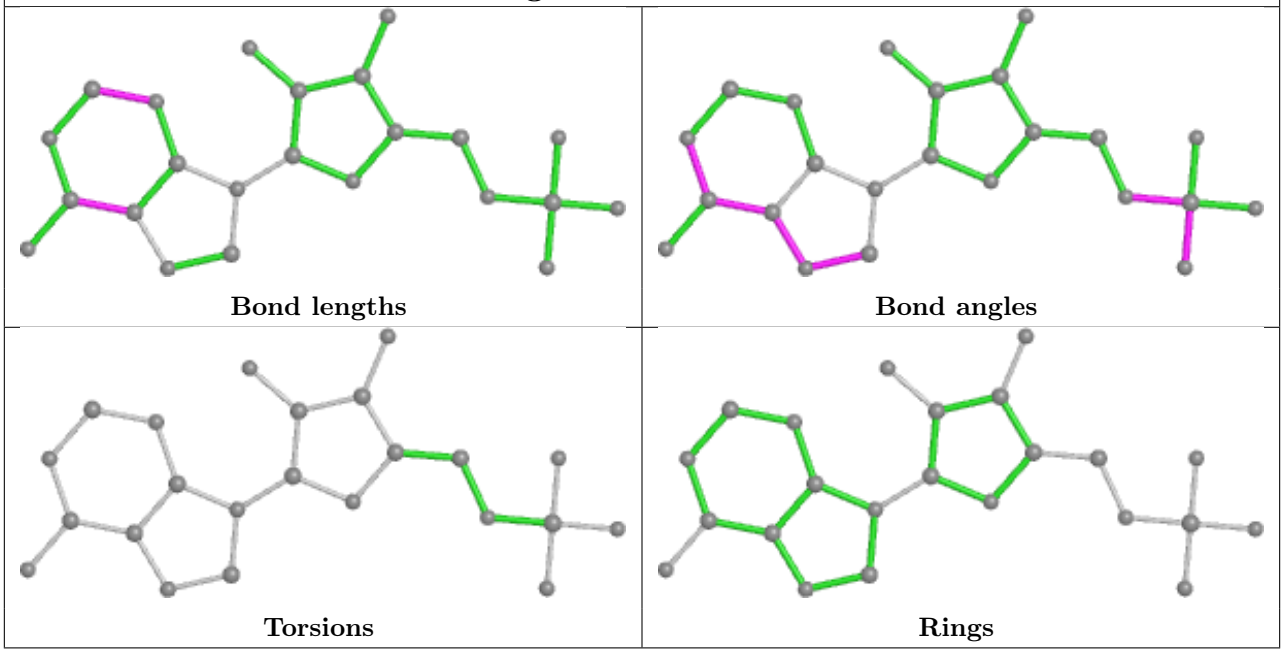
Ligand 8LA D 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand IMP C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand IMP E 501



Ligand IMP D 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.53	11 (3%)	49	51	23, 35, 58, 97	0
1	B	350/384 (91%)	0.50	10 (2%)	51	53	24, 37, 61, 95	0
1	C	349/384 (90%)	0.67	24 (6%)	16	18	24, 38, 62, 86	0
1	D	350/384 (91%)	0.55	8 (2%)	60	62	24, 37, 64, 91	0
1	E	350/384 (91%)	0.83	32 (9%)	9	10	26, 45, 68, 95	0
1	F	351/384 (91%)	0.74	32 (9%)	9	10	26, 43, 68, 95	0
1	G	349/384 (90%)	0.66	22 (6%)	20	21	26, 42, 68, 93	0
1	H	348/384 (90%)	0.54	16 (4%)	32	35	24, 39, 63, 90	0
All	All	2798/3072 (91%)	0.63	155 (5%)	25	27	23, 39, 65, 97	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	228	GLY	7.5
1	E	-4	PHE	6.4
1	G	-2	SER	4.8
1	H	231	ALA	4.8
1	E	-3	GLN	4.6
1	E	237	ILE	4.6
1	E	235	THR	4.4
1	A	380	TYR	4.4
1	G	380	TYR	4.1
1	C	-2	SER	4.0
1	C	70	GLY	4.0
1	H	413	LEU	4.0
1	G	231	ALA	4.0
1	G	269	ALA	3.9
1	F	264	VAL	3.9
1	G	287	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	90	ARG	3.8
1	B	79	GLU	3.8
1	C	244	SER	3.8
1	F	79	GLU	3.7
1	H	269	ALA	3.7
1	C	413	LEU	3.7
1	E	379	ILE	3.6
1	E	227	VAL	3.6
1	D	231	ALA	3.5
1	F	242	LYS	3.5
1	C	239	ALA	3.5
1	F	230	THR	3.5
1	E	244	SER	3.4
1	F	487	LEU	3.4
1	C	235	THR	3.4
1	H	24	ASP	3.4
1	F	241	VAL	3.4
1	A	-3	GLN	3.3
1	F	380	TYR	3.3
1	H	239	ALA	3.2
1	F	394	VAL	3.1
1	G	376	GLU	3.1
1	C	231	ALA	3.1
1	F	232	ASP	3.1
1	B	92	GLY	3.0
1	H	-1	ASN	3.0
1	E	242	LYS	3.0
1	E	274	LEU	3.0
1	F	266	GLU	3.0
1	E	241	VAL	3.0
1	F	80	GLN	3.0
1	F	51	MET	2.9
1	E	239	ALA	2.9
1	C	374	PRO	2.9
1	G	413	LEU	2.9
1	A	230	THR	2.9
1	C	80	GLN	2.9
1	D	380	TYR	2.9
1	B	231	ALA	2.8
1	A	75	ASN	2.8
1	F	377	THR	2.8
1	C	88	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	251	ASP	2.8
1	G	233	ALA	2.8
1	D	234	MET	2.8
1	A	-1	ASN	2.8
1	E	-2	SER	2.8
1	A	242	LYS	2.8
1	C	377	THR	2.8
1	E	80	GLN	2.8
1	E	84	GLN	2.8
1	A	231	ALA	2.7
1	F	248	ILE	2.7
1	D	269	ALA	2.7
1	A	377	THR	2.7
1	F	0	ALA	2.7
1	F	240	LEU	2.7
1	C	241	VAL	2.7
1	E	0	ALA	2.7
1	D	479	THR	2.6
1	E	377	THR	2.6
1	G	290	LEU	2.6
1	F	76	MET	2.5
1	E	273	SER	2.5
1	H	88	VAL	2.5
1	G	79	GLU	2.5
1	F	260	VAL	2.5
1	E	424	TYR	2.5
1	C	453	PHE	2.4
1	E	229	VAL	2.4
1	H	82	ALA	2.4
1	F	75	ASN	2.4
1	F	375	GLY	2.4
1	C	370	VAL	2.4
1	E	271	TYR	2.4
1	B	239	ALA	2.4
1	H	235	THR	2.4
1	H	266	GLU	2.4
1	B	383	ARG	2.4
1	G	421	ARG	2.4
1	F	233	ALA	2.4
1	G	36	LEU	2.3
1	D	-2	SER	2.3
1	G	379	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	23	SER	2.3
1	E	245	VAL	2.3
1	B	376	GLU	2.3
1	H	383	ARG	2.3
1	H	412	LYS	2.3
1	C	480	LYS	2.3
1	B	413	LEU	2.2
1	F	235	THR	2.2
1	D	90	ARG	2.2
1	H	21	ALA	2.2
1	E	10	GLY	2.2
1	C	86	ASP	2.2
1	C	57	ALA	2.2
1	A	376	GLU	2.2
1	G	328	ALA	2.2
1	H	221	LEU	2.2
1	F	229	VAL	2.2
1	E	232	ASP	2.2
1	E	261	ILE	2.2
1	C	486	SER	2.2
1	G	0	ALA	2.2
1	D	383	ARG	2.2
1	G	479	THR	2.2
1	E	70	GLY	2.2
1	E	75	ASN	2.1
1	C	267	VAL	2.1
1	F	391	MET	2.1
1	C	82	ALA	2.1
1	F	396	ALA	2.1
1	E	26	LEU	2.1
1	F	395	GLY	2.1
1	F	468	LEU	2.1
1	C	269	ALA	2.1
1	F	231	ALA	2.1
1	G	377	THR	2.1
1	C	90	ARG	2.1
1	B	240	LEU	2.1
1	A	232	ASP	2.1
1	G	477	GLN	2.1
1	C	368	ALA	2.1
1	E	79	GLU	2.1
1	F	83	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	348	GLY	2.1
1	H	273	SER	2.1
1	E	453	PHE	2.1
1	G	83	GLU	2.0
1	B	-1	ASN	2.0
1	E	76	MET	2.0
1	G	486	SER	2.0
1	H	380	TYR	2.0
1	A	-2	SER	2.0
1	B	-2	SER	2.0
1	E	458	ALA	2.0
1	F	54	VAL	2.0
1	C	91	SER	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	GOL	D	503	6/6	0.80	0.26	41,46,50,50	0
8	PEG	E	504	7/7	0.87	0.14	45,48,49,50	0
6	PO4	C	503	5/5	0.88	0.25	79,80,81,81	0
3	8LA	B	501	33/33	0.89	0.18	26,44,59,65	0
3	8LA	H	501	33/33	0.90	0.17	32,49,58,61	0
3	8LA	E	502	33/33	0.90	0.19	45,50,56,68	0
3	8LA	F	501	33/33	0.91	0.20	35,46,61,63	0
3	8LA	C	502	33/33	0.91	0.18	38,47,60,72	0
5	EDO	A	504	4/4	0.91	0.28	44,46,47,48	0
3	8LA	A	502	33/33	0.92	0.18	35,45,53,56	0

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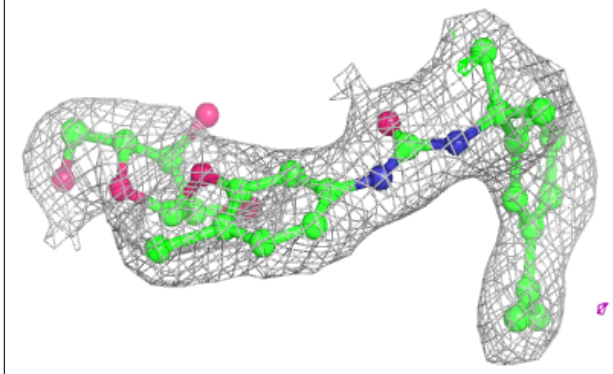
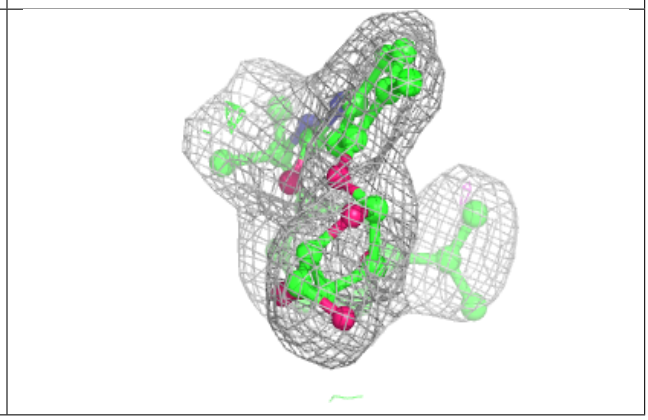
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	8LA	G	501	33/33	0.93	0.16	29,34,46,57	0
6	PO4	E	505	5/5	0.94	0.16	65,65,66,67	0
3	8LA	D	502	33/33	0.94	0.16	24,38,46,53	0
6	PO4	C	504	5/5	0.94	0.22	68,68,71,77	0
2	IMP	A	501	23/23	0.95	0.16	23,32,40,42	0
4	K	A	503	1/1	0.95	0.12	40,40,40,40	0
2	IMP	C	501	23/23	0.96	0.16	23,33,40,42	0
2	IMP	F	500	23/23	0.96	0.14	23,33,37,40	0
2	IMP	H	500	23/23	0.96	0.15	20,28,32,34	0
4	K	E	503	1/1	0.97	0.07	38,38,38,38	0
4	K	G	502	1/1	0.97	0.10	36,36,36,36	0
2	IMP	B	500	23/23	0.97	0.16	22,32,37,41	0
2	IMP	G	500	23/23	0.97	0.14	21,30,40,41	0
2	IMP	D	501	23/23	0.97	0.14	19,28,36,38	0
2	IMP	E	501	23/23	0.97	0.13	31,37,39,41	0
4	K	A	505	1/1	0.97	0.07	37,37,37,37	0
4	K	B	502	1/1	0.97	0.10	37,37,37,37	0
4	K	E	506	1/1	0.98	0.12	38,38,38,38	0
4	K	C	505	1/1	0.98	0.07	39,39,39,39	0
4	K	F	502	1/1	0.99	0.10	38,38,38,38	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 8LA B 501:

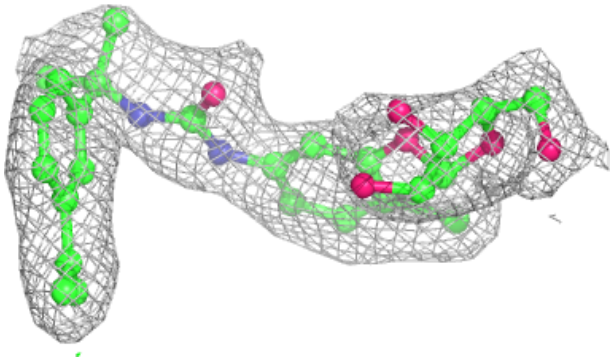
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

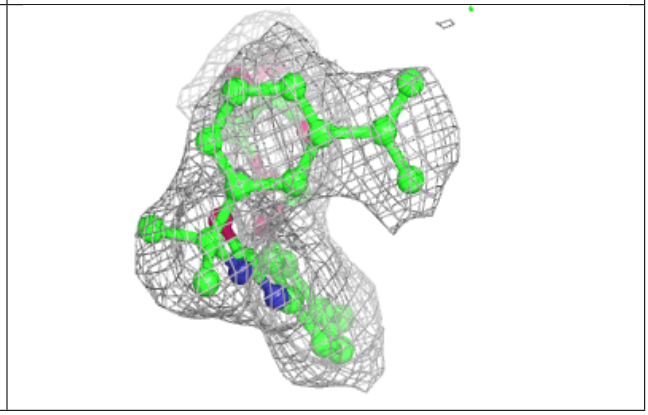




Electron density around 8LA H 501:

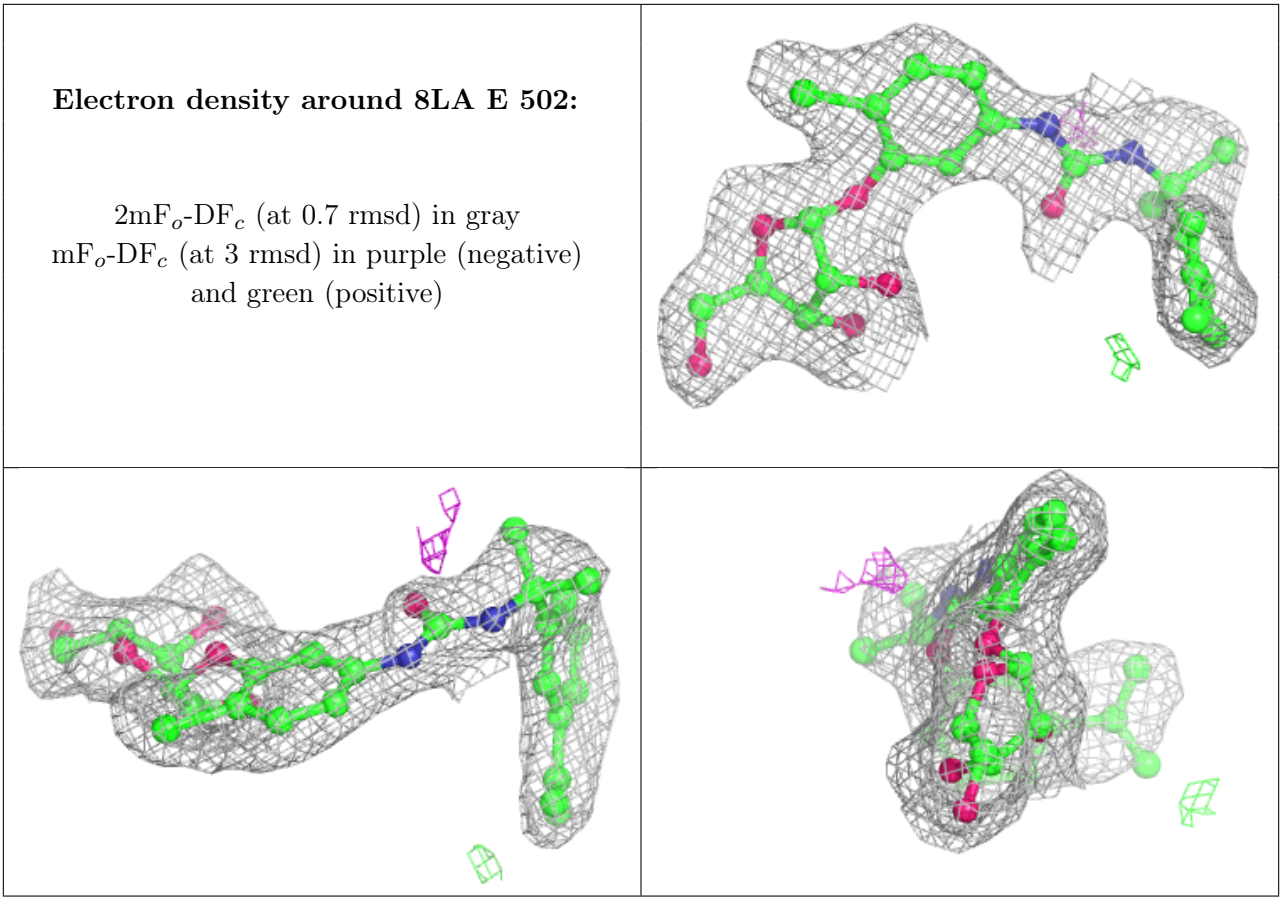
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





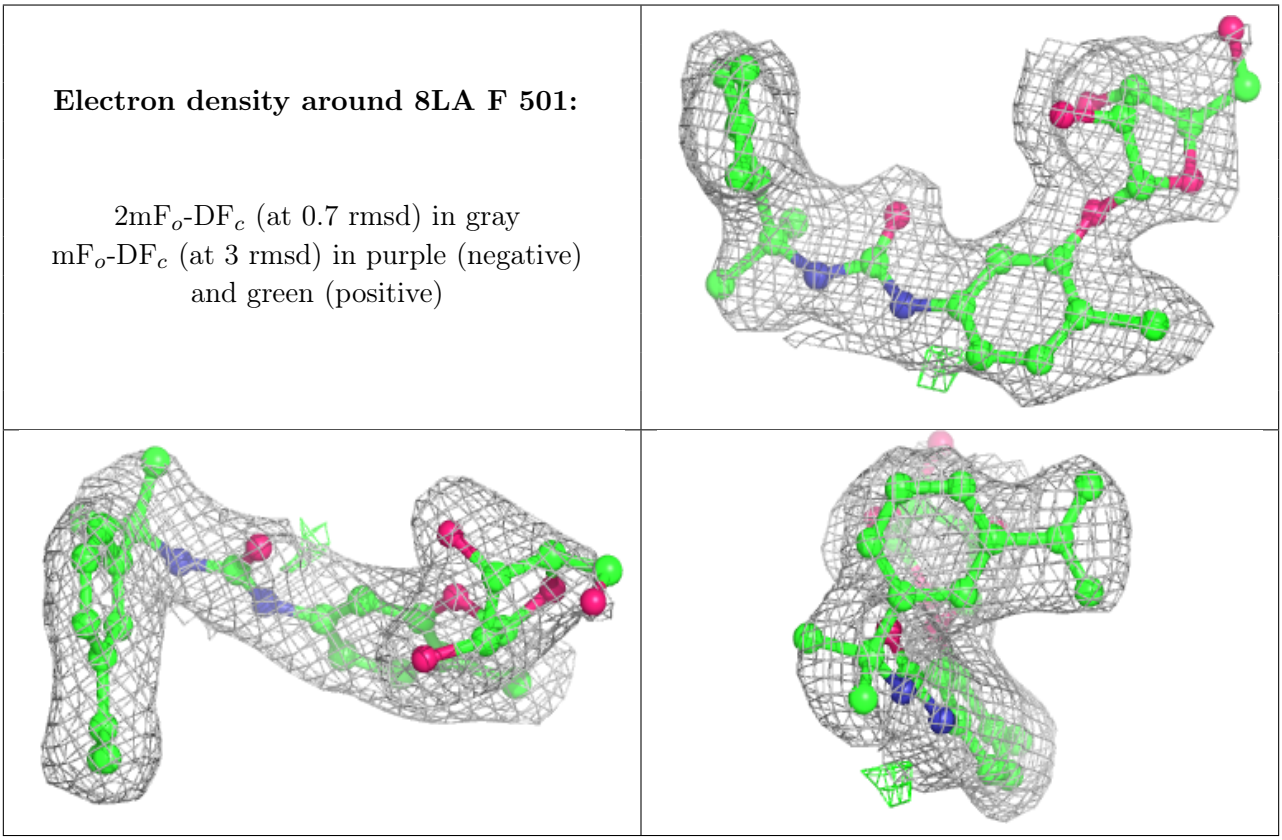
Electron density around 8LA E 502:

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



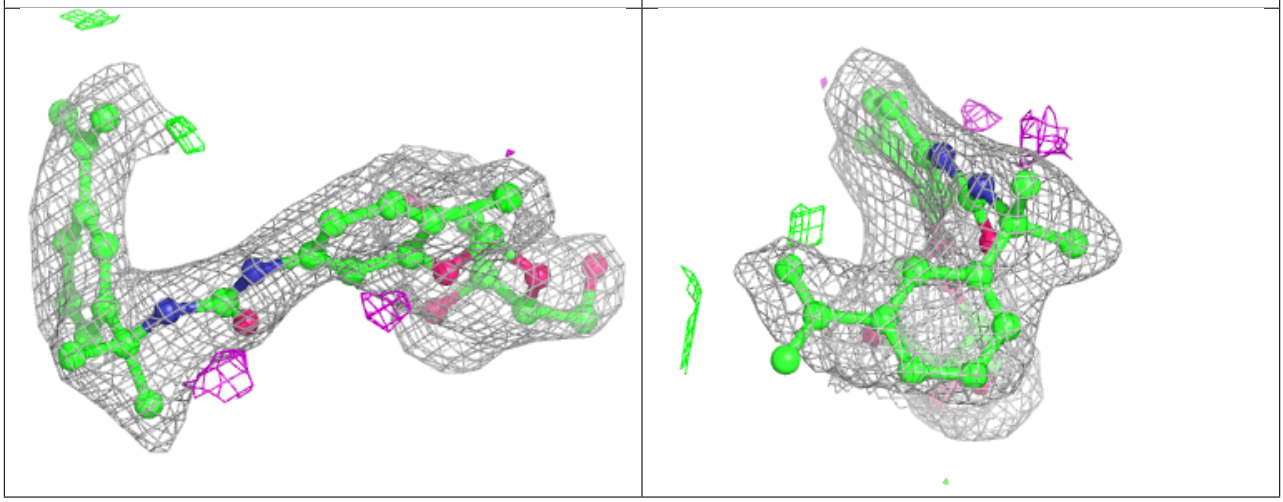
Electron density around 8LA F 501:

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



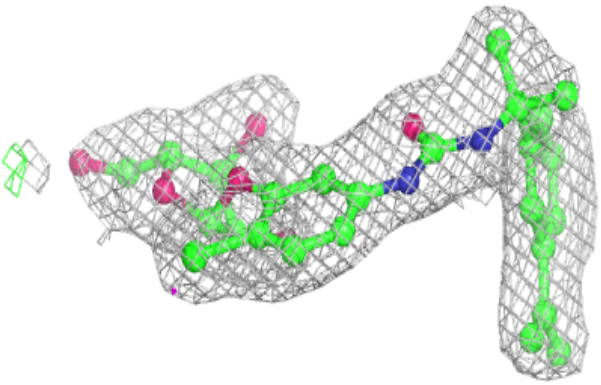
Electron density around 8LA C 502:

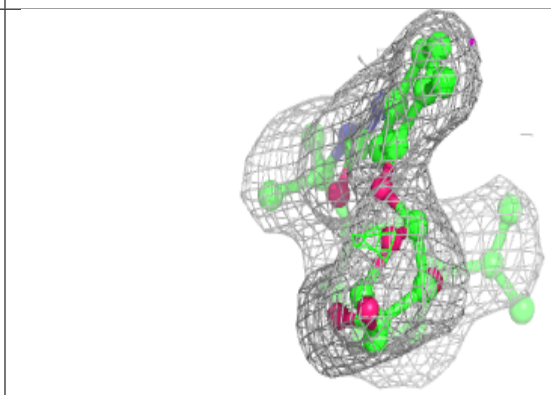
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

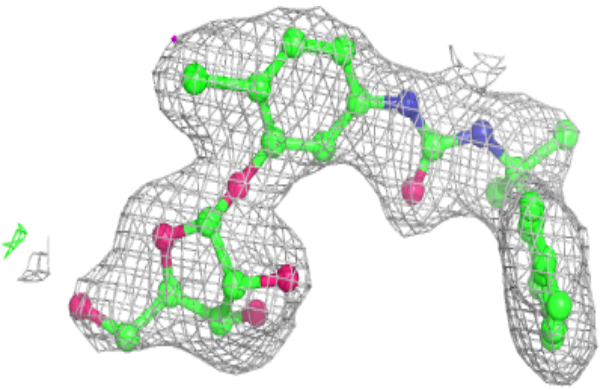


Electron density around 8LA A 502:

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

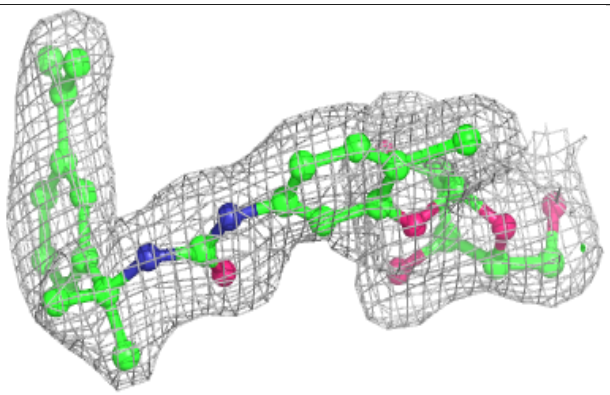


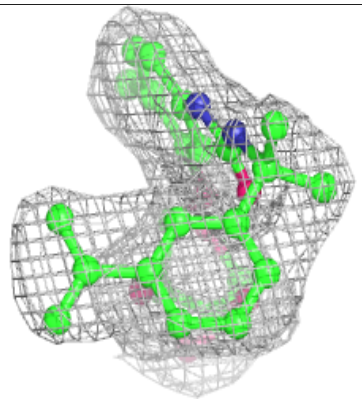


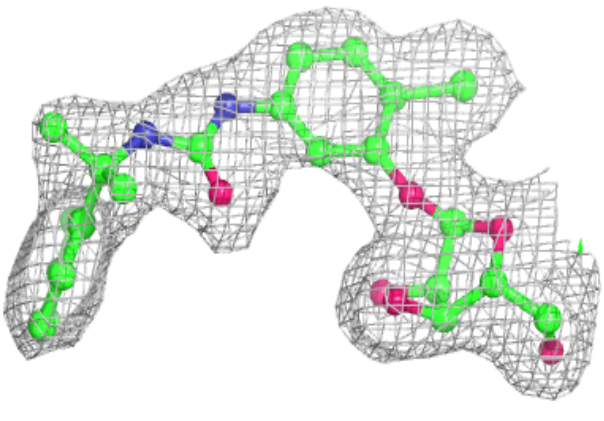


Electron density around 8LA G 501:

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

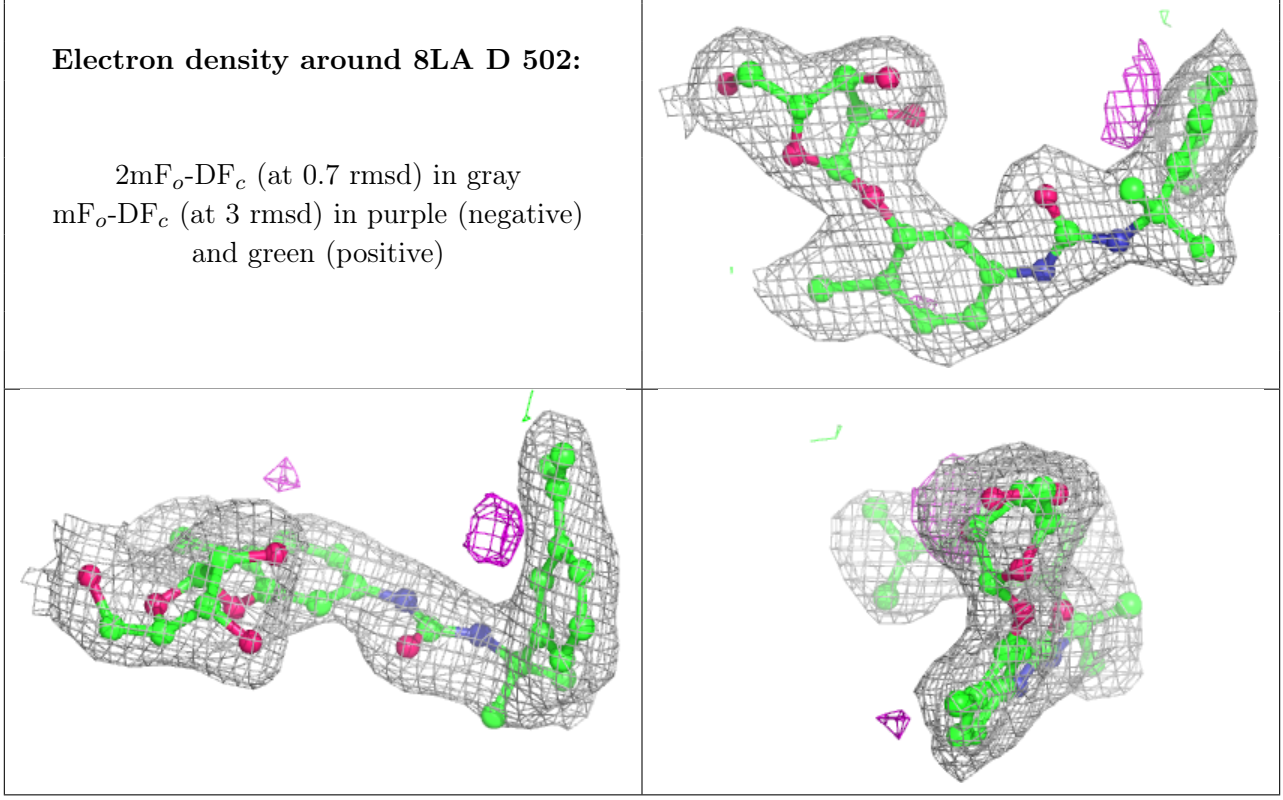






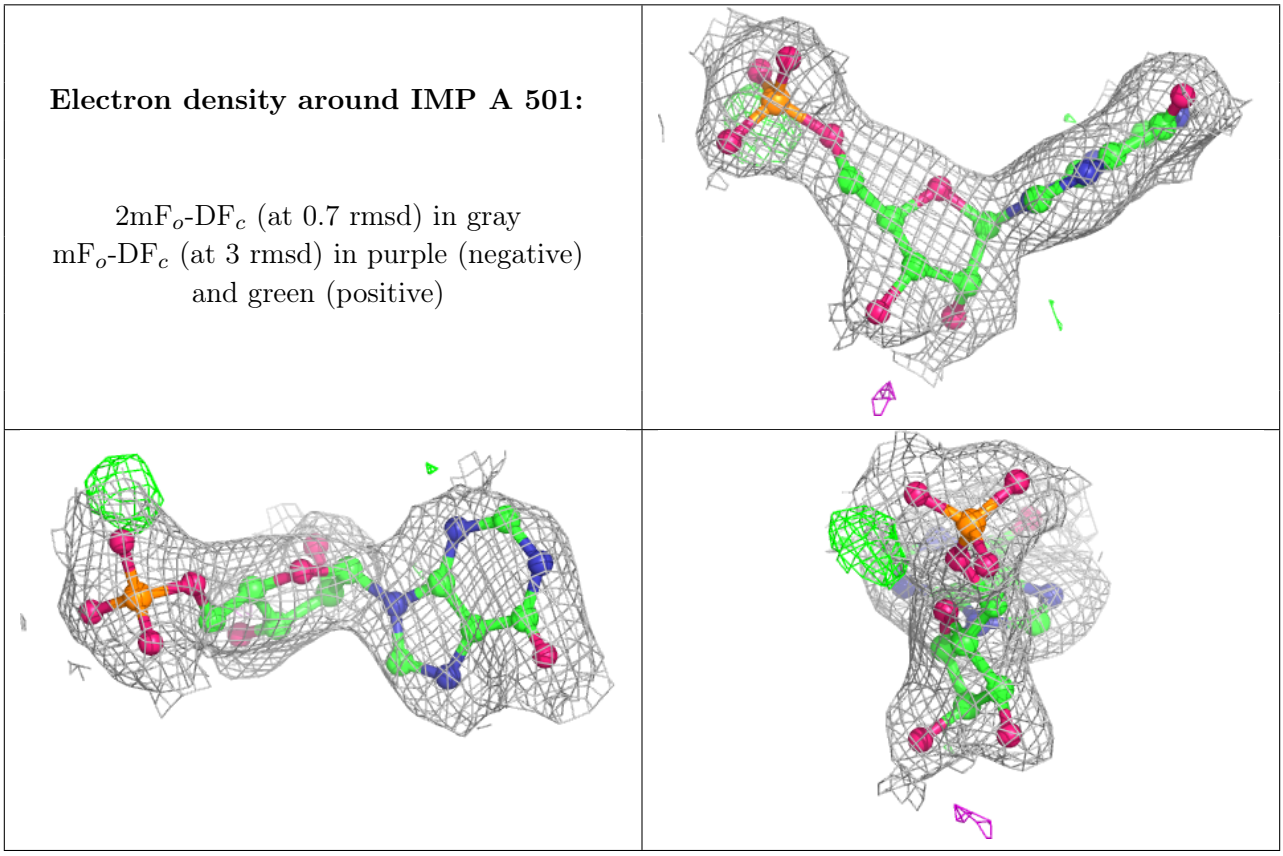
Electron density around 8LA D 502:

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



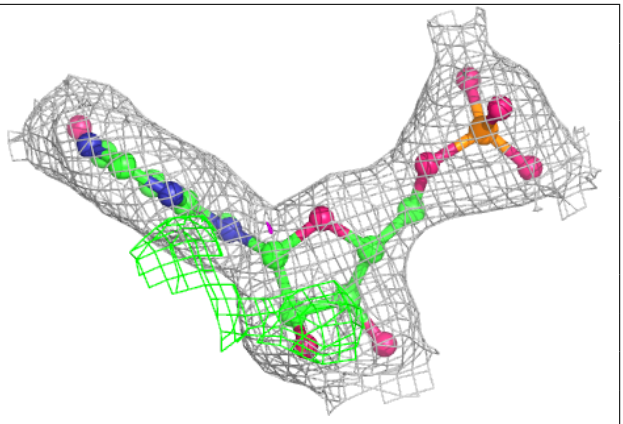
Electron density around IMP A 501:

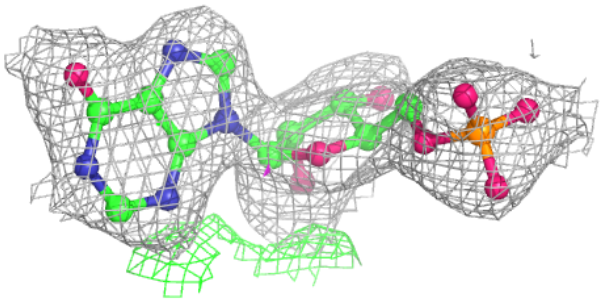
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

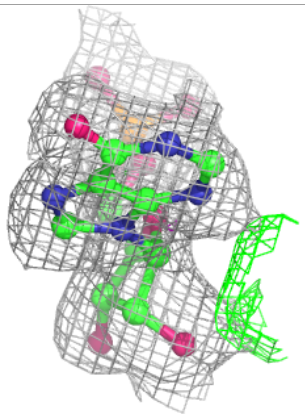


Electron density around IMP C 501:

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

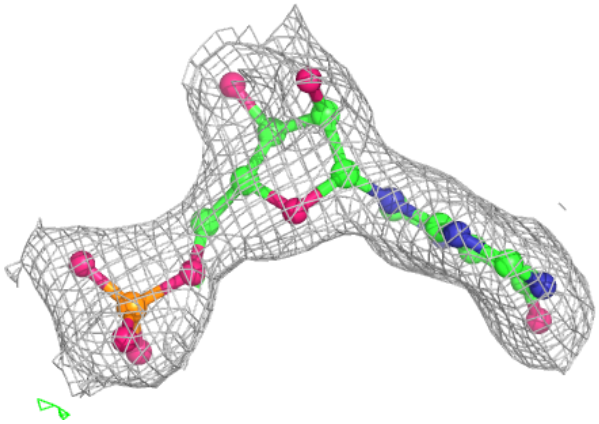


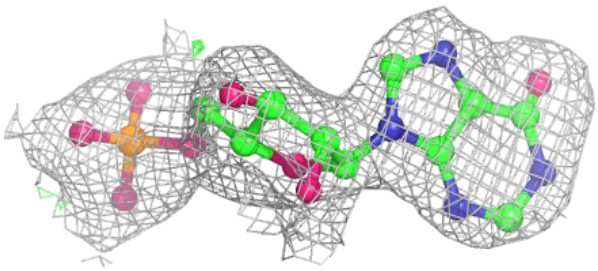


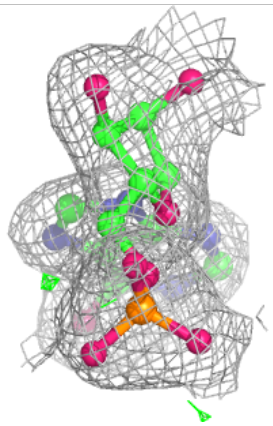


Electron density around IMP F 500:

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

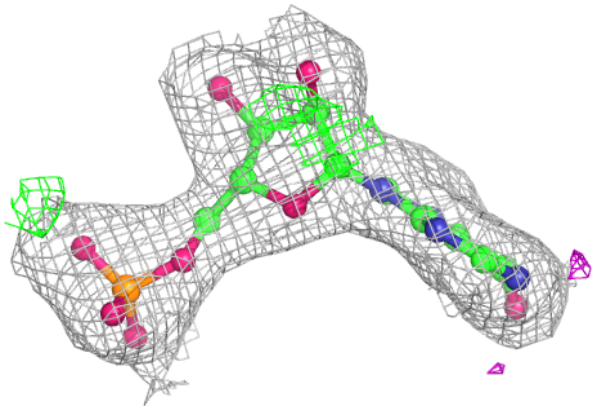


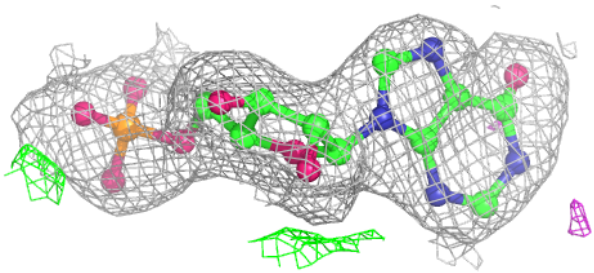




Electron density around IMP H 500:

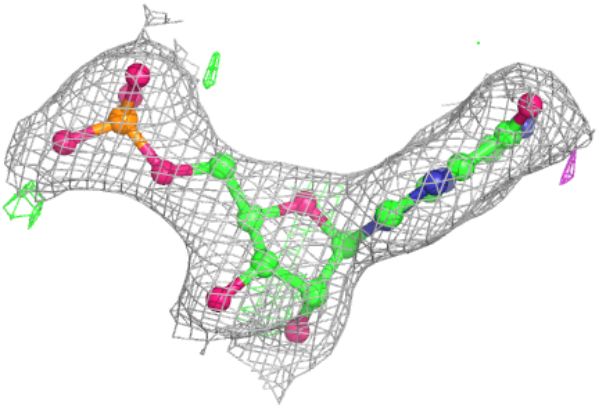
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

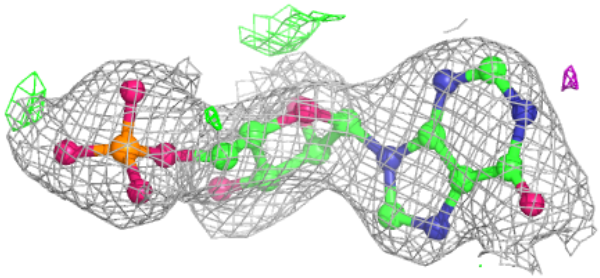


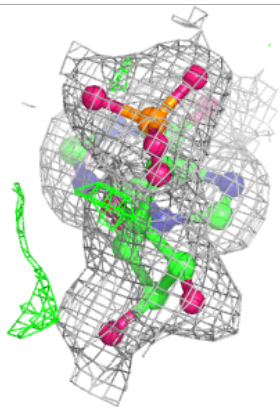


Electron density around IMP B 500:

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

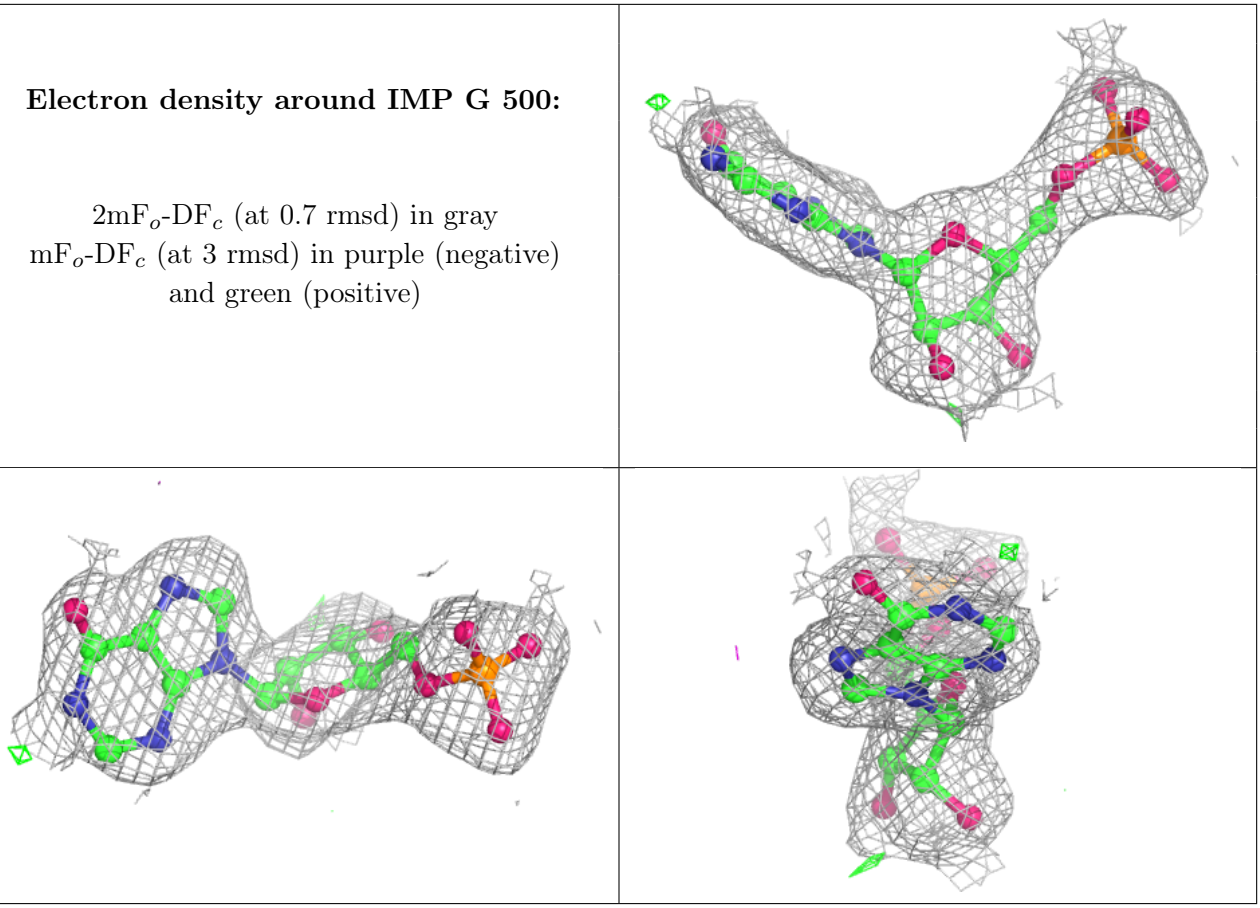






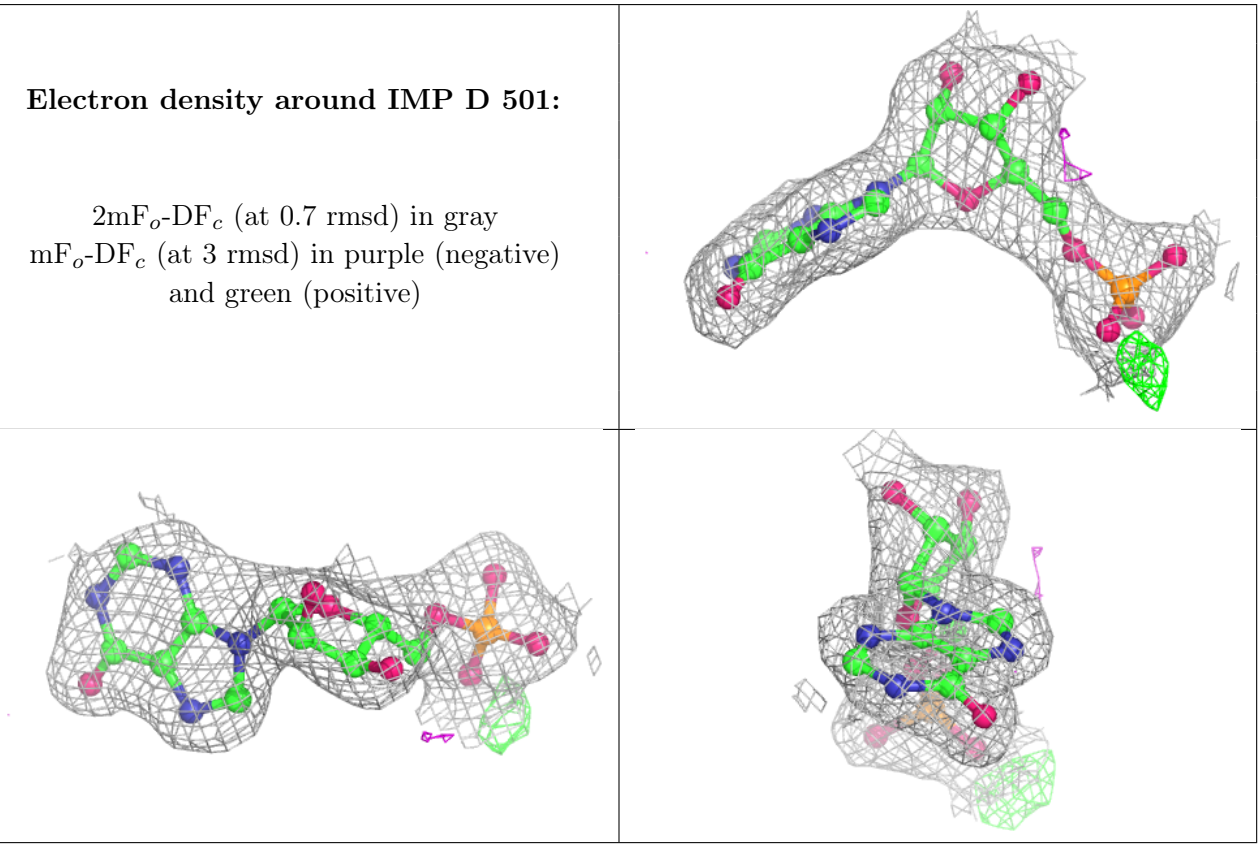
Electron density around IMP G 500:

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



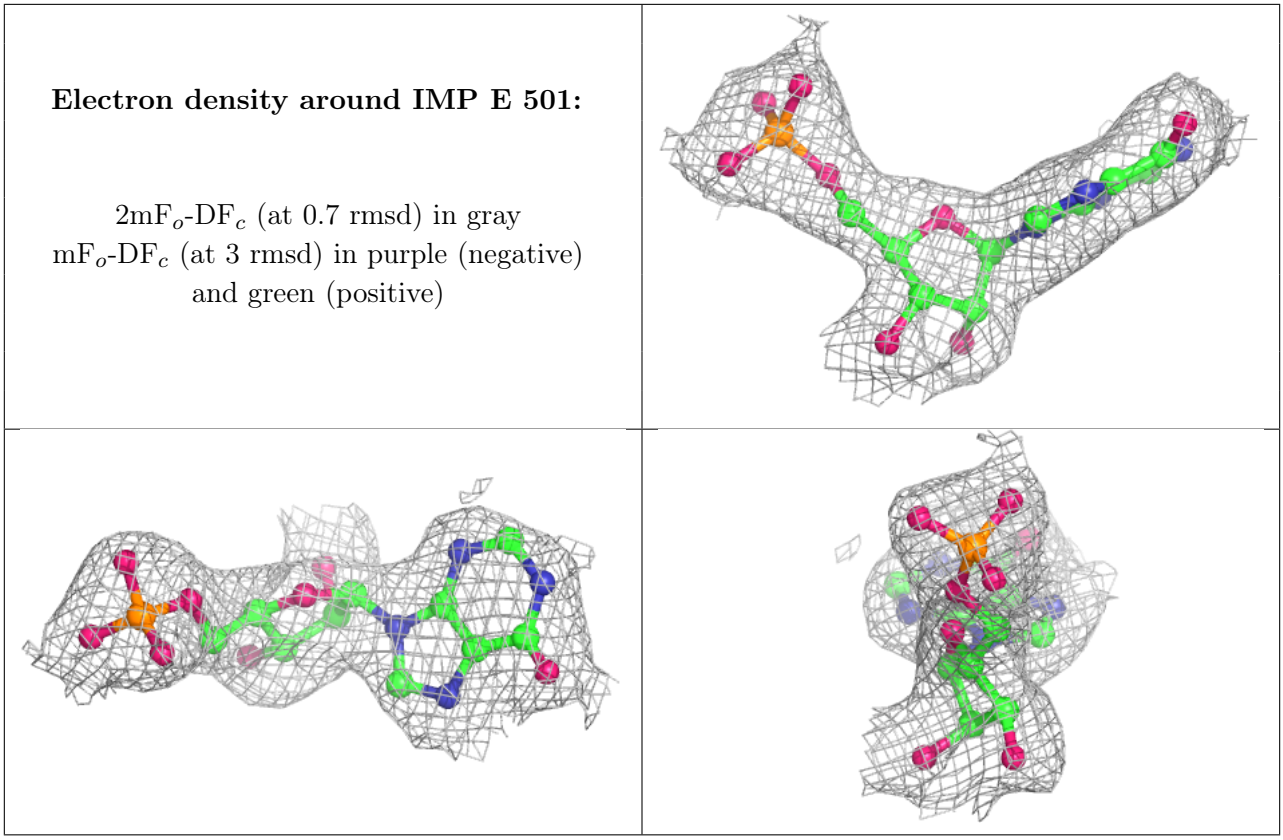
Electron density around IMP D 501:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.