wwPDB X-ray Structure Validation Summary Report (i)

Mar 17, 2022 – 04:09 PM EDT

PDB ID	:	5UWX
Title	:	Crystal Structure of Inosine 5'-monophosphate Dehydrogenase from Clostridium perfringens Complexed with IMP and P176
Authors	:	Maltseva, N.; Kim, Y.; Mulligan, R.; Makowska-Grzyska, M.; Gu, M.; Gollapalli, D.R.; Hedstrom, L.; Joachimiak, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2017-02-21
Resolution	:	1.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

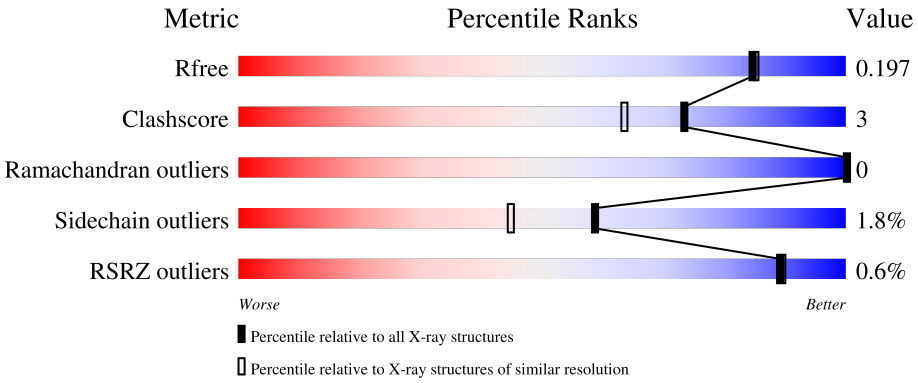
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	363	87% 7% • 5%
1	B	363	86% 9% 5%
1	C	363	87% 9% 5%
1	D	363	85% 9% 6%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11017 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,Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	4	0
			2578	1616	444	497	21			
1	B	344	Total	C	N	O	S	0	7	0
			2594	1630	449	494	21			
1	C	346	Total	C	N	O	S	0	0	0
			2542	1594	440	488	20			
1	D	341	Total	C	N	O	S	0	5	0
			2550	1598	439	492	21			

There are 24 discrepancies between the modelled and reference sequences:

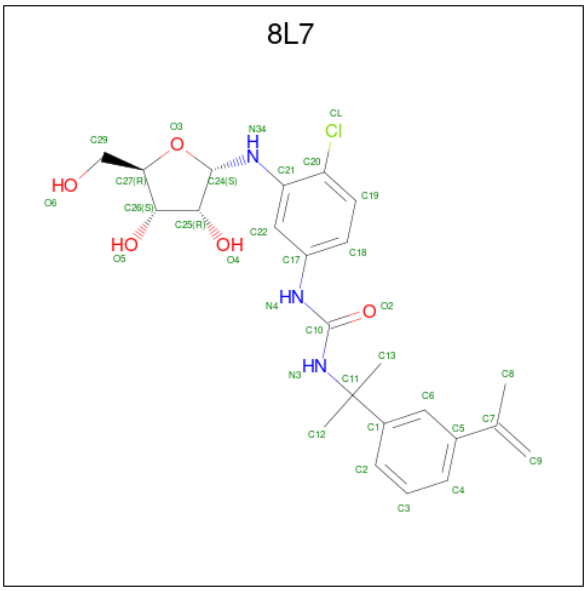
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A127ELD1
A	-1	ASN	-	expression tag	UNP A0A127ELD1
A	0	ALA	-	expression tag	UNP A0A127ELD1
A	89	SER	-	linker	UNP A0A127ELD1
A	90	GLY	-	linker	UNP A0A127ELD1
A	91	GLY	-	linker	UNP A0A127ELD1
B	-2	SER	-	expression tag	UNP A0A127ELD1
B	-1	ASN	-	expression tag	UNP A0A127ELD1
B	0	ALA	-	expression tag	UNP A0A127ELD1
B	89	SER	-	linker	UNP A0A127ELD1
B	90	GLY	-	linker	UNP A0A127ELD1
B	91	GLY	-	linker	UNP A0A127ELD1
C	-2	SER	-	expression tag	UNP A0A127ELD1
C	-1	ASN	-	expression tag	UNP A0A127ELD1
C	0	ALA	-	expression tag	UNP A0A127ELD1
C	89	SER	-	linker	UNP A0A127ELD1
C	90	GLY	-	linker	UNP A0A127ELD1
C	91	GLY	-	linker	UNP A0A127ELD1
D	-2	SER	-	expression tag	UNP A0A127ELD1
D	-1	ASN	-	expression tag	UNP A0A127ELD1

Continued on next page...

Continued from previous page...

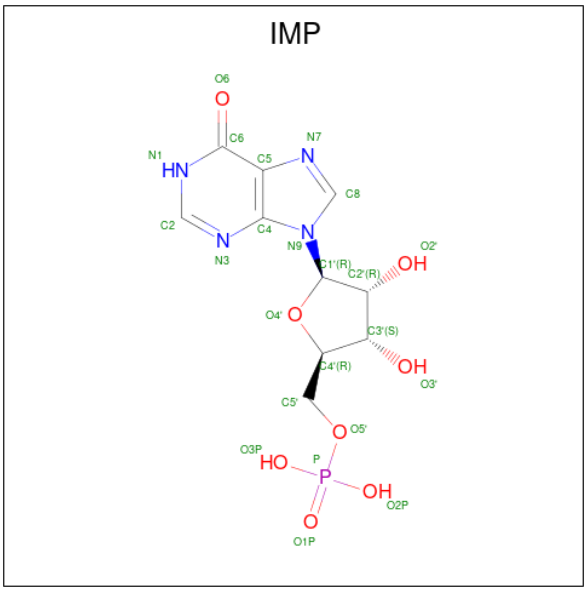
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ALA	-	expression tag	UNP A0A127ELD1
D	89	SER	-	linker	UNP A0A127ELD1
D	90	GLY	-	linker	UNP A0A127ELD1
D	91	GLY	-	linker	UNP A0A127ELD1

- Molecule 2 is N-{2-chloro-5-[({2-[3-(prop-1-en-2-yl)phenyl]propan-2-yl}carbamoyl)amino]phenyl}-alpha-D-ribofuranosylamine (three-letter code: 8L7) (formula: $C_{24}H_{30}ClN_3O_5$).



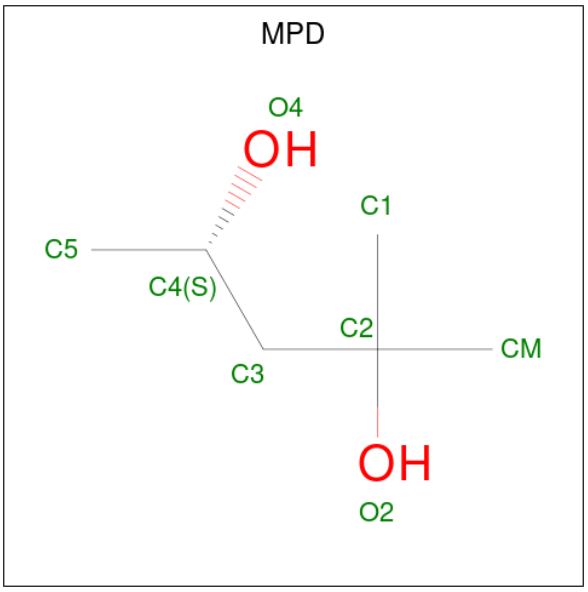
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		
2	B	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		
2	C	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		
2	D	1	Total	C	Cl	N	O	0	0
			33	24	1	3	5		

- Molecule 3 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



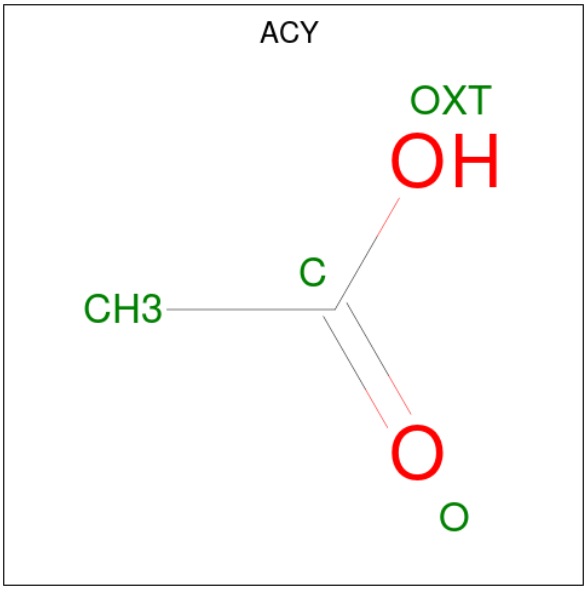
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



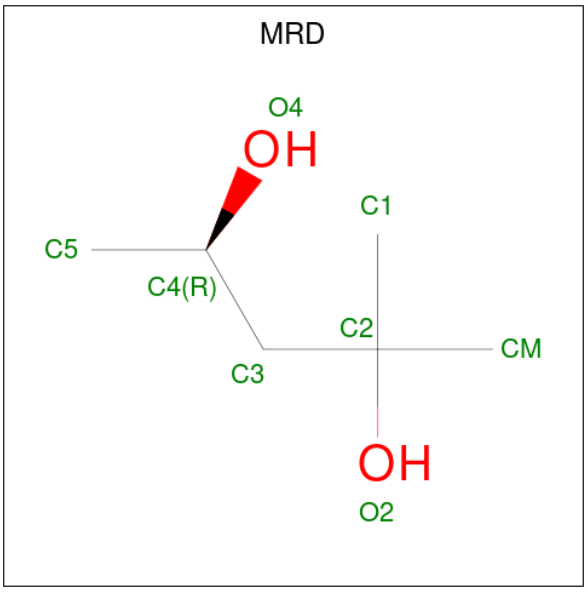
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	C	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 8 6 2	0	0

- Molecule 7 is water.

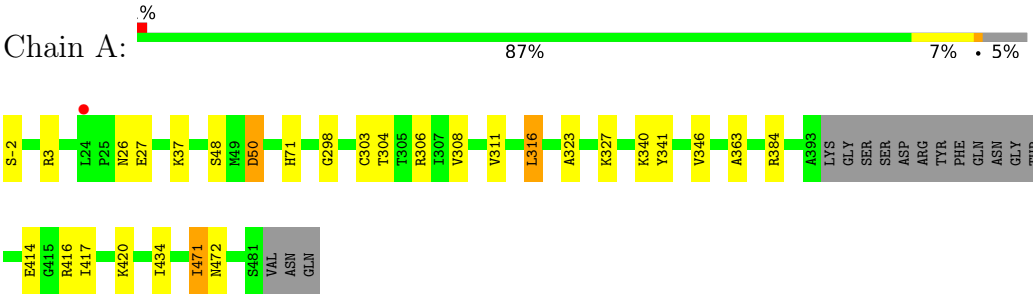
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	150	Total O 150 150	0	0
7	B	140	Total O 140 140	0	0
7	C	103	Total O 103 103	0	0
7	D	84	Total O 84 84	0	0

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.

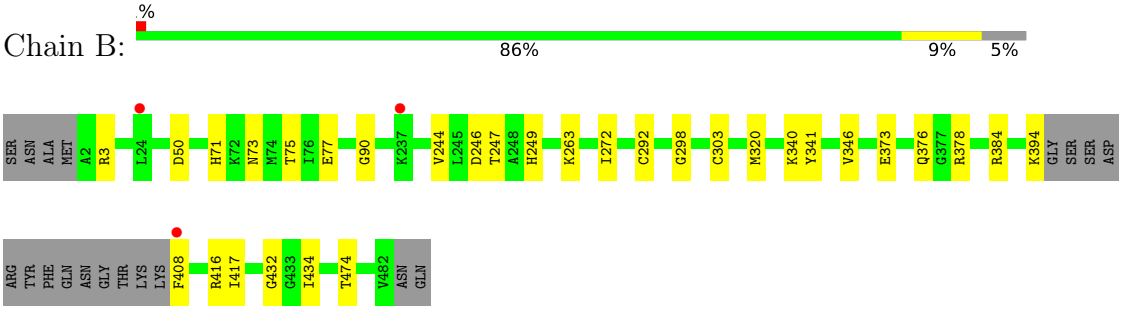
• Molecule 1: Inosine-5'-monophosphate dehydrogenase,Inosine-5'-monophosphate dehydrogenase

Chain A:



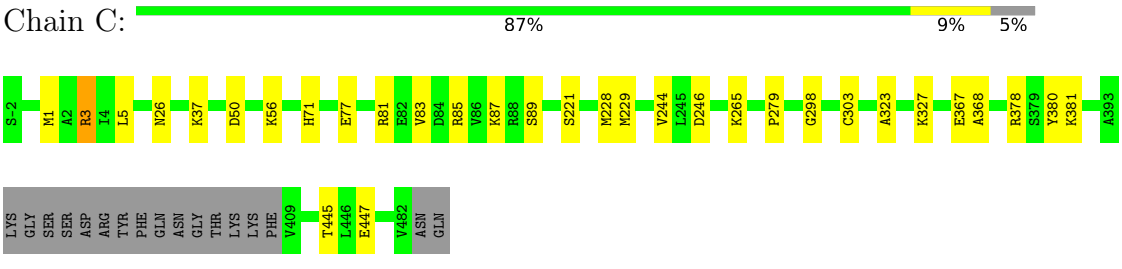
• Molecule 1: Inosine-5'-monophosphate dehydrogenase,Inosine-5'-monophosphate dehydrogenase

Chain B:



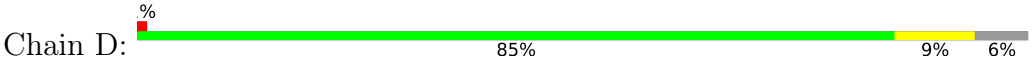
• Molecule 1: Inosine-5'-monophosphate dehydrogenase,Inosine-5'-monophosphate dehydrogenase

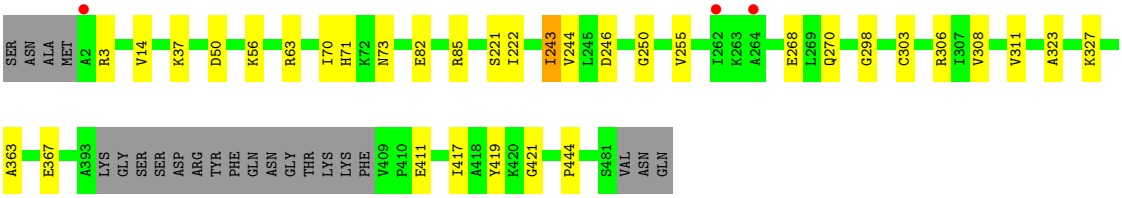
Chain C:



• Molecule 1: Inosine-5'-monophosphate dehydrogenase,Inosine-5'-monophosphate dehydrogenase

Chain D:




SER ASN ALA MET A2 R3 V14 K37 D50 K56 R63 I70 H71 K72 N73 E82 R85 S221 I222 I243 V244 L245 D246 G250 V255 I262 K263 A264 E268 L269 Q270 G298 C303 R306 I307 V308 V311 A323 K327

A363 E367 A393 LYS GLY SER SER ASP ARG TYR PHE GLN ASN GLY THR LYS LYS PHE V409 P410 E411 I417 A418 Y419 K420 G421 P444 S481 VAL ASN GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.28Å 118.94Å 96.99Å 90.00° 102.88° 90.00°	Depositor
Resolution (Å)	47.50 – 1.85 47.51 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.50-1.85) 97.2 (47.51-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.163 , 0.197 0.162 , 0.197	Depositor DCC
R_{free} test set	5794 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.5	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	0.97	EDS
Total number of atoms	11017	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: IMP, 8L7, MPD, ACY, MRD

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	0.43	0/2611	0.59	2/3522 (0.1%)
1	B	0.44	0/2627	0.59	0/3542
1	C	0.41	0/2574	0.56	0/3474
1	D	0.38	0/2582	0.56	0/3483
All	All	0.42	0/10394	0.58	2/14021 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	316	LEU	CA-CB-CG	-5.32	103.07	115.30
1	A	50	ASP	CB-CG-OD1	5.18	122.96	118.30

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	2578	0	2633	18	0
1	B	2594	0	2664	18	0
1	C	2542	0	2611	18	0
1	D	2550	0	2604	19	0
2	A	33	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	33	0	0	0	0
2	C	33	0	0	0	0
2	D	33	0	0	0	0
3	A	23	0	11	1	0
3	B	23	0	11	1	0
3	C	23	0	11	2	0
3	D	23	0	11	1	0
4	A	8	0	14	0	0
4	B	8	0	14	1	0
4	C	8	0	14	1	0
4	D	8	0	14	0	0
5	A	4	0	3	0	0
5	C	4	0	3	0	0
5	D	4	0	3	0	0
6	B	8	0	14	1	0
7	A	150	0	0	1	0
7	B	140	0	0	0	0
7	C	103	0	0	0	0
7	D	84	0	0	0	0
All	All	11017	0	10635	69	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 3.

The worst 5 of 69 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:VAL:HG21	1:B:432:GLY:HA3	1.77	0.65
1:C:303:CYS:SG	3:C:501:IMP:H2	2.39	0.63
4:B:502:MPD:O2	4:B:502:MPD:H52	2.01	0.61
1:B:376:GLN:O	1:C:378:ARG:NH2	2.34	0.61
1:B:90:GLY:HA2	1:D:444:PRO:HG3	1.84	0.59

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	346/363 (95%)	337 (97%)	9 (3%)	0	100	100
1	B	347/363 (96%)	337 (97%)	10 (3%)	0	100	100
1	C	342/363 (94%)	333 (97%)	9 (3%)	0	100	100
1	D	342/363 (94%)	333 (97%)	9 (3%)	0	100	100
All	All	1377/1452 (95%)	1340 (97%)	37 (3%)	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	271/282 (96%)	268 (99%)	3 (1%)	73	65
1	B	273/282 (97%)	269 (98%)	4 (2%)	65	53
1	C	267/282 (95%)	261 (98%)	6 (2%)	52	36
1	D	268/282 (95%)	262 (98%)	6 (2%)	52	36
All	All	1079/1128 (96%)	1060 (98%)	19 (2%)	59	45

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	14	VAL
1	D	221	SER
1	D	243	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	73	ASN
1	C	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	33	GLN
1	B	73	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	IMP	C	501	-	21,25,25	1.30	3 (14%)	23,38,38	1.35	2 (8%)
2	8L7	C	500	-	35,35,35	1.26	6 (17%)	48,51,51	1.15	4 (8%)
3	IMP	B	501	-	21,25,25	1.21	3 (14%)	23,38,38	1.69	4 (17%)
3	IMP	A	501	-	21,25,25	1.30	3 (14%)	23,38,38	1.49	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MPD	A	502	-	7,7,7	0.32	0	9,10,10	0.55	0
4	MPD	C	503	-	7,7,7	0.28	0	9,10,10	0.64	0
5	ACY	A	503	-	1,3,3	1.44	0	0,3,3	-	-
4	MPD	D	502	-	7,7,7	0.31	0	9,10,10	0.45	0
2	8L7	B	500	-	35,35,35	1.25	5 (14%)	48,51,51	1.31	4 (8%)
3	IMP	D	501	-	21,25,25	1.23	3 (14%)	23,38,38	1.44	3 (13%)
2	8L7	D	500	-	35,35,35	1.34	6 (17%)	48,51,51	2.47	4 (8%)
4	MPD	B	502	-	7,7,7	0.39	0	9,10,10	0.39	0
2	8L7	A	500	-	35,35,35	1.30	6 (17%)	48,51,51	1.19	6 (12%)
5	ACY	C	502	-	1,3,3	1.50	0	0,3,3	-	-
6	MRD	B	503	-	7,7,7	0.39	0	9,10,10	0.48	0
5	ACY	D	503	-	1,3,3	1.53	0	0,3,3	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMP	C	501	-	-	0/6/26/26	0/3/3/3
2	8L7	C	500	-	-	7/25/41/41	0/3/3/3
3	IMP	B	501	-	-	0/6/26/26	0/3/3/3
3	IMP	A	501	-	-	0/6/26/26	0/3/3/3
4	MPD	A	502	-	-	4/5/5/5	-
4	MPD	C	503	-	-	4/5/5/5	-
4	MPD	D	502	-	-	0/5/5/5	-
2	8L7	B	500	-	-	7/25/41/41	0/3/3/3
3	IMP	D	501	-	-	0/6/26/26	0/3/3/3
2	8L7	D	500	-	-	4/25/41/41	0/3/3/3
4	MPD	B	502	-	-	1/5/5/5	-
2	8L7	A	500	-	-	6/25/41/41	0/3/3/3
6	MRD	B	503	-	-	4/5/5/5	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	8L7	C21-C20	4.42	1.50	1.39
3	C	501	IMP	C2-N3	3.79	1.38	1.32
3	A	501	IMP	C2-N3	3.70	1.38	1.32
2	C	500	8L7	C21-C20	3.64	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	8L7	C21-C20	3.60	1.48	1.39

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	8L7	C20-C21-N34	14.54	127.34	120.43
2	B	500	8L7	C21-N34-C24	-5.00	118.04	123.16
3	B	501	IMP	N3-C2-N1	-4.67	121.39	128.68
3	A	501	IMP	N3-C2-N1	-4.47	121.70	128.68
3	D	501	IMP	N3-C2-N1	-4.25	122.04	128.68

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	8L7	C20-C21-N34-C24
2	B	500	8L7	C22-C21-N34-C24
2	C	500	8L7	C20-C21-N34-C24
2	C	500	8L7	O3-C24-N34-C21
2	D	500	8L7	C20-C21-N34-C24

There are no ring outliers.

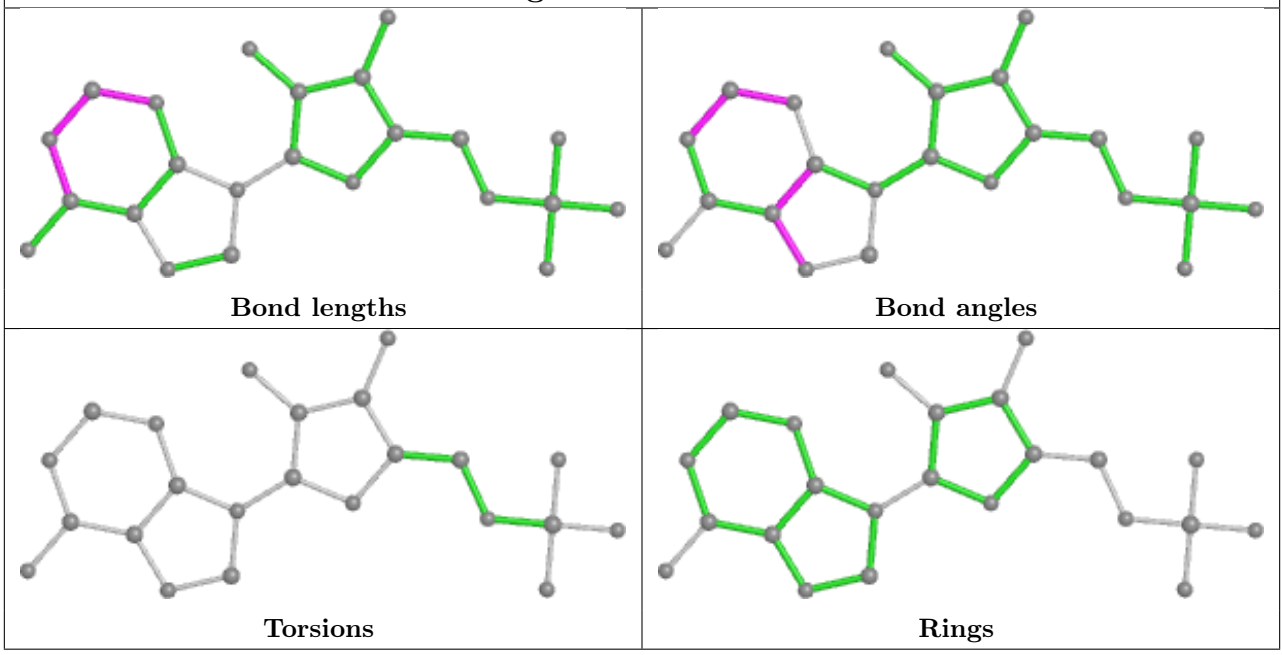
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	IMP	2	0
3	B	501	IMP	1	0
3	A	501	IMP	1	0
4	C	503	MPD	1	0
3	D	501	IMP	1	0
4	B	502	MPD	1	0
6	B	503	MRD	1	0

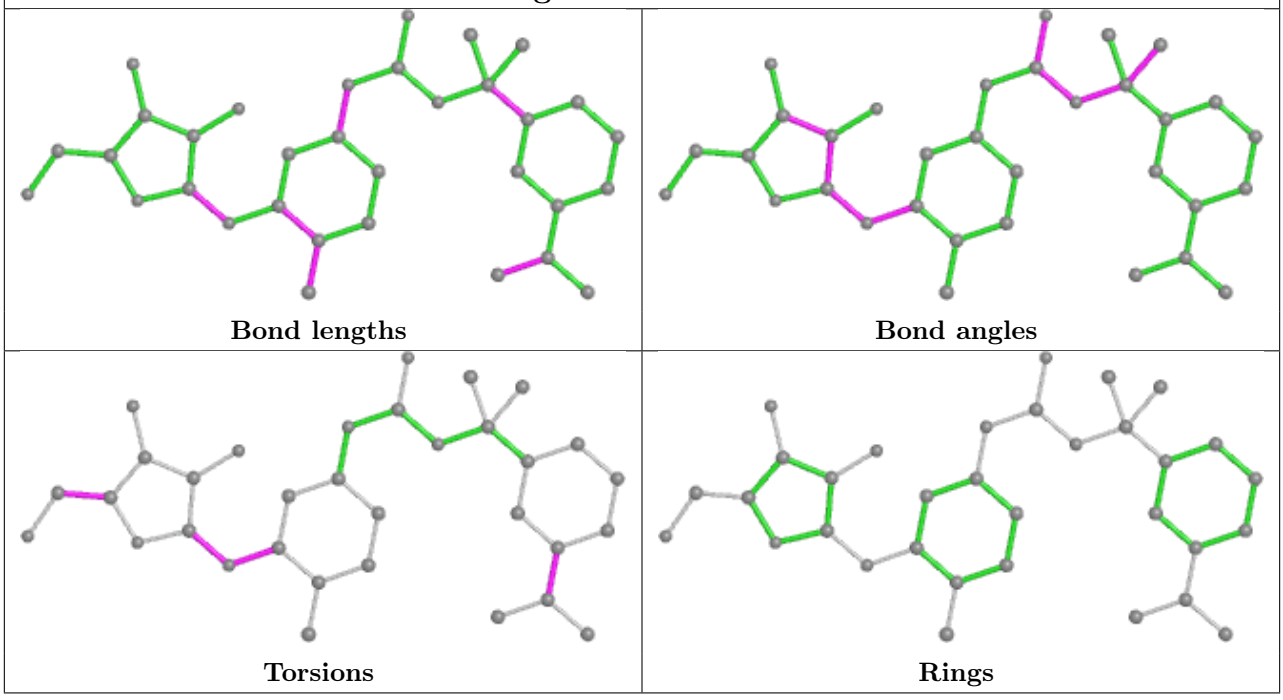
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

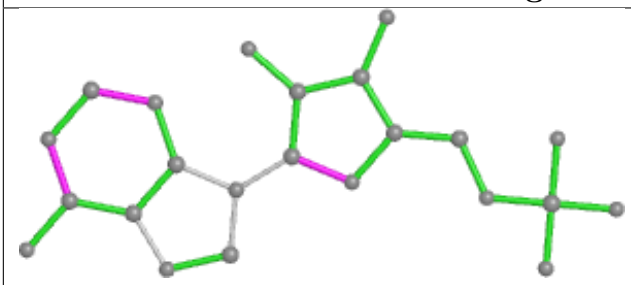
Ligand IMP C 501



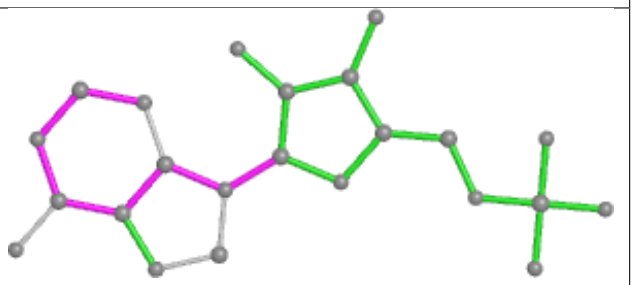
Ligand 8L7 C 500



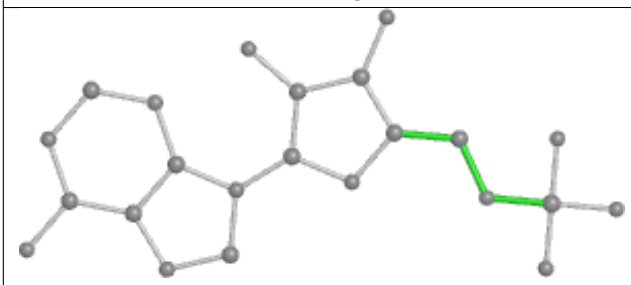
Ligand IMP B 501



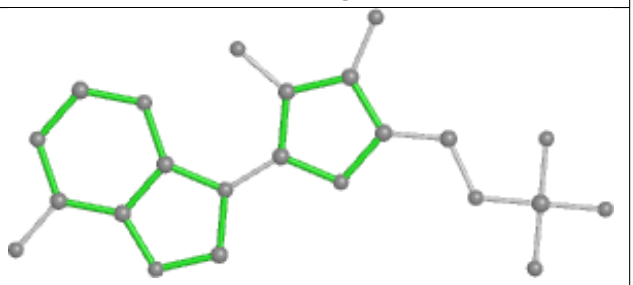
Bond lengths



Bond angles

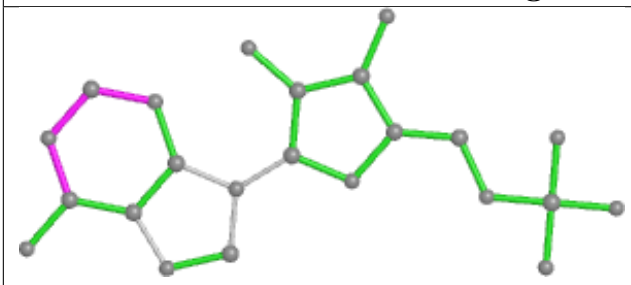


Torsions

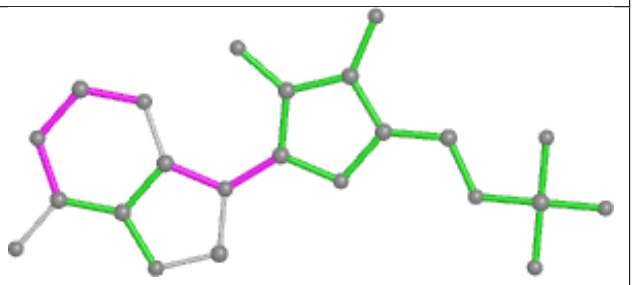


Rings

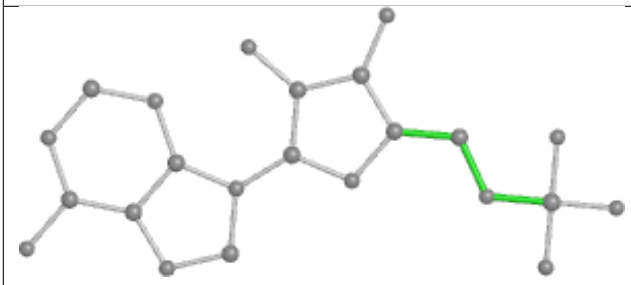
Ligand IMP A 501



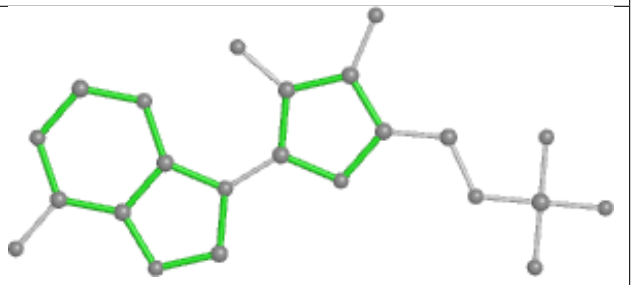
Bond lengths



Bond angles

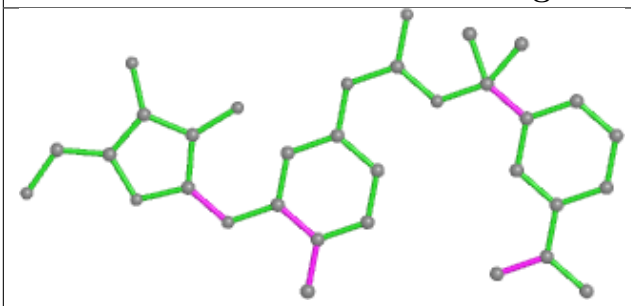


Torsions

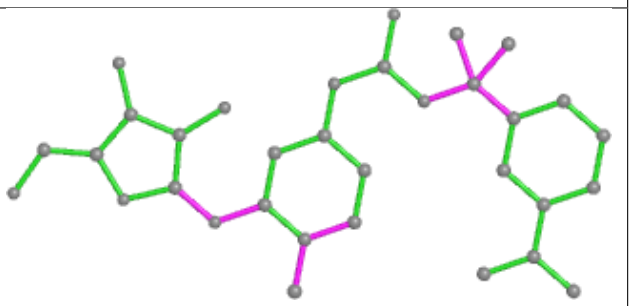


Rings

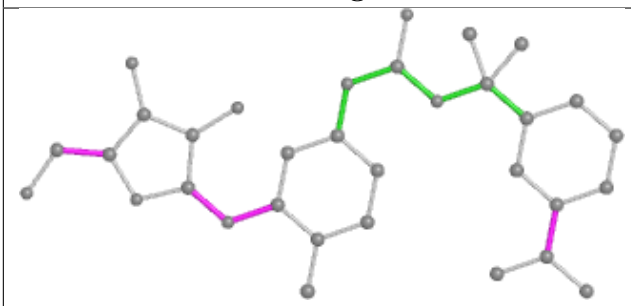
Ligand 8L7 B 500



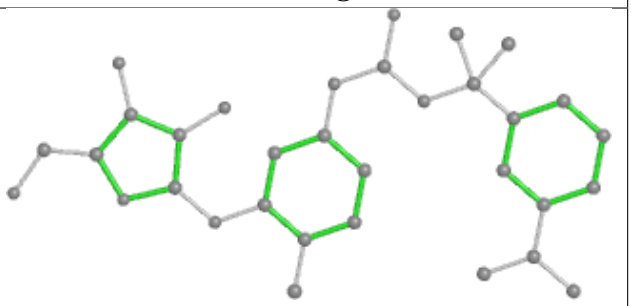
Bond lengths



Bond angles

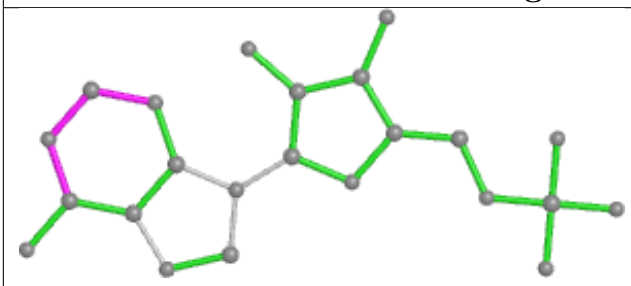


Torsions

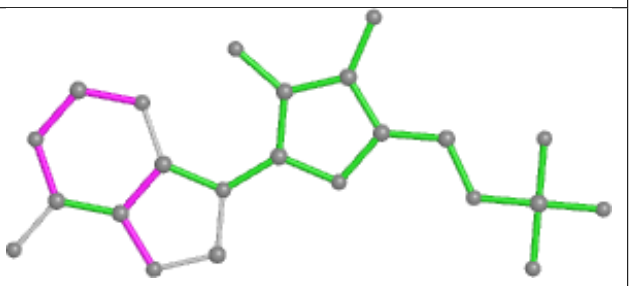


Rings

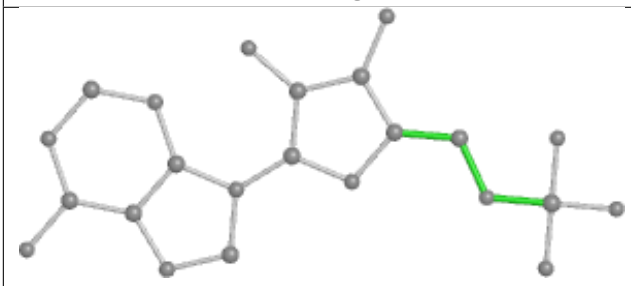
Ligand IMP D 501



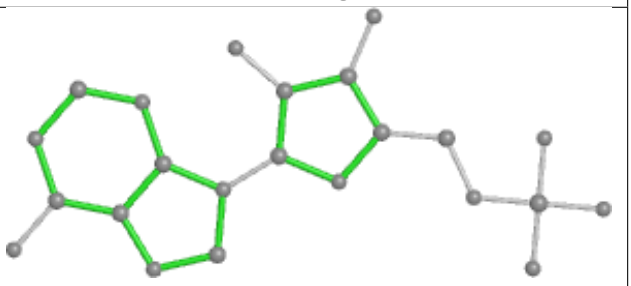
Bond lengths



Bond angles

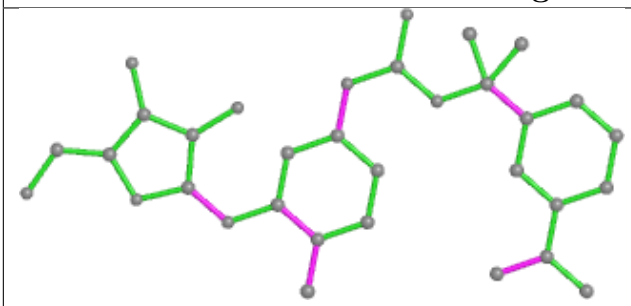


Torsions

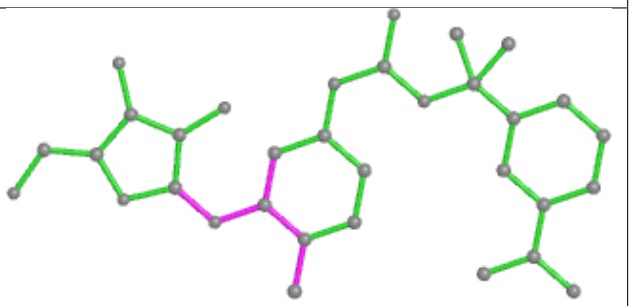


Rings

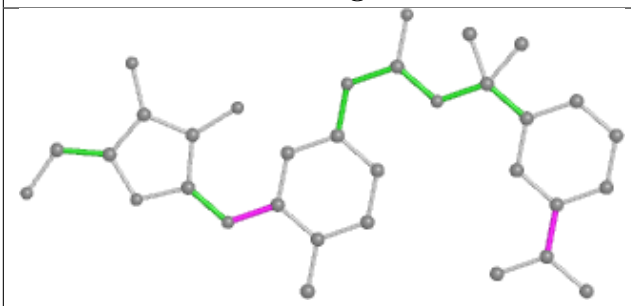
Ligand 8L7 D 500



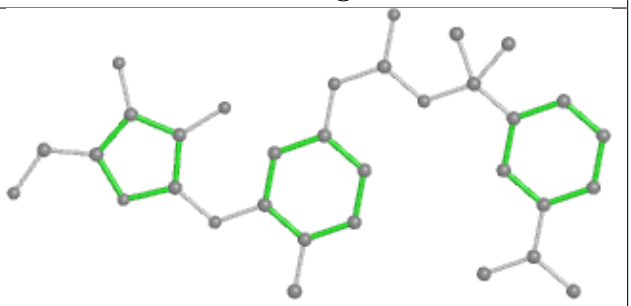
Bond lengths



Bond angles

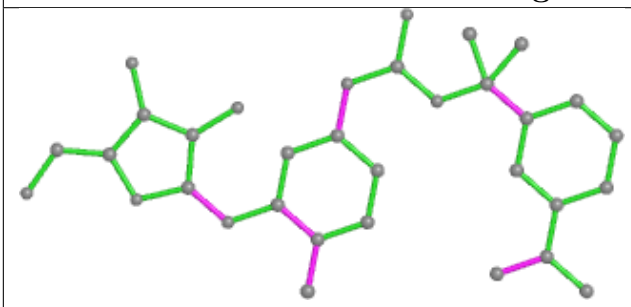


Torsions

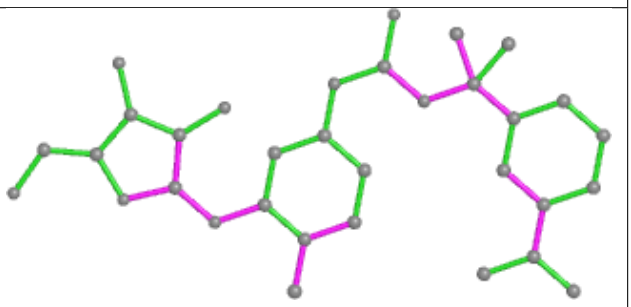


Rings

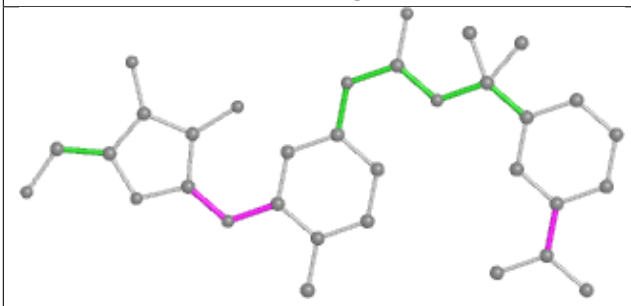
Ligand 8L7 A 500



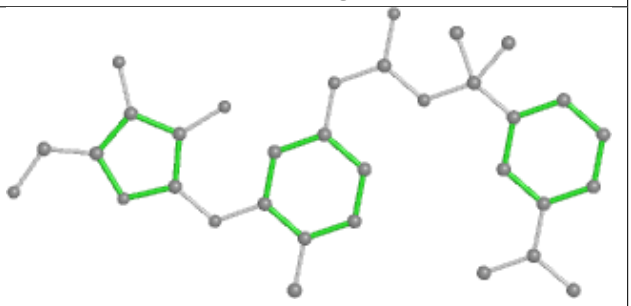
Bond lengths



Bond angles



Torsions



Rings

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	346/363 (95%)	-0.33	2 (0%)	89	89	26, 36, 61, 82	1 (0%)
1	B	344/363 (94%)	-0.35	3 (0%)	84	84	23, 38, 64, 88	3 (0%)
1	C	346/363 (95%)	-0.33	0	100	100	23, 40, 67, 87	0
1	D	341/363 (93%)	-0.15	3 (0%)	84	84	27, 47, 71, 86	0
All	All	1377/1452 (94%)	-0.29	8 (0%)	89	89	23, 39, 67, 88	4 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	PHE	6.7
1	B	408	PHE	5.6
1	D	262	ILE	3.9
1	D	2	ALA	3.5
1	B	237	LYS	3.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

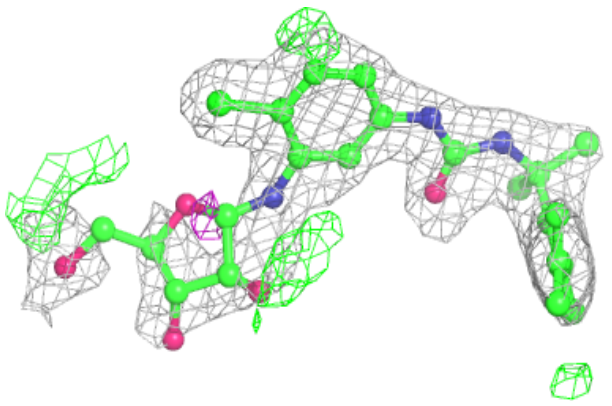
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

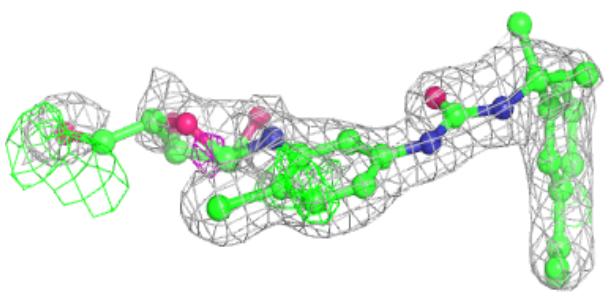
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACY	D	503	4/4	0.74	0.14	70,74,75,77	0
2	8L7	D	500	33/33	0.80	0.19	39,46,75,78	33
5	ACY	C	502	4/4	0.84	0.19	63,67,67,68	0
4	MPD	B	502	8/8	0.84	0.16	49,56,62,62	0
2	8L7	A	500	33/33	0.86	0.19	32,42,73,77	33
5	ACY	A	503	4/4	0.86	0.09	54,60,63,68	0
6	MRD	B	503	8/8	0.88	0.13	65,72,74,77	0
4	MPD	A	502	8/8	0.90	0.12	37,55,59,59	0
4	MPD	D	502	8/8	0.90	0.12	44,53,58,58	0
4	MPD	C	503	8/8	0.91	0.11	43,46,50,56	0
2	8L7	C	500	33/33	0.91	0.20	42,53,90,91	0
2	8L7	B	500	33/33	0.91	0.17	34,41,84,85	0
3	IMP	D	501	23/23	0.97	0.07	31,34,39,40	0
3	IMP	A	501	23/23	0.98	0.07	26,29,31,34	0
3	IMP	B	501	23/23	0.98	0.07	23,26,31,33	0
3	IMP	C	501	23/23	0.98	0.06	25,32,36,40	0

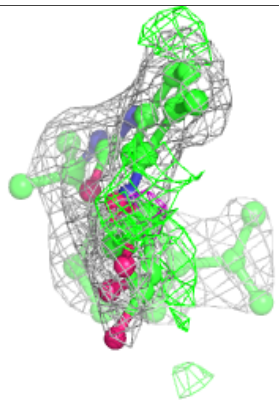
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8L7 D 500:

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

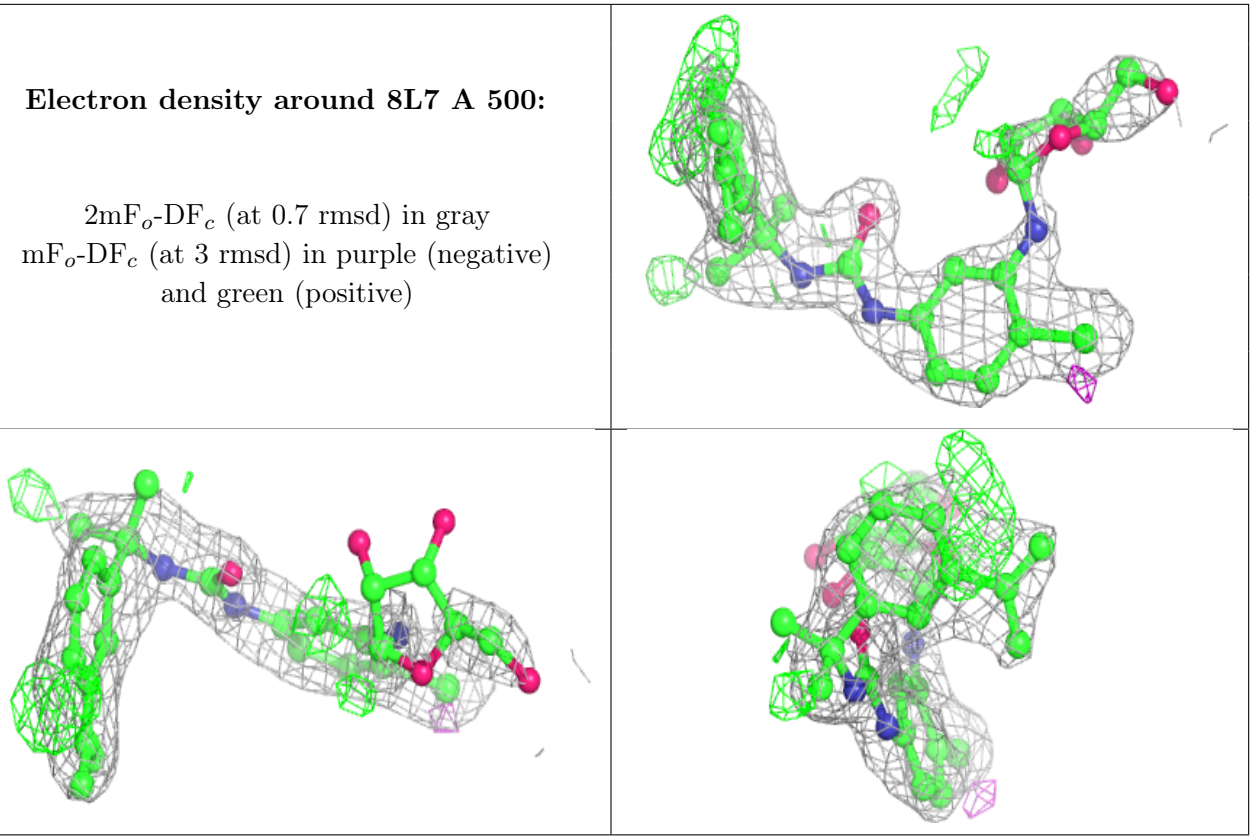






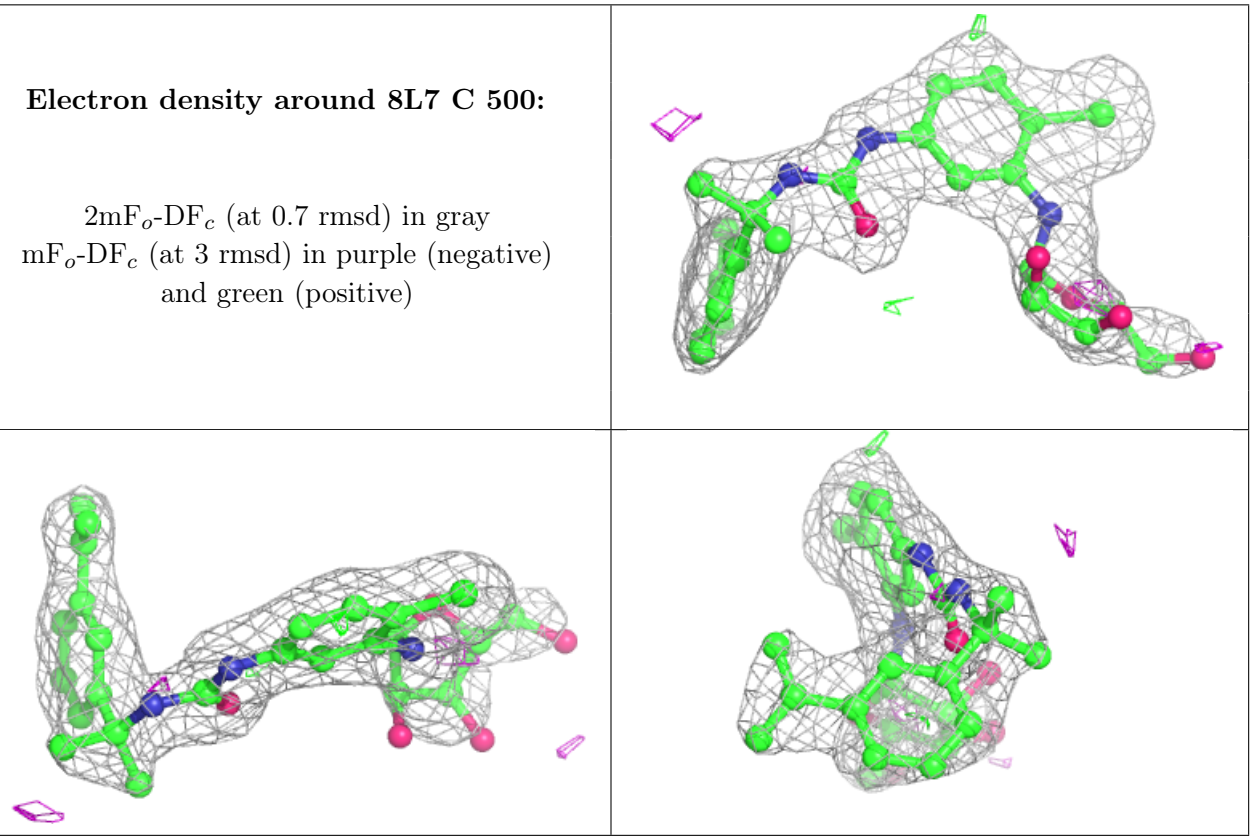
Electron density around 8L7 A 500:

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



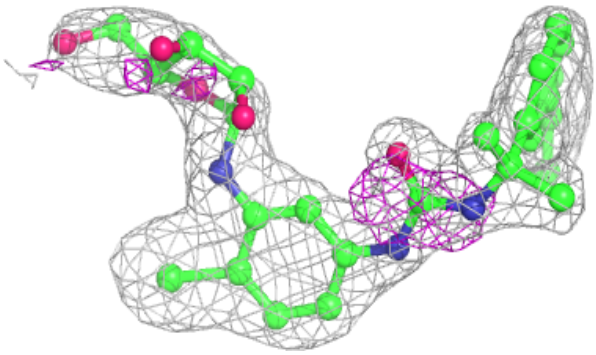
Electron density around 8L7 C 500:

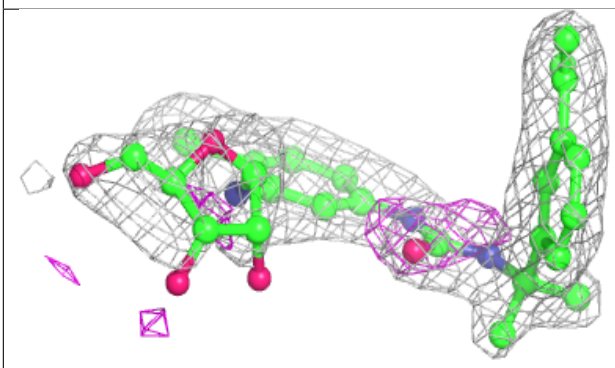
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

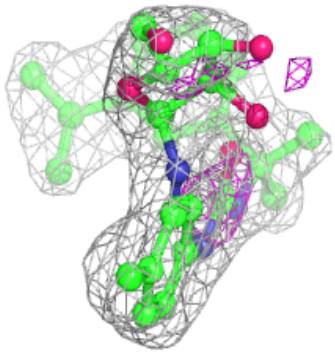


Electron density around 8L7 B 500:

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

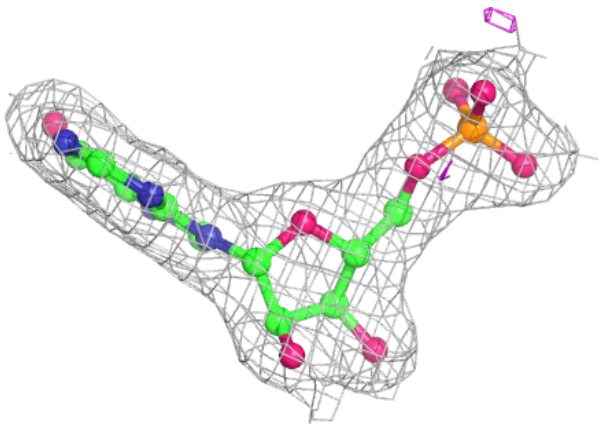


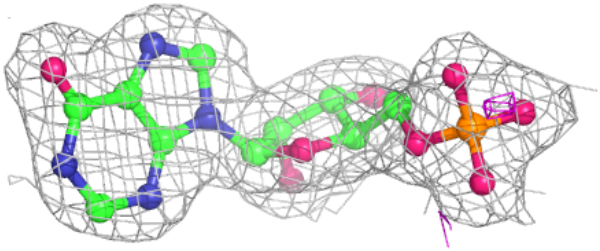


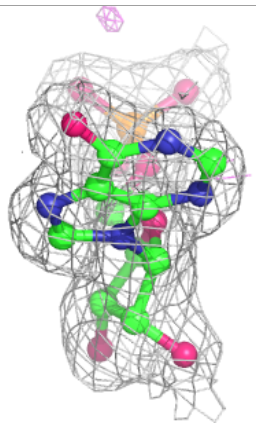


Electron density around IMP D 501:

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

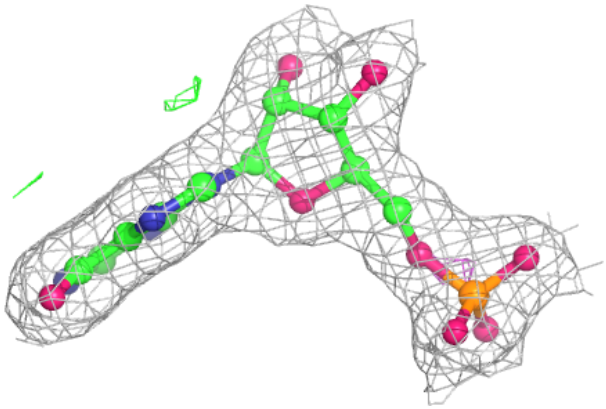


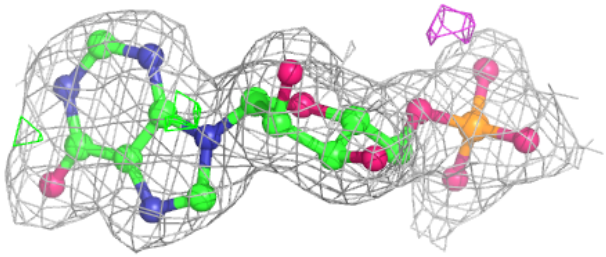


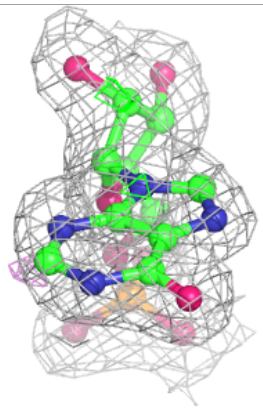


Electron density around IMP A 501:

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

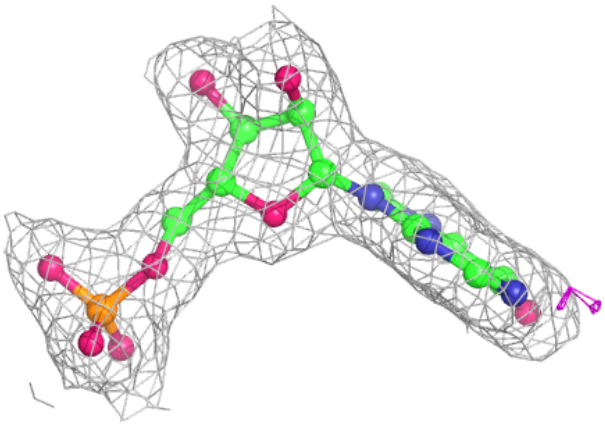


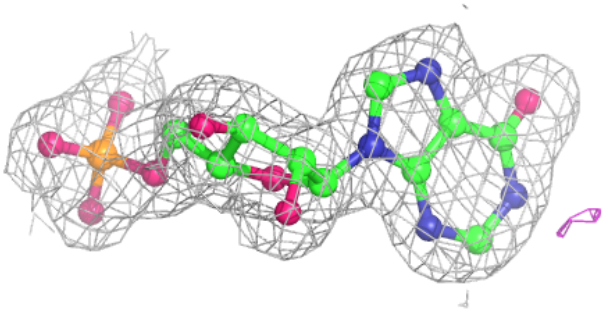


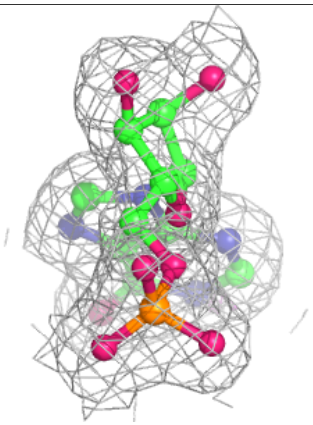


Electron density around IMP B 501:

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

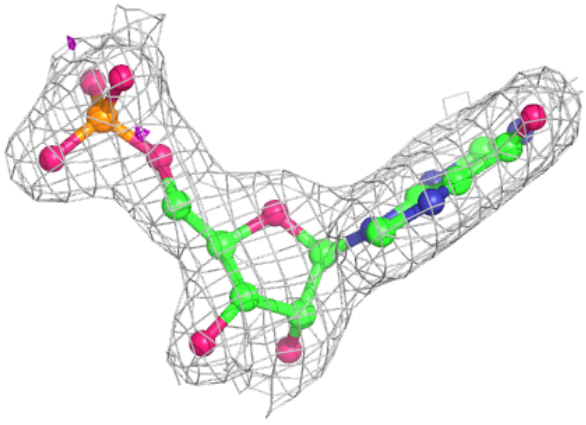


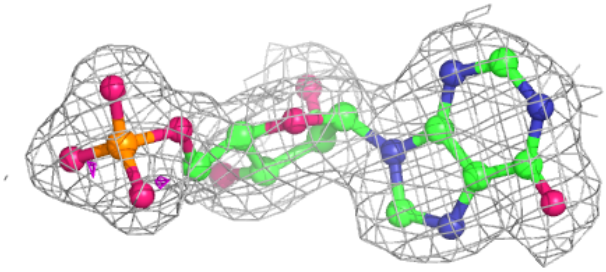


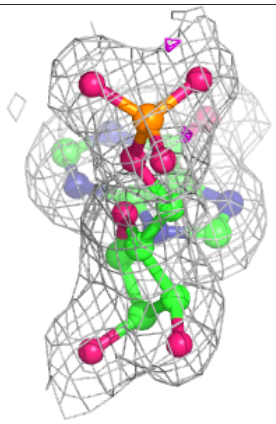


Electron density around IMP C 501:

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







6.5 Other polymers

There are no such residues in this entry.