



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:29 am BST

PDB ID : 5UXE  
Title : Crystal Structure of Inosine 5'-monophosphate Dehydrogenase from *Clostridium perfringens* Complexed with IMP and P178  
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 : 2017-02-22  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

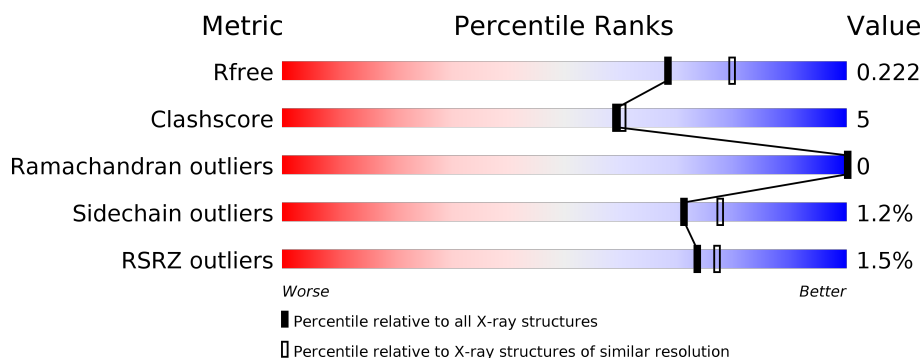
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	363	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>6%</div> </div> </div>
1	B	363	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
1	C	363	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>
1	D	363	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10766 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	343	Total	C	N	O	S	0	3	0
			2550	1602	440	489	19			
1	B	346	Total	C	N	O	S	0	6	0
			2598	1631	447	499	21			
1	C	343	Total	C	N	O	S	0	7	0
			2586	1624	447	495	20			
1	D	342	Total	C	N	O	S	0	4	0
			2549	1598	441	491	19			

There are 24 discrepancies between the modelled and reference sequences:

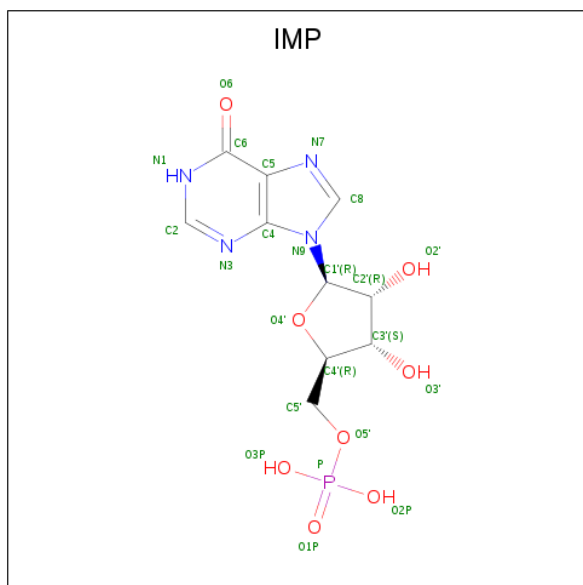
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP A0A127ELD1
A	-1	ASN	-	expression tag	UNP A0A127ELD1
A	0	ALA	-	expression tag	UNP A0A127ELD1
A	89	SER	-	linker	UNP A0A127ELD1
A	90	GLY	-	linker	UNP A0A127ELD1
A	91	GLY	-	linker	UNP A0A127ELD1
B	-2	SER	-	expression tag	UNP A0A127ELD1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

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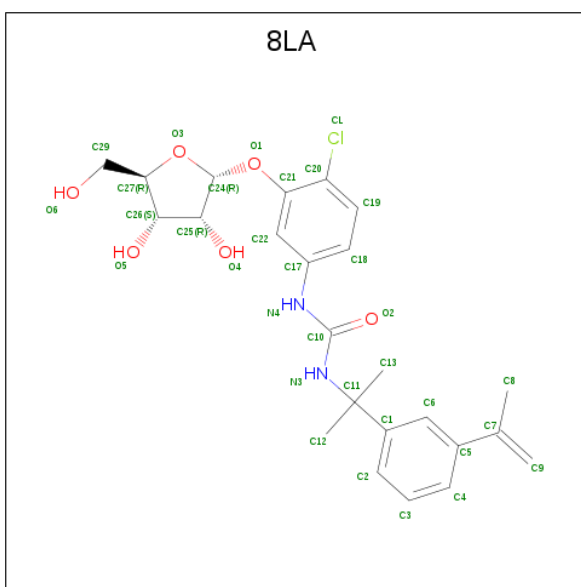
Chain	Residue	Modelled	Actual	Comment	Reference
D	89	SER	-	linker	UNP A0A127ELD1
D	90	GLY	-	linker	UNP A0A127ELD1
D	91	GLY	-	linker	UNP A0A127ELD1

- 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		

- 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	0	0
			33	24	1	2	6		
3	B	1	Total	C	Cl	N	O	0	0
			33	24	1	2	6		
3	C	1	Total	C	Cl	N	O	0	0
			33	24	1	2	6		
3	D	1	Total	C	Cl	N	O	0	0
			33	24	1	2	6		

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

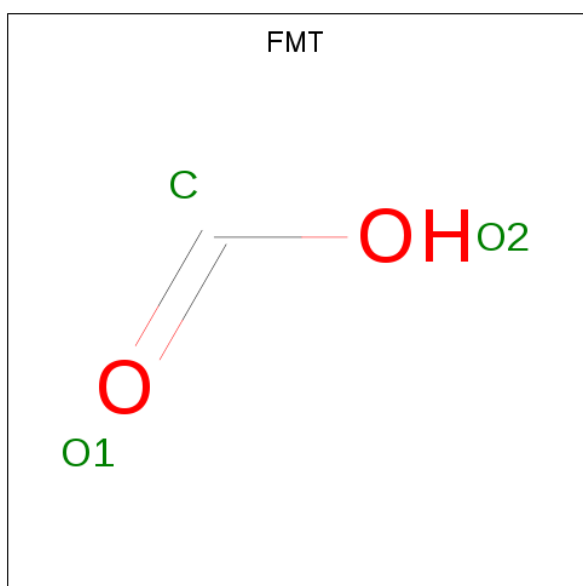
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



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

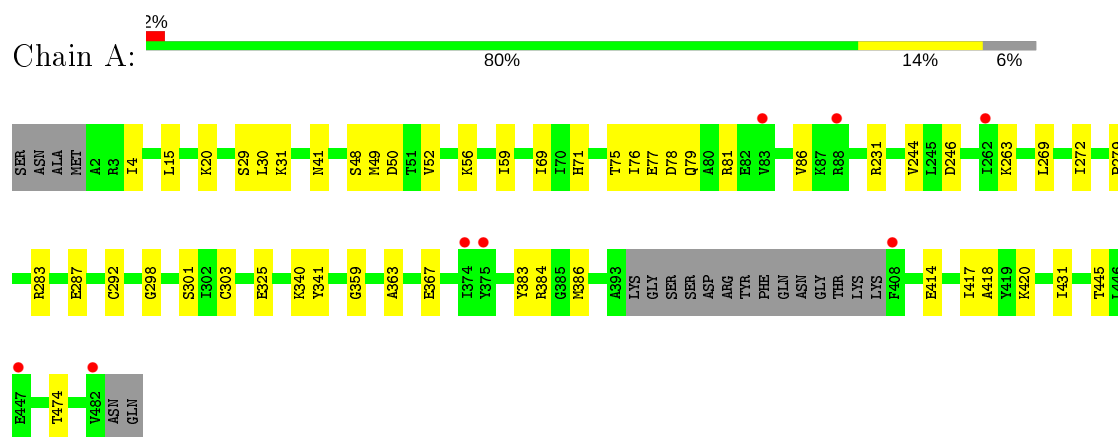
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	39	Total	O	0	0
			39	39		
8	B	61	Total	O	0	0
			61	61		
8	C	70	Total	O	0	0
			70	70		
8	D	62	Total	O	0	0
			62	62		

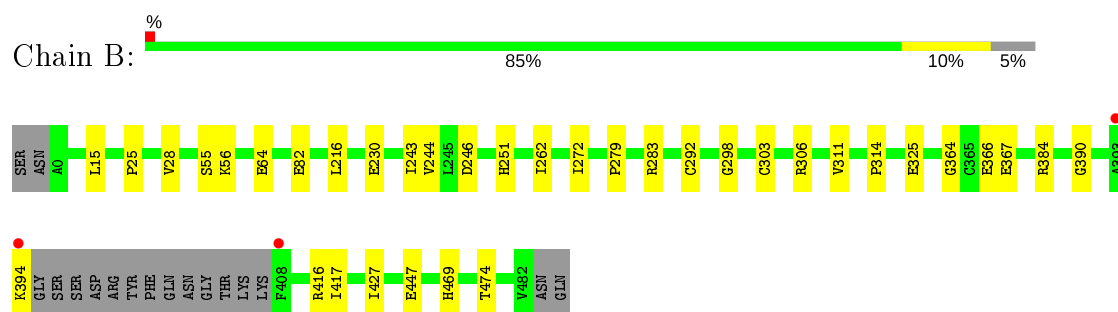
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

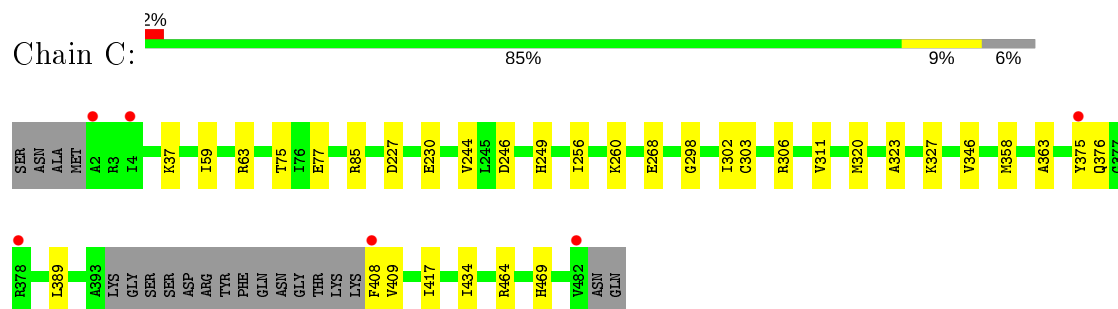
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase

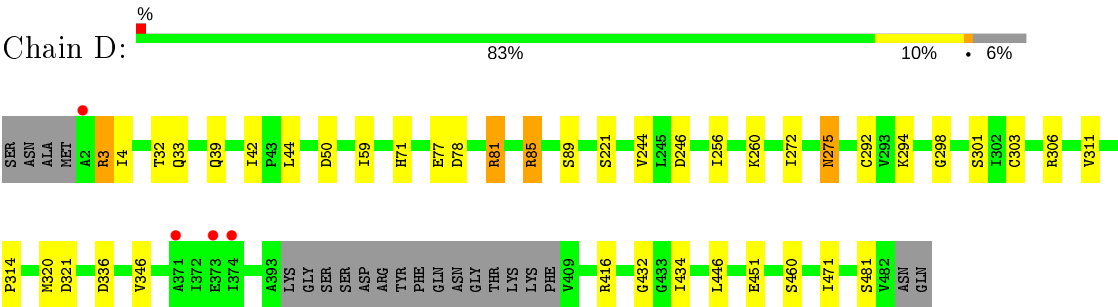


- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.94Å 119.10Å 96.97Å 90.00° 102.86° 90.00°	Depositor
Resolution (Å)	39.25 – 2.10 43.07 – 2.07	Depositor EDS
% Data completeness (in resolution range)	92.6 (39.25-2.10) 92.6 (43.07-2.07)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.06Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.173 , 0.223 0.172 , 0.222	Depositor DCC
$R_{free}$ test set	3908 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, K, 8LA, IMP, SO4, FMT

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	0.35	0/2583	0.54	0/3485
1	B	0.38	0/2631	0.54	0/3547
1	C	0.37	0/2619	0.56	0/3532
1	D	0.42	0/2581	0.56	0/3483
All	All	0.38	0/10414	0.55	0/14047

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2550	0	2613	36	0
1	B	2598	0	2661	27	0
1	C	2586	0	2648	21	0
1	D	2549	0	2608	27	0
2	A	23	0	11	2	0
2	B	23	0	11	1	0
2	C	23	0	11	0	0
2	D	23	0	11	1	0
3	A	33	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	0	0	0
3	C	33	0	0	0	0
3	D	33	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	8	0	14	1	0
5	D	8	0	14	2	0
6	C	3	0	1	1	0
7	C	5	0	0	0	0
8	A	39	0	0	0	0
8	B	61	0	0	0	0
8	C	70	0	0	2	0
8	D	62	0	0	0	0
All	All	10766	0	10603	100	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 5.

All (100) 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:49:MET:HE3	1:A:383:TYR:HE1	1.52	0.73
1:C:409:VAL:HG21	1:D:432:GLY:HA3	1.72	0.71
1:D:272:ILE:HG12	1:D:292:CYS:HB3	1.73	0.69
1:A:49:MET:HE1	1:A:359:GLY:HA3	1.76	0.67
1:A:49:MET:HE3	1:A:383:TYR:CE1	2.31	0.64
1:C:37:LYS:NZ	1:C:268:GLU:OE1	2.25	0.62
1:B:303:CYS:SG	2:B:501:IMP:H2	2.40	0.62
1:A:49:MET:HA	1:A:386:MET:SD	2.41	0.61
1:D:321:ASP:OD2	5:D:504:MPD:H12	2.01	0.60
1:A:244:VAL:HG12	1:A:246:ASP:HB2	1.83	0.60
1:A:49:MET:HE2	1:A:52:VAL:HG21	1.84	0.59
1:D:303:CYS:SG	2:D:502:IMP:H2	2.42	0.59
1:A:272:ILE:HG12	1:A:292:CYS:HB3	1.84	0.58
1:A:49:MET:SD	2:A:500:IMP:H8	2.44	0.57
1:C:244:VAL:HG12	1:C:246:ASP:HB3	1.86	0.56
1:A:384:ARG:HB3	1:A:414[B]:GLU:HG3	1.86	0.56
1:A:303:CYS:SG	2:A:500:IMP:H2	2.46	0.56
1:A:79:GLN:NE2	1:A:231:ARG:HH11	2.04	0.56
1:A:298:GLY:HA2	1:A:303:CYS:SG	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:ARG:HD3	1:D:81:ARG:C	2.26	0.54
1:A:79:GLN:HE22	1:A:231:ARG:HD3	1.73	0.54
1:A:4:ILE:HD11	1:C:320:MET:HE1	1.90	0.53
1:C:302:ILE:HG22	1:D:471:ILE:HD13	1.90	0.53
1:A:59:ILE:HG13	1:A:86:VAL:HG22	1.90	0.53
1:B:384:ARG:HH12	1:B:394:LYS:HE2	1.73	0.52
1:D:275:ASN:HD21	1:D:294:LYS:NZ	2.07	0.52
1:D:244:VAL:HG12	1:D:246[A]:ASP:HB3	1.92	0.51
1:D:77[A]:GLU:HG3	1:D:78:ASP:N	2.25	0.51
1:C:375:TYR:CD2	1:C:376:GLN:HG3	2.45	0.51
1:A:474:THR:HG21	1:B:416:ARG:HD2	1.92	0.51
1:B:384:ARG:HH22	1:B:394:LYS:HG3	1.74	0.50
1:B:64:GLU:HG3	1:B:427:ILE:HD12	1.94	0.50
1:A:49:MET:CE	1:A:52:VAL:HG21	2.41	0.50
1:B:230:GLU:OE2	1:B:230:GLU:N	2.42	0.50
1:D:32:THR:HB	1:D:446:LEU:HD12	1.94	0.49
1:C:227:ASP:O	1:C:230:GLU:HG2	2.13	0.49
1:A:263:LYS:HE2	1:A:269:LEU:O	2.13	0.49
1:B:56:LYS:NZ	1:B:366:GLU:OE2	2.46	0.49
1:A:30:LEU:HD13	1:A:431:ILE:HD12	1.93	0.49
1:B:298:GLY:HA2	1:B:303:CYS:SG	2.52	0.49
6:C:501:FMT:H	1:D:460:SER:OG	2.13	0.48
1:A:283:ARG:O	1:A:287:GLU:HG2	2.13	0.48
1:A:15:LEU:HD13	1:B:306:ARG:HD3	1.95	0.48
1:C:346:VAL:HG22	1:C:434:ILE:HA	1.96	0.48
1:A:56:LYS:HE3	1:A:367:GLU:HA	1.95	0.47
1:C:256:ILE:O	1:C:260:LYS:HG3	2.14	0.47
1:D:3:ARG:HD3	1:D:4:ILE:H	1.79	0.47
1:D:50:ASP:HA	1:D:71:HIS:CD2	2.49	0.47
1:D:346:VAL:HG22	1:D:434:ILE:HA	1.97	0.47
1:C:249:HIS:HD2	8:C:643:HOH:O	1.98	0.47
1:B:272:ILE:HG12	1:B:292:CYS:HB3	1.97	0.46
1:B:364:GLY:N	1:B:417:ILE:HD11	2.30	0.46
1:B:474:THR:HG21	1:D:416:ARG:NE	2.30	0.46
1:A:31:LYS:HG2	1:A:41:ASN:HA	1.98	0.45
1:B:279:PRO:HB3	1:B:325:GLU:HB2	1.98	0.45
1:B:306:ARG:HG2	1:B:311:VAL:O	2.16	0.45
1:A:29:SER:HB3	1:A:445:THR:HG22	1.96	0.45
1:A:48:SER:HB3	1:A:69:ILE:HB	1.97	0.45
1:A:418:ALA:HB3	1:A:420[B]:LYS:HE3	1.99	0.45
1:B:244:VAL:HG12	1:B:246:ASP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HD12	1:B:314:PRO:HD3	1.99	0.45
1:C:302:ILE:CG2	1:D:471:ILE:HD13	2.47	0.45
1:C:323:ALA:O	1:C:327:LYS:HG2	2.16	0.44
5:D:504:MPD:H11	5:D:504:MPD:H52	2.00	0.44
1:A:76:ILE:HG23	1:A:231:ARG:HA	1.99	0.44
1:B:15:LEU:HD12	1:D:314:PRO:HD3	2.00	0.44
1:C:77[B]:GLU:H	1:C:77[B]:GLU:CD	2.21	0.44
1:C:298:GLY:HA2	1:C:303:CYS:SG	2.58	0.44
1:D:306:ARG:HG2	1:D:311:VAL:O	2.17	0.44
1:D:256:ILE:O	1:D:260:LYS:HG3	2.18	0.44
1:D:320:MET:HE3	1:D:320:MET:HB2	1.91	0.44
1:A:363:ALA:HB3	1:A:417:ILE:HD11	2.00	0.43
1:D:59:ILE:HD11	1:D:85:ARG:HG3	2.00	0.43
1:C:358[A]:MET:HB2	8:C:642:HOH:O	2.18	0.43
1:A:78:ASP:OD1	1:A:81:ARG:NH1	2.52	0.42
1:C:346:VAL:CG2	1:C:434:ILE:HA	2.48	0.42
1:B:243:ILE:HD11	1:B:262:ILE:HD13	2.00	0.42
1:C:59:ILE:O	1:C:63:ARG:HG3	2.18	0.42
1:D:298:GLY:HA3	1:D:306:ARG:HG3	2.01	0.42
1:C:306:ARG:HG2	1:C:311:VAL:O	2.20	0.42
1:C:75:THR:OG1	1:C:77[A]:GLU:HG2	2.19	0.42
1:D:33:GLN:HE22	1:D:39:GLN:HB2	1.84	0.42
1:A:279:PRO:HB3	1:A:325:GLU:HB2	2.01	0.42
1:D:294:LYS:NZ	1:D:336:ASP:OD2	2.53	0.42
1:C:363:ALA:HB3	1:C:417:ILE:HD11	2.01	0.42
1:A:20:LYS:HB2	1:B:251:HIS:CE1	2.55	0.41
1:A:301:SER:HB2	1:C:469:HIS:O	2.20	0.41
1:A:340:LYS:HE2	1:A:341:TYR:CZ	2.55	0.41
1:B:55:SER:OG	1:B:82:GLU:OE1	2.38	0.41
1:D:85:ARG:HE	1:D:89:SER:HG	1.68	0.41
1:B:364:GLY:CA	1:B:417:ILE:HD11	2.50	0.41
1:B:390:GLY:O	1:B:394:LYS:HG2	2.20	0.41
1:B:469:HIS:O	1:D:301:SER:HB2	2.20	0.41
1:A:50:ASP:HA	1:A:71:HIS:CD2	2.56	0.41
1:B:279:PRO:O	1:B:283:ARG:HG3	2.21	0.41
1:A:75:THR:OG1	1:A:77:GLU:HG2	2.21	0.40
1:B:56:LYS:HE3	1:B:367:GLU:HA	2.03	0.40
1:B:279:PRO:HD2	5:B:503:MPD:H53	2.01	0.40
1:D:42:ILE:HD12	1:D:44:LEU:HD12	2.03	0.40
1:B:25:PRO:O	1:B:28:VAL:HG22	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/363 (94%)	334 (98%)	8 (2%)	0	100	100
1	B	348/363 (96%)	340 (98%)	8 (2%)	0	100	100
1	C	346/363 (95%)	335 (97%)	11 (3%)	0	100	100
1	D	342/363 (94%)	335 (98%)	7 (2%)	0	100	100
All	All	1378/1452 (95%)	1344 (98%)	34 (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	268/282 (95%)	268 (100%)	0	100	100
1	B	273/282 (97%)	270 (99%)	3 (1%)	73	79
1	C	272/282 (96%)	266 (98%)	6 (2%)	52	57
1	D	268/282 (95%)	261 (97%)	7 (3%)	46	50
All	All	1081/1128 (96%)	1065 (98%)	16 (2%)	71	71

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	216	LEU
1	B	447[A]	GLU

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Mol	Chain	Res	Type
1	B	447[B]	GLU
1	C	85	ARG
1	C	389[A]	LEU
1	C	389[B]	LEU
1	C	408	PHE
1	C	464[A]	ARG
1	C	464[B]	ARG
1	D	3	ARG
1	D	81	ARG
1	D	85	ARG
1	D	221	SER
1	D	275	ASN
1	D	451	GLU
1	D	481	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	429	GLN
1	A	452	ASN
1	B	249	HIS
1	C	249	HIS
1	C	270	GLN
1	D	33	GLN
1	D	275	ASN
1	D	454	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 carbohydrates in this entry.



## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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$
3	8LA	B	502	-	35,35,35	1.46	6 (17%)	50,51,51	1.41	2 (4%)
3	8LA	D	503	-	35,35,35	1.44	6 (17%)	50,51,51	1.27	2 (4%)
3	8LA	C	503	-	35,35,35	1.38	5 (14%)	50,51,51	1.13	2 (4%)
2	IMP	A	500	-	21,25,25	1.31	3 (14%)	23,38,38	1.41	3 (13%)
7	SO4	C	504	-	4,4,4	0.14	0	6,6,6	0.08	0
5	MPD	B	503	-	7,7,7	0.30	0	9,10,10	0.43	0
5	MPD	D	504	-	7,7,7	0.35	0	9,10,10	0.43	0
2	IMP	D	502	-	21,25,25	1.29	3 (14%)	23,38,38	1.57	4 (17%)
2	IMP	B	501	-	21,25,25	1.31	3 (14%)	23,38,38	1.41	2 (8%)
3	8LA	A	501	-	35,35,35	1.46	5 (14%)	50,51,51	1.75	3 (6%)
6	FMT	C	501	-	0,2,2	0.00	-	0,1,1	0.00	-
2	IMP	C	502	-	21,25,25	1.21	2 (9%)	23,38,38	1.54	2 (8%)

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	8LA	B	502	-	-	5/24/41/41	0/3/3/3
3	8LA	D	503	-	-	4/24/41/41	0/3/3/3
3	8LA	C	503	-	-	4/24/41/41	0/3/3/3
2	IMP	A	500	-	-	0/6/26/26	0/3/3/3
5	MPD	B	503	-	-	2/5/5/5	-
5	MPD	D	504	-	-	1/5/5/5	-
2	IMP	D	502	-	-	0/6/26/26	0/3/3/3
2	IMP	B	501	-	-	0/6/26/26	0/3/3/3
3	8LA	A	501	-	-	7/24/41/41	0/3/3/3
2	IMP	C	502	-	-	0/6/26/26	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	8LA	C21-C20	5.71	1.49	1.39
3	D	503	8LA	C21-C20	5.59	1.49	1.39
3	C	503	8LA	C21-C20	5.30	1.48	1.39
3	B	502	8LA	C21-C20	5.10	1.48	1.39
2	B	501	IMP	C2-N3	4.13	1.38	1.32
2	D	502	IMP	C2-N3	4.08	1.38	1.32
2	A	500	IMP	C2-N3	3.90	1.38	1.32
2	C	502	IMP	C2-N3	3.56	1.37	1.32
3	B	502	8LA	C11-C1	-3.53	1.49	1.53
3	D	503	8LA	C20-CL	3.29	1.81	1.73
2	B	501	IMP	C6-N1	3.16	1.38	1.33
3	A	501	8LA	C11-C1	-3.14	1.49	1.53
2	C	502	IMP	C6-N1	3.01	1.38	1.33
3	B	502	8LA	C8-C7	-2.87	1.32	1.46
3	D	503	8LA	C8-C7	-2.82	1.32	1.46
2	A	500	IMP	C6-N1	2.77	1.37	1.33
3	A	501	8LA	C8-C7	-2.70	1.33	1.46
2	A	500	IMP	C2-N1	2.69	1.38	1.33
3	C	503	8LA	C8-C7	-2.68	1.33	1.46
3	A	501	8LA	C20-CL	2.68	1.80	1.73
2	D	502	IMP	C6-N1	2.65	1.37	1.33
3	B	502	8LA	C20-CL	2.56	1.79	1.73
3	D	503	8LA	C11-C1	-2.49	1.50	1.53
3	C	503	8LA	C11-C1	-2.48	1.50	1.53
3	C	503	8LA	C20-CL	2.46	1.79	1.73
2	D	502	IMP	C2-N1	2.35	1.38	1.33
3	C	503	8LA	C17-N4	-2.34	1.36	1.41
3	A	501	8LA	C17-N4	-2.31	1.37	1.41
3	B	502	8LA	C17-N4	-2.29	1.37	1.41
3	B	502	8LA	O1-C24	2.24	1.44	1.41
2	B	501	IMP	C2-N1	2.21	1.38	1.33
3	D	503	8LA	C17-N4	-2.07	1.37	1.41
3	D	503	8LA	O1-C24	2.03	1.44	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	8LA	O1-C21-C20	9.30	124.31	116.13
3	B	502	8LA	O1-C21-C20	6.79	122.11	116.13
3	D	503	8LA	O1-C21-C20	5.54	121.00	116.13
2	C	502	IMP	N3-C2-N1	-5.05	120.78	128.68
2	D	502	IMP	N3-C2-N1	-4.98	120.89	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	IMP	N3-C2-N1	-4.61	121.48	128.68
2	A	500	IMP	N3-C2-N1	-4.36	121.86	128.68
3	C	503	8LA	O1-C21-C20	4.06	119.70	116.13
3	A	501	8LA	C21-O1-C24	4.02	125.77	118.09
3	C	503	8LA	C21-O1-C24	3.62	125.00	118.09
3	B	502	8LA	C21-O1-C24	3.41	124.60	118.09
2	C	502	IMP	C2-N1-C6	3.21	121.26	115.88
3	D	503	8LA	C21-O1-C24	3.01	123.84	118.09
2	D	502	IMP	C1'-N9-C4	-2.94	121.47	126.64
2	D	502	IMP	C2-N1-C6	2.69	120.38	115.88
3	A	501	8LA	O1-C21-C22	-2.43	118.30	123.79
2	B	501	IMP	C4-C5-N7	-2.25	107.05	109.40
2	A	500	IMP	C1'-N9-C4	-2.19	122.79	126.64
2	D	502	IMP	C4-C5-N7	-2.16	107.15	109.40
2	A	500	IMP	C2-N1-C6	2.13	119.45	115.88

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	8LA	C20-C21-O1-C24
3	D	503	8LA	C20-C21-O1-C24
3	C	503	8LA	C20-C21-O1-C24
5	B	503	MPD	C2-C3-C4-O4
5	D	504	MPD	C2-C3-C4-O4
3	A	501	8LA	C20-C21-O1-C24
3	A	501	8LA	C26-C27-C29-O6
3	A	501	8LA	O3-C27-C29-O6
3	B	502	8LA	C22-C21-O1-C24
3	D	503	8LA	C22-C21-O1-C24
3	C	503	8LA	C22-C21-O1-C24
3	A	501	8LA	C22-C21-O1-C24
3	A	501	8LA	O3-C24-O1-C21
5	B	503	MPD	CM-C2-C3-C4
3	B	502	8LA	C4-C5-C7-C8
3	D	503	8LA	C4-C5-C7-C8
3	B	502	8LA	C6-C5-C7-C8
3	D	503	8LA	C6-C5-C7-C8
3	A	501	8LA	C4-C5-C7-C8
3	C	503	8LA	C4-C5-C7-C8
3	C	503	8LA	C6-C5-C7-C8
3	A	501	8LA	C6-C5-C7-C8

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Mol	Chain	Res	Type	Atoms
3	B	502	8LA	O3-C24-O1-C21

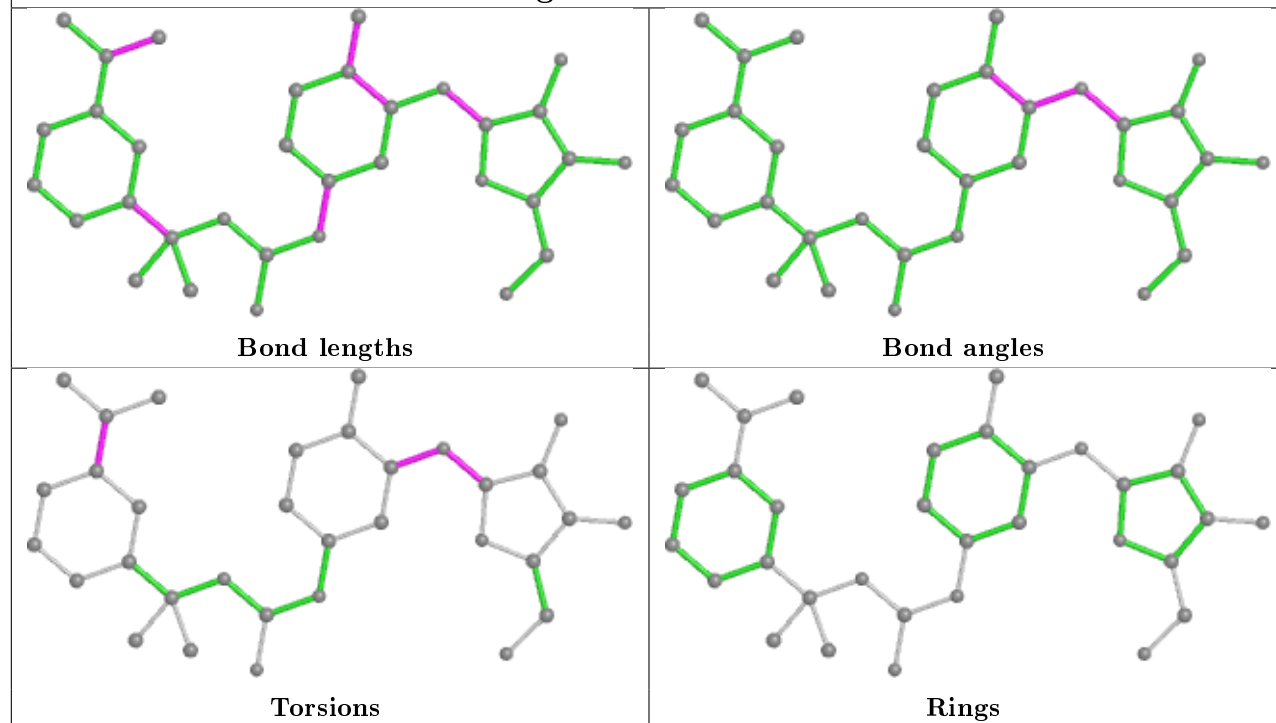
There are no ring outliers.

6 monomers are involved in 8 short contacts:

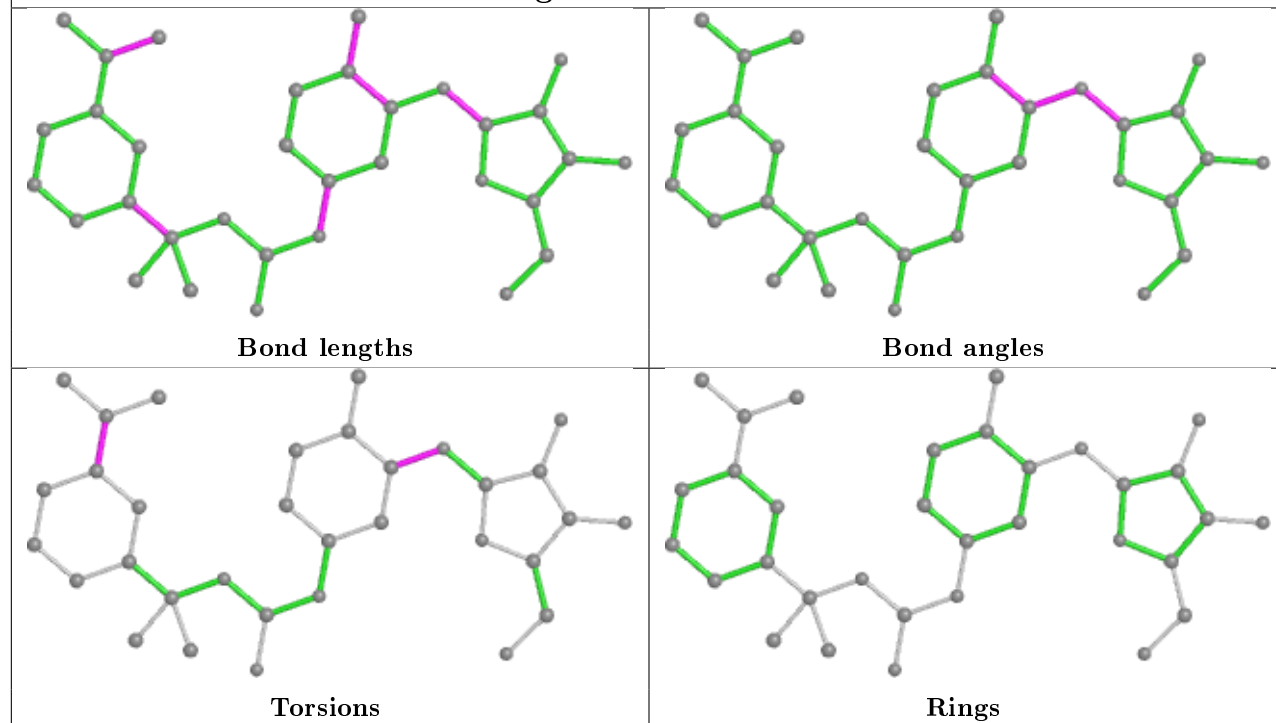
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	IMP	2	0
5	B	503	MPD	1	0
5	D	504	MPD	2	0
2	D	502	IMP	1	0
2	B	501	IMP	1	0
6	C	501	FMT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

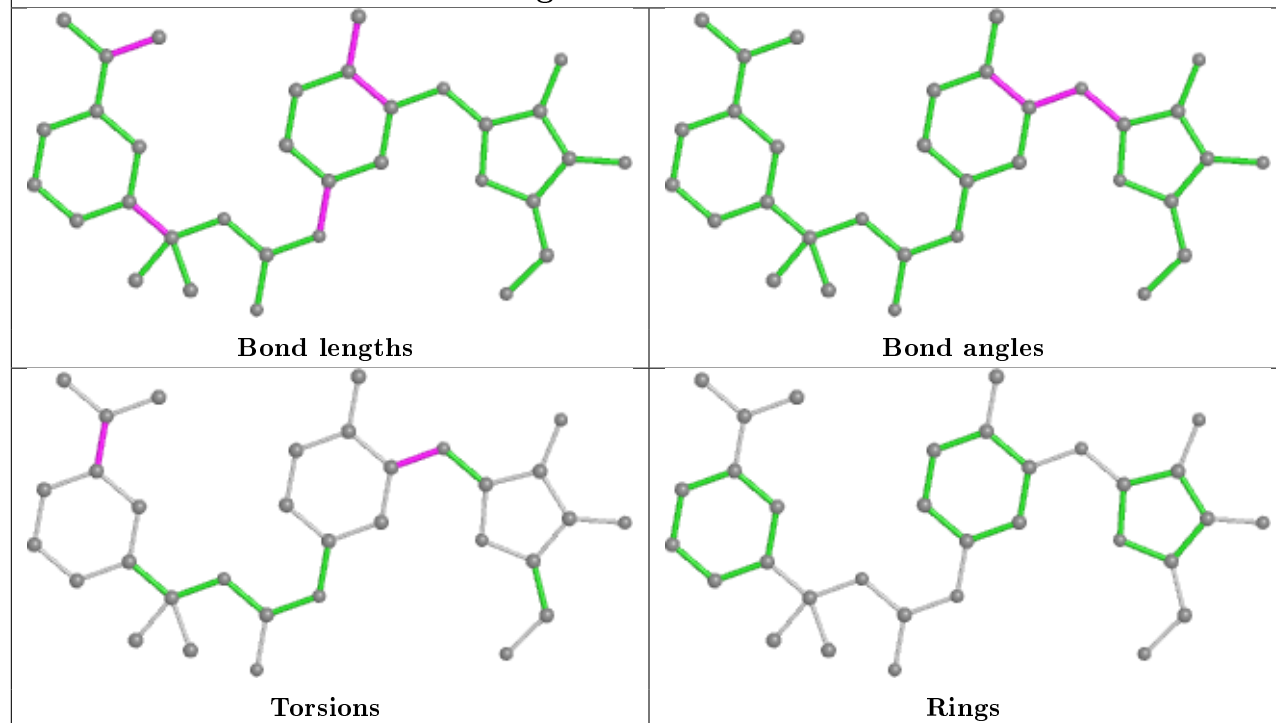
## Ligand 8LA B 502



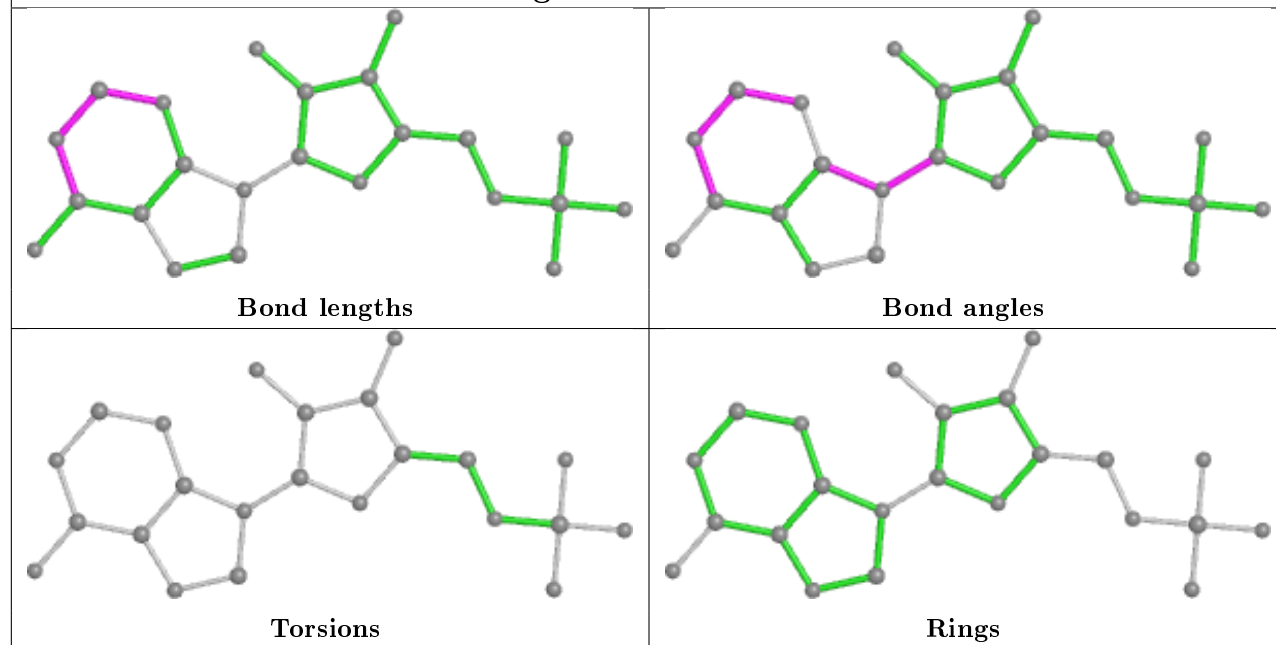
## Ligand 8LA D 503



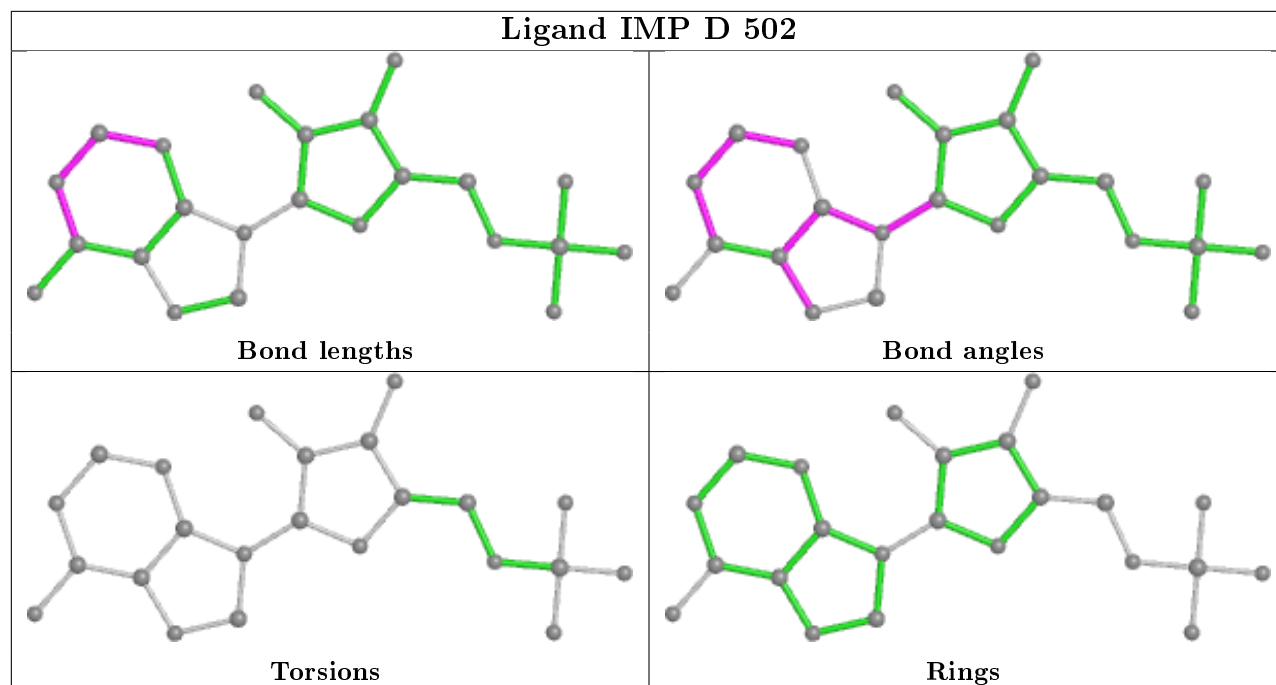
## Ligand 8LA C 503



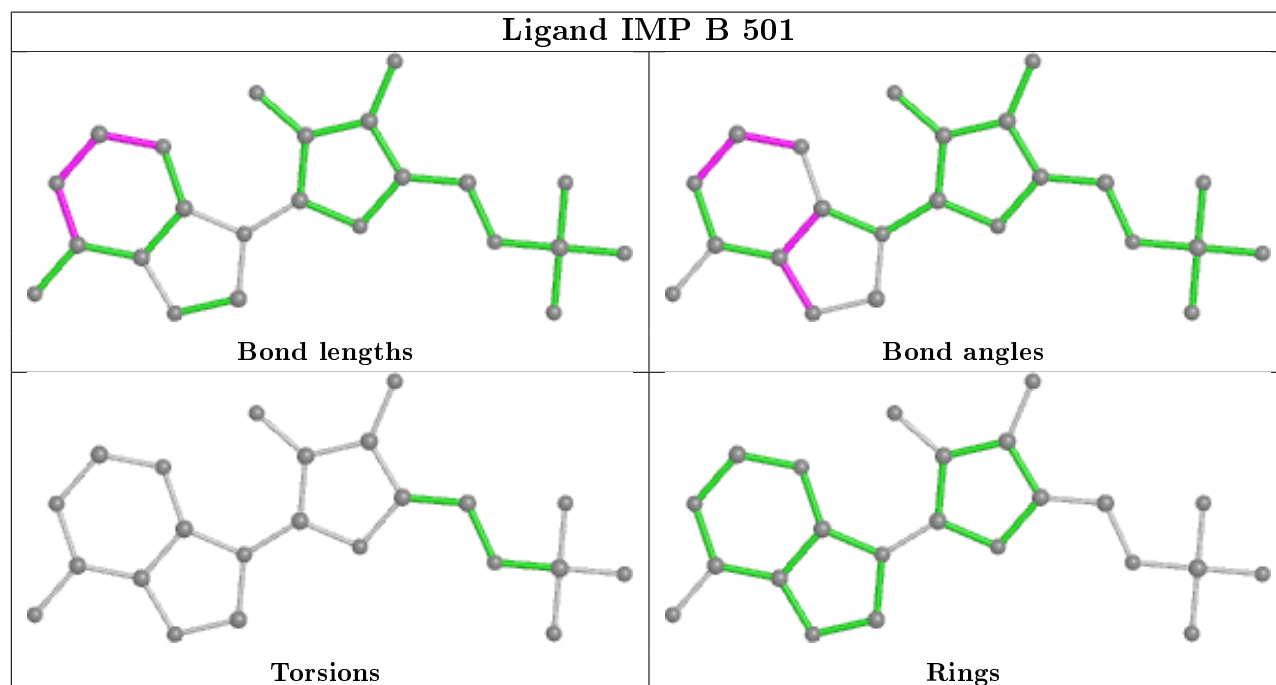
## Ligand IMP A 500

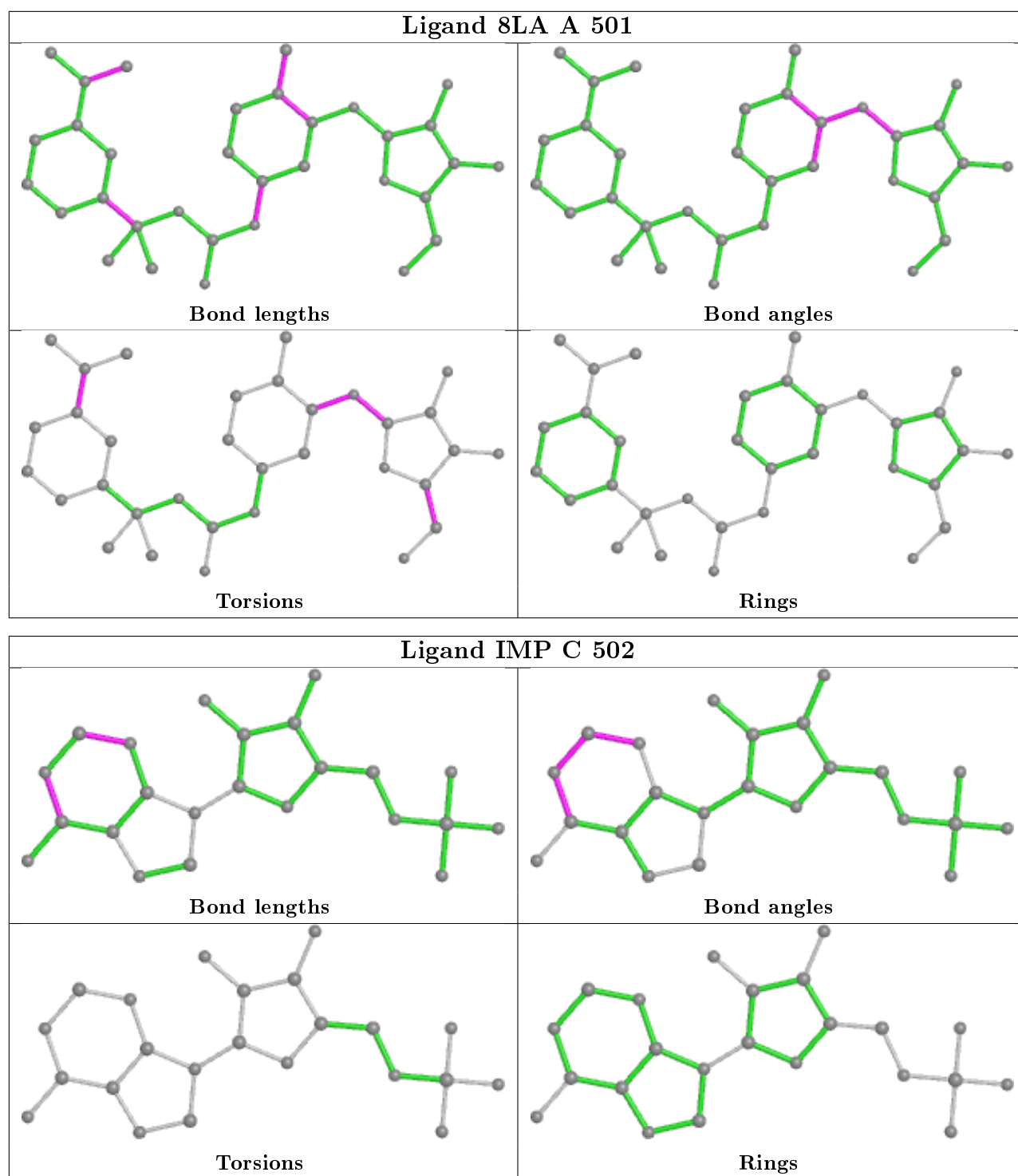


## Ligand IMP D 502



## Ligand IMP B 501





## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	343/363 (94%)	0.14	8 (2%) 60 65	24, 43, 65, 96	5 (1%)
1	B	346/363 (95%)	-0.14	3 (0%) 84 86	21, 38, 61, 80	3 (0%)
1	C	343/363 (94%)	-0.16	6 (1%) 70 74	25, 36, 56, 91	2 (0%)
1	D	342/363 (94%)	-0.14	4 (1%) 79 82	24, 38, 58, 75	4 (1%)
All	All	1374/1452 (94%)	-0.07	21 (1%) 73 77	21, 38, 62, 96	14 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	PHE	5.1
1	C	482	VAL	4.8
1	A	482	VAL	4.5
1	A	262	ILE	3.8
1	C	2	ALA	3.6
1	B	394	LYS	3.2
1	C	408	PHE	3.1
1	D	2	ALA	3.0
1	C	4	ILE	2.7
1	A	374	ILE	2.6
1	A	88	ARG	2.5
1	D	374	ILE	2.4
1	C	375	TYR	2.3
1	D	371	ALA	2.3
1	B	393	ALA	2.3
1	A	83	VAL	2.2
1	A	375	TYR	2.2
1	C	378	ARG	2.2
1	A	447	GLU	2.2
1	D	373	GLU	2.2
1	B	408	PHE	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

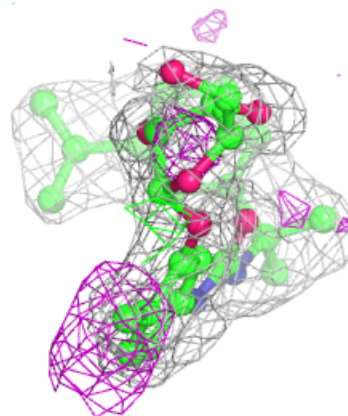
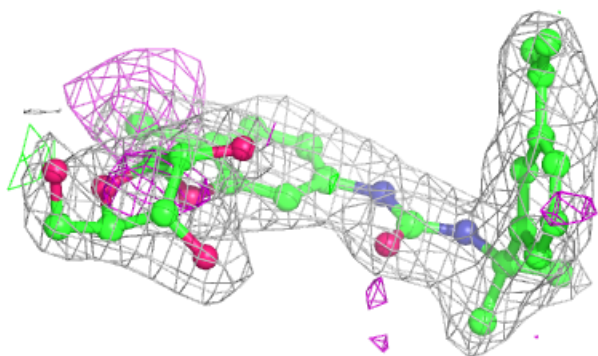
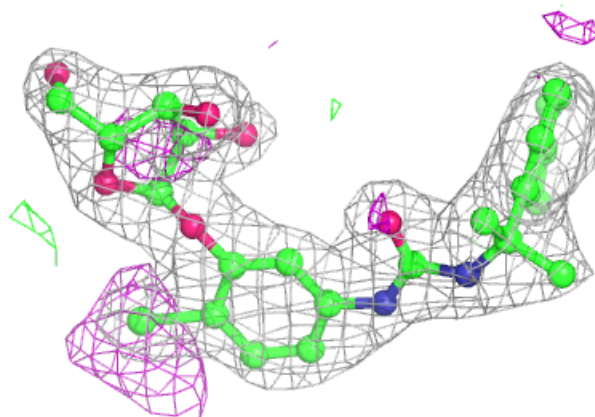
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MPD	D	504	8/8	0.86	0.23	51,55,60,62	0
3	8LA	C	503	33/33	0.87	0.17	33,38,43,47	0
3	8LA	A	501	33/33	0.88	0.15	39,46,53,61	0
7	SO4	C	504	5/5	0.90	0.31	88,88,88,89	5
5	MPD	B	503	8/8	0.91	0.18	51,55,57,58	0
4	K	A	502	1/1	0.94	0.11	78,78,78,78	0
3	8LA	D	503	33/33	0.95	0.10	29,38,42,43	0
3	8LA	B	502	33/33	0.96	0.09	29,37,44,54	0
4	K	B	504	1/1	0.96	0.08	67,67,67,67	0
2	IMP	D	502	23/23	0.98	0.10	24,27,31,32	0
2	IMP	B	501	23/23	0.98	0.11	26,30,33,38	0
2	IMP	A	500	23/23	0.98	0.10	30,33,38,39	0
6	FMT	C	501	3/3	0.98	0.36	44,44,46,47	0
2	IMP	C	502	23/23	0.98	0.12	23,29,33,35	0
4	K	D	501	1/1	0.99	0.07	54,54,54,54	0

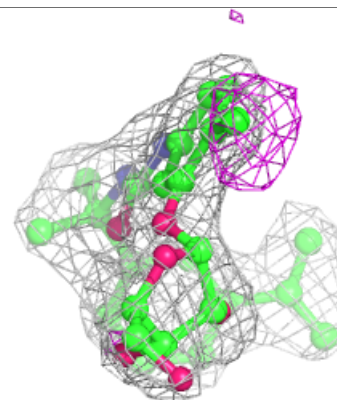
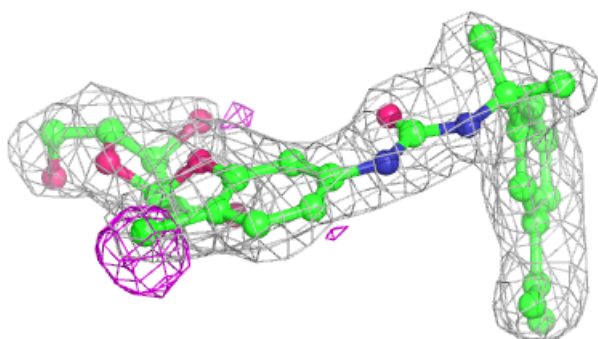
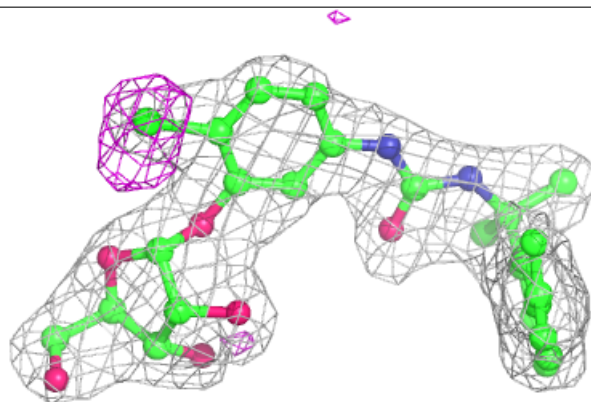
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 8LA C 503:**

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

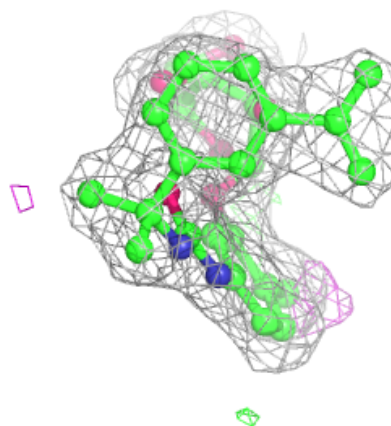
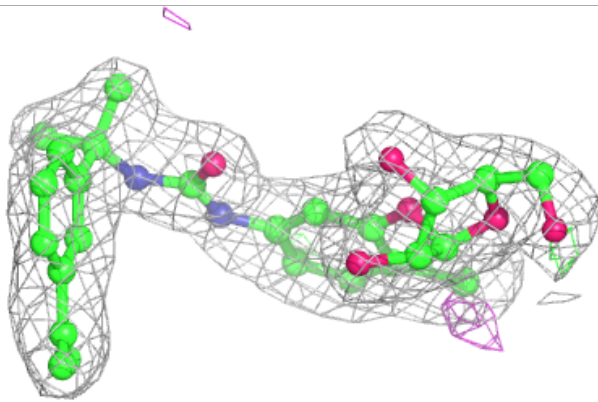
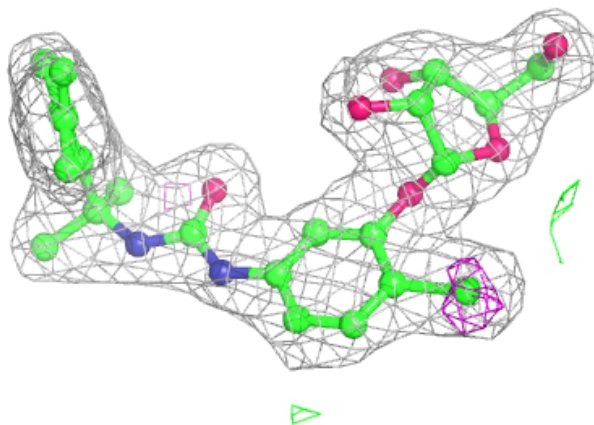
**Electron density around 8LA A 501:**

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



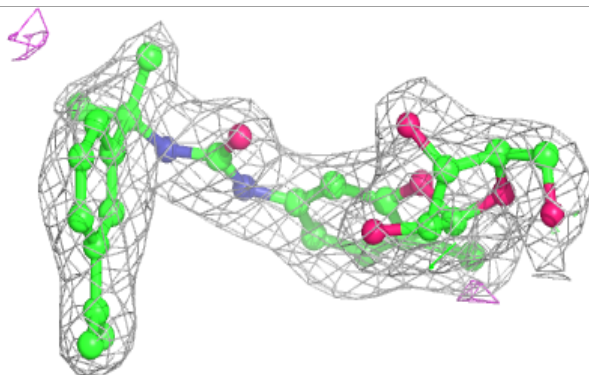
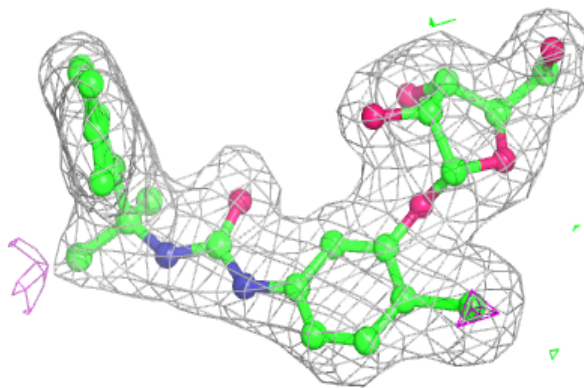
**Electron density around 8LA D 503:**

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

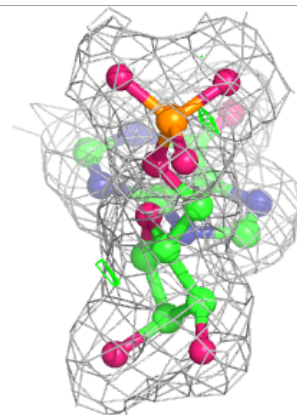
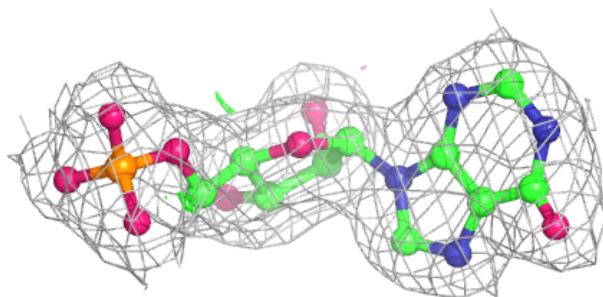
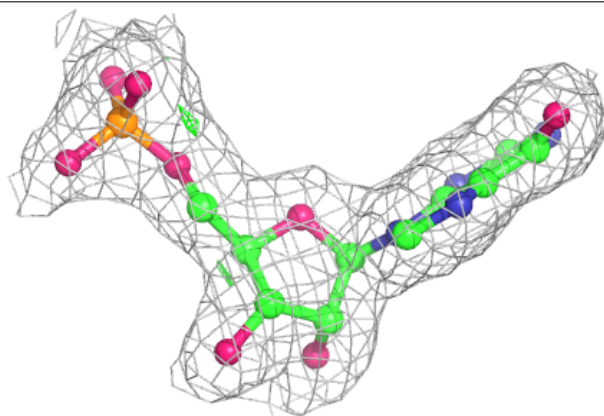


**Electron density around 8LA B 502:**

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

**Electron density around IMP D 502:**

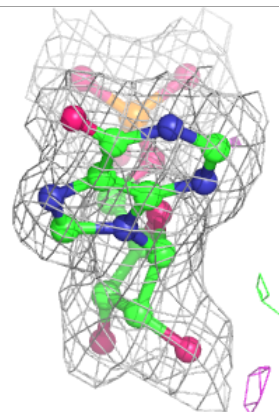
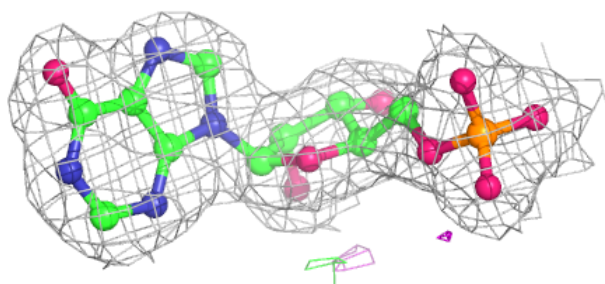
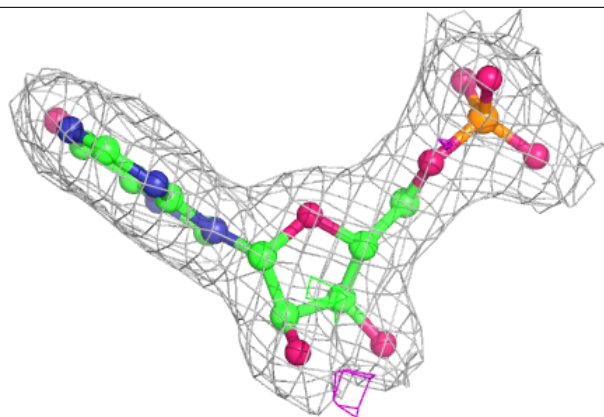
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



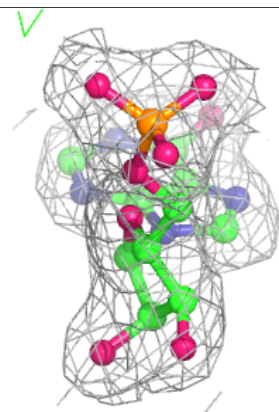
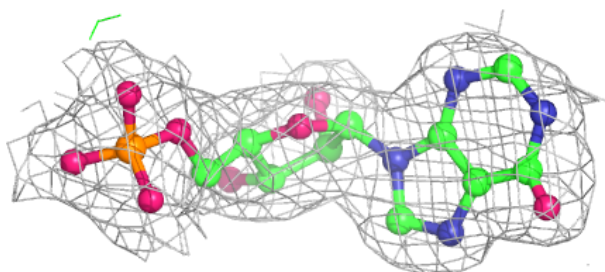
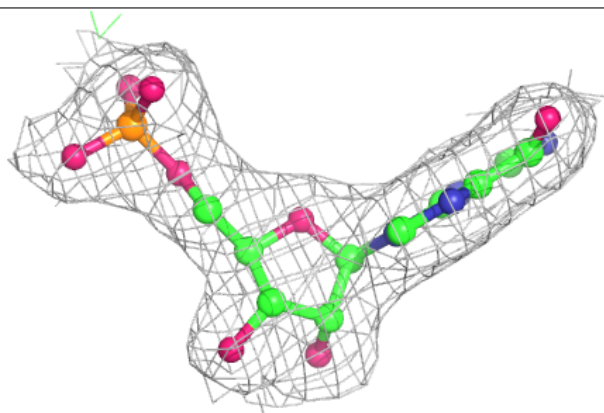


**Electron density around IMP B 501:**

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

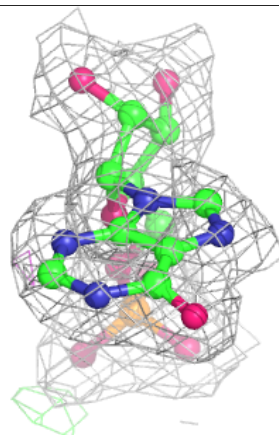
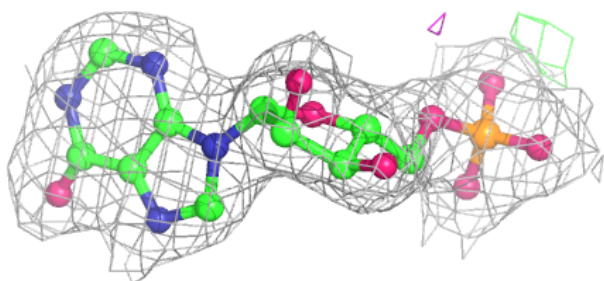
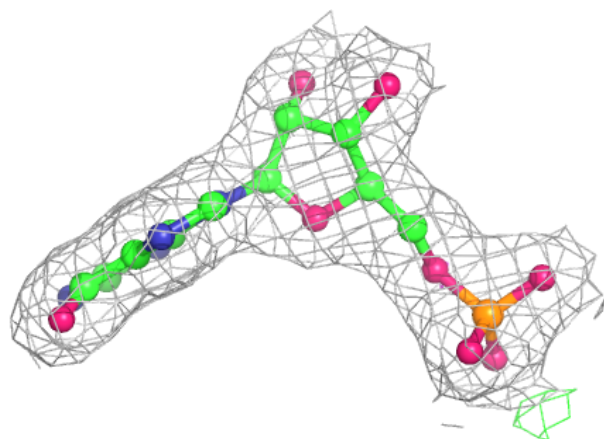
**Electron density around IMP A 500:**

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



**Electron density around IMP C 502:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.