



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:52 pm BST

PDB ID : 5UQF
Title : Crystal Structure of the Catalytic Domain of the Inosine Monophosphate Dehydrogenase from *Campylobacter jejuni* in the complex with IMP and the inhibitor P225
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 : 2017-02-08
Resolution : 2.73 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 ⓘ symbol.

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

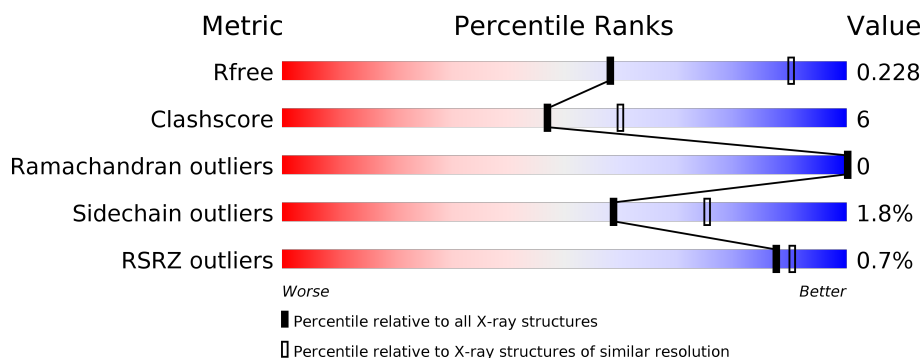
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 ≥ 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	406	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, orange 11%, yellow 13%, green 76%, grey 100%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; text-align: center;"> </div> </div> </div>
1	B	406	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, green 79%, yellow 88%, grey 100%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; text-align: center;"> </div> </div> </div>
1	C	406	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, green 72%, yellow 87%, grey 100%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; text-align: center;"> </div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	A	506	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8232 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	354	Total	C	N	O	S	0	0	0
			2630	1656	464	496	14			
1	B	355	Total	C	N	O	S	0	0	0
			2639	1662	466	497	14			
1	C	355	Total	C	N	O	S	0	1	0
			2649	1668	469	498	14			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
A	-22	HIS	-	expression tag	UNP A0A1B3XFT6
A	-21	HIS	-	expression tag	UNP A0A1B3XFT6
A	-20	HIS	-	expression tag	UNP A0A1B3XFT6
A	-19	HIS	-	expression tag	UNP A0A1B3XFT6
A	-18	HIS	-	expression tag	UNP A0A1B3XFT6
A	-17	HIS	-	expression tag	UNP A0A1B3XFT6
A	-16	SER	-	expression tag	UNP A0A1B3XFT6
A	-15	SER	-	expression tag	UNP A0A1B3XFT6
A	-14	GLY	-	expression tag	UNP A0A1B3XFT6
A	-13	VAL	-	expression tag	UNP A0A1B3XFT6
A	-12	ASP	-	expression tag	UNP A0A1B3XFT6
A	-11	LEU	-	expression tag	UNP A0A1B3XFT6
A	-10	GLY	-	expression tag	UNP A0A1B3XFT6
A	-9	THR	-	expression tag	UNP A0A1B3XFT6
A	-8	GLU	-	expression tag	UNP A0A1B3XFT6
A	-7	ASN	-	expression tag	UNP A0A1B3XFT6
A	-6	LEU	-	expression tag	UNP A0A1B3XFT6
A	-5	TYR	-	expression tag	UNP A0A1B3XFT6
A	-4	PHE	-	expression tag	UNP A0A1B3XFT6
A	-3	GLN	-	expression tag	UNP A0A1B3XFT6
A	-2	SER	-	expression tag	UNP A0A1B3XFT6
A	-1	ASN	-	expression tag	UNP A0A1B3XFT6

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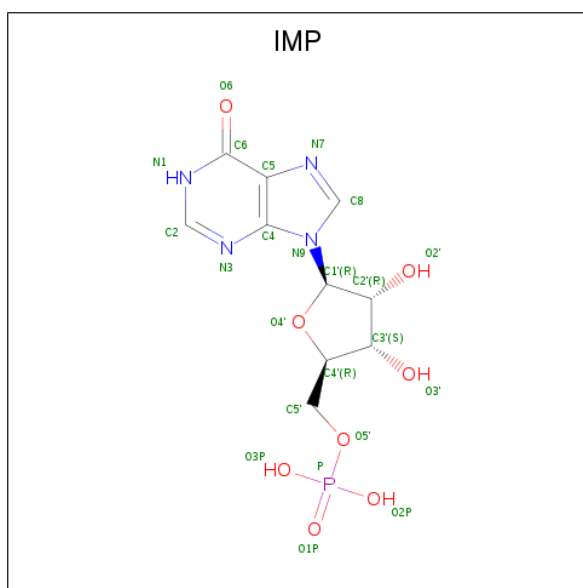
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP A0A1B3XFT6
A	195	GLY	-	linker	UNP A0A1B3XFT6
B	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
B	-22	HIS	-	expression tag	UNP A0A1B3XFT6
B	-21	HIS	-	expression tag	UNP A0A1B3XFT6
B	-20	HIS	-	expression tag	UNP A0A1B3XFT6
B	-19	HIS	-	expression tag	UNP A0A1B3XFT6
B	-18	HIS	-	expression tag	UNP A0A1B3XFT6
B	-17	HIS	-	expression tag	UNP A0A1B3XFT6
B	-16	SER	-	expression tag	UNP A0A1B3XFT6
B	-15	SER	-	expression tag	UNP A0A1B3XFT6
B	-14	GLY	-	expression tag	UNP A0A1B3XFT6
B	-13	VAL	-	expression tag	UNP A0A1B3XFT6
B	-12	ASP	-	expression tag	UNP A0A1B3XFT6
B	-11	LEU	-	expression tag	UNP A0A1B3XFT6
B	-10	GLY	-	expression tag	UNP A0A1B3XFT6
B	-9	THR	-	expression tag	UNP A0A1B3XFT6
B	-8	GLU	-	expression tag	UNP A0A1B3XFT6
B	-7	ASN	-	expression tag	UNP A0A1B3XFT6
B	-6	LEU	-	expression tag	UNP A0A1B3XFT6
B	-5	TYR	-	expression tag	UNP A0A1B3XFT6
B	-4	PHE	-	expression tag	UNP A0A1B3XFT6
B	-3	GLN	-	expression tag	UNP A0A1B3XFT6
B	-2	SER	-	expression tag	UNP A0A1B3XFT6
B	-1	ASN	-	expression tag	UNP A0A1B3XFT6
B	0	ALA	-	expression tag	UNP A0A1B3XFT6
B	195	GLY	-	linker	UNP A0A1B3XFT6
C	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
C	-22	HIS	-	expression tag	UNP A0A1B3XFT6
C	-21	HIS	-	expression tag	UNP A0A1B3XFT6
C	-20	HIS	-	expression tag	UNP A0A1B3XFT6
C	-19	HIS	-	expression tag	UNP A0A1B3XFT6
C	-18	HIS	-	expression tag	UNP A0A1B3XFT6
C	-17	HIS	-	expression tag	UNP A0A1B3XFT6
C	-16	SER	-	expression tag	UNP A0A1B3XFT6
C	-15	SER	-	expression tag	UNP A0A1B3XFT6
C	-14	GLY	-	expression tag	UNP A0A1B3XFT6
C	-13	VAL	-	expression tag	UNP A0A1B3XFT6
C	-12	ASP	-	expression tag	UNP A0A1B3XFT6
C	-11	LEU	-	expression tag	UNP A0A1B3XFT6
C	-10	GLY	-	expression tag	UNP A0A1B3XFT6
C	-9	THR	-	expression tag	UNP A0A1B3XFT6

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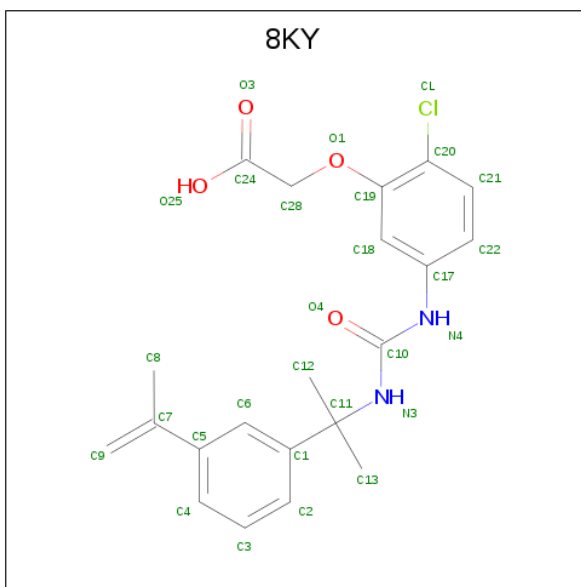
Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLU	-	expression tag	UNP A0A1B3XFT6
C	-7	ASN	-	expression tag	UNP A0A1B3XFT6
C	-6	LEU	-	expression tag	UNP A0A1B3XFT6
C	-5	TYR	-	expression tag	UNP A0A1B3XFT6
C	-4	PHE	-	expression tag	UNP A0A1B3XFT6
C	-3	GLN	-	expression tag	UNP A0A1B3XFT6
C	-2	SER	-	expression tag	UNP A0A1B3XFT6
C	-1	ASN	-	expression tag	UNP A0A1B3XFT6
C	0	ALA	-	expression tag	UNP A0A1B3XFT6
C	195	GLY	-	linker	UNP A0A1B3XFT6

- 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		

- Molecule 3 is {2-chloro-5-[(2-[3-(prop-1-en-2-yl)phenyl]propan-2-yl}carbamoyl)amino]phenoxy}acetic acid (three-letter code: 8KY) (formula: $C_{21}H_{23}ClN_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	
			28	21	1	2	4	0
3	B	1	Total	C	Cl	N	O	
			28	21	1	2	4	0
3	C	1	Total	C	Cl	N	O	
			28	21	1	2	4	0

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

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	2	Total	Cl	0	0
			2	2		

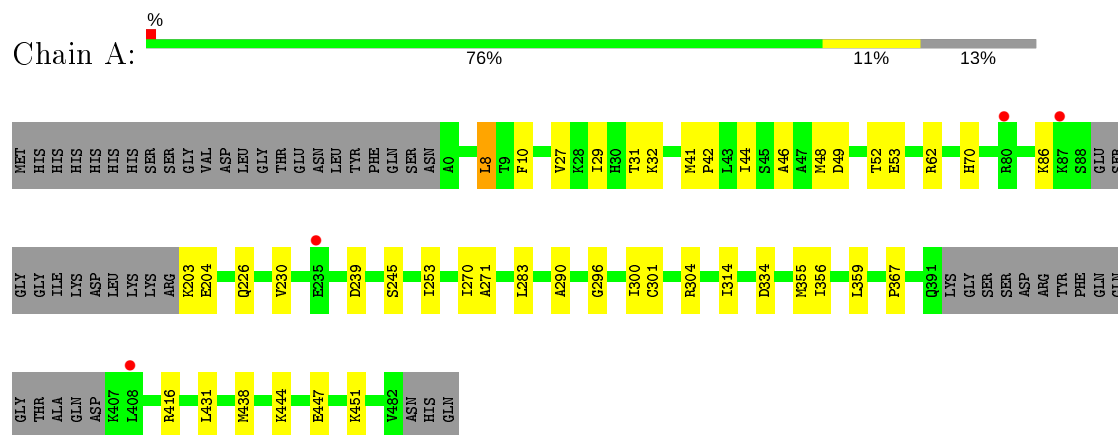
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	28	Total	O	0	0
			28	28		
9	B	27	Total	O	0	0
			27	27		
9	C	15	Total	O	0	0
			15	15		

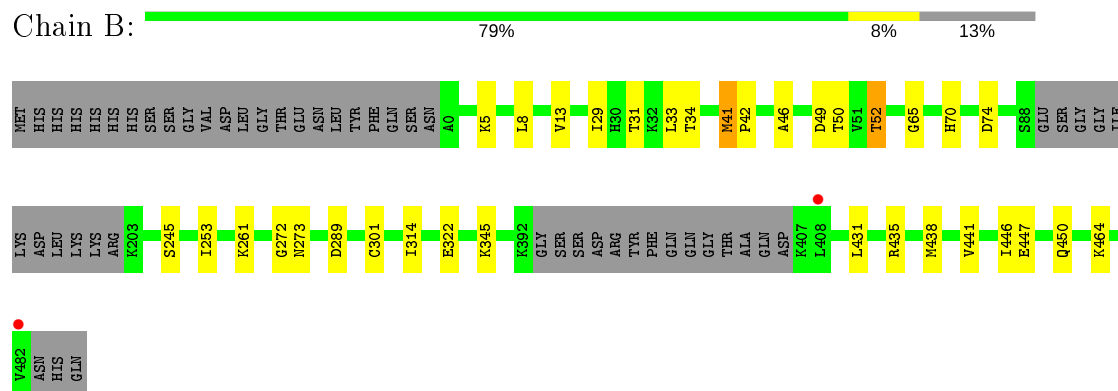
3 Residue-property plots [i](#)

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.

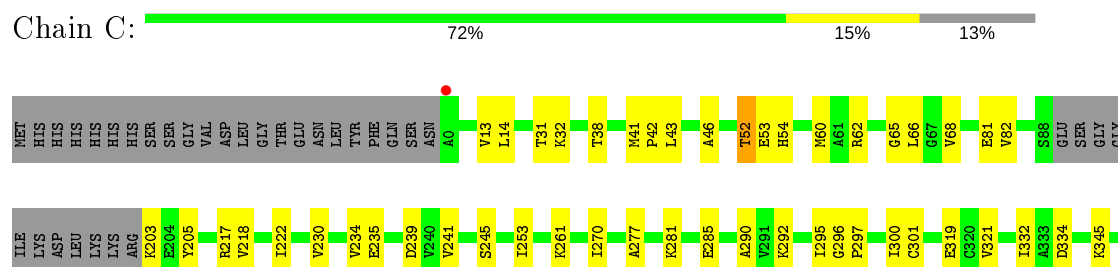
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

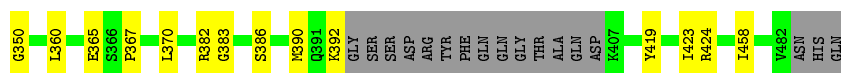


- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.53 Å 118.53 Å 451.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.55 – 2.73 46.55 – 2.72	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.55-2.73) 98.9 (46.55-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.73 Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.175 , 0.228 0.174 , 0.228	Depositor DCC
R_{free} test set	2092 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8232	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, CL, K, EDO, IMP, 8KY, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/2664	0.60	0/3591
1	B	0.41	0/2673	0.61	0/3602
1	C	0.42	0/2684	0.62	0/3617
All	All	0.42	0/8021	0.61	0/10810

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	2630	0	2722	40	0
1	B	2639	0	2735	22	0
1	C	2649	0	2741	40	0
2	A	23	0	11	6	0
2	B	23	0	11	1	0
2	C	23	0	11	2	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
3	C	28	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	15	0	0	0	0
5	B	25	0	0	0	0
5	C	10	0	0	0	0
6	A	16	0	24	2	0
6	B	8	0	12	1	0
7	B	6	0	8	0	0
7	C	6	0	8	0	0
8	C	2	0	0	0	0
9	A	28	0	0	0	0
9	B	27	0	0	2	0
9	C	15	0	0	0	0
All	All	8232	0	8283	102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:SER:HB2	1:C:253:ILE:HD11	1.65	0.78
1:C:301:CYS:SG	2:C:501:IMP:H2	2.29	0.72
1:A:53:GLU:HG3	1:A:367:PRO:CG	2.24	0.68
1:C:41:MET:HE2	1:C:65:GLY:HA3	1.77	0.67
1:B:41:MET:SD	1:B:431:LEU:HD11	2.34	0.67
1:A:46:ALA:CB	1:A:48:MET:HE2	2.27	0.64
1:C:270:ILE:HG12	1:C:290:ALA:HB3	1.79	0.64
1:A:62:ARG:HH22	6:A:508:EDO:H21	1.61	0.64
1:B:41:MET:HG3	1:B:431:LEU:HD21	1.80	0.63
1:B:435:ARG:NH2	9:B:601:HOH:O	2.31	0.63
1:B:245:SER:HB2	1:B:253:ILE:HD11	1.80	0.63
1:A:86:LYS:NZ	1:A:239:ASP:OD1	2.31	0.63
1:A:245:SER:HB2	1:A:253:ILE:HD11	1.81	0.62
1:A:53:GLU:HG3	1:A:367:PRO:HG3	1.81	0.62
1:B:446:ILE:O	1:B:450:GLN:HG3	1.99	0.62
1:C:32:LYS:HD2	1:C:38:THR:HG22	1.84	0.60
1:A:32:LYS:HB2	1:A:32:LYS:NZ	2.17	0.60
1:A:301:CYS:SG	2:A:500:IMP:H2	2.42	0.59
1:A:334:ASP:OD2	2:A:500:IMP:O3'	2.19	0.59
1:A:41:MET:SD	1:A:431:LEU:HD11	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ALA:HB3	1:A:48:MET:HE2	1.84	0.59
1:C:222:ILE:HG12	1:C:241:VAL:HG13	1.84	0.59
1:A:270:ILE:HG12	1:A:290:ALA:HB3	1.85	0.59
1:C:382:ARG:HH22	1:C:392:LYS:HE3	1.68	0.58
1:C:41:MET:HE2	1:C:65:GLY:CA	2.33	0.58
1:C:13:VAL:O	1:C:345:LYS:HE2	2.04	0.57
1:A:334:ASP:OD1	2:A:500:IMP:O2'	2.23	0.57
1:B:49:ASP:HA	1:B:70:HIS:CD2	2.40	0.57
1:C:46:ALA:O	1:C:52:THR:HG23	2.05	0.56
1:A:204:GLU:OE1	1:A:204:GLU:N	2.39	0.56
1:A:32:LYS:HB2	1:A:32:LYS:HZ3	1.69	0.55
1:A:53:GLU:HG3	1:A:367:PRO:HG2	1.88	0.55
1:C:52:THR:OG1	1:C:68:VAL:O	2.25	0.55
1:A:49:ASP:HA	1:A:70:HIS:CD2	2.42	0.54
1:B:301:CYS:SG	2:B:500:IMP:H2	2.48	0.54
1:A:296:GLY:HA3	1:A:304:ARG:HG3	1.90	0.53
1:C:41:MET:CE	1:C:65:GLY:HA3	2.37	0.53
1:C:301:CYS:SG	2:C:501:IMP:C2	2.96	0.53
1:A:10:PHE:HA	1:A:314:ILE:HG13	1.92	0.51
1:A:8:LEU:O	1:A:314:ILE:HB	2.10	0.51
1:B:13:VAL:O	1:B:345:LYS:NZ	2.43	0.51
1:B:8:LEU:O	1:B:314:ILE:HG22	2.11	0.51
1:C:53:GLU:HG3	1:C:367:PRO:HG3	1.91	0.51
1:C:300:ILE:HD13	1:C:383:GLY:CA	2.41	0.51
1:C:31:THR:HG21	1:C:42:PRO:HB3	1.94	0.50
1:A:32:LYS:NZ	1:A:32:LYS:CB	2.73	0.50
1:C:54:HIS:ND1	1:C:81:GLU:OE1	2.44	0.50
1:A:48:MET:HE1	2:A:500:IMP:H5'2	1.93	0.49
1:A:300:ILE:C	1:A:300:ILE:HD12	2.33	0.49
1:C:370:LEU:HD21	1:C:419:TYR:CD1	2.49	0.48
1:C:230:VAL:O	1:C:234:VAL:HG23	2.14	0.48
1:C:296:GLY:N	1:C:297:PRO:HD3	2.29	0.48
1:B:74:ASP:OD1	1:B:74:ASP:N	2.47	0.47
1:C:300:ILE:HD12	1:C:300:ILE:C	2.34	0.47
1:B:33:LEU:HG	1:B:34:THR:HG23	1.97	0.47
1:A:203:LYS:HB3	1:A:204:GLU:H	1.50	0.47
1:B:447:GLU:CD	1:B:447:GLU:H	2.18	0.47
1:C:281:LYS:O	1:C:285:GLU:HG3	2.16	0.46
1:C:292:LYS:HE3	1:C:334:ASP:OD2	2.15	0.46
1:C:292:LYS:HG3	1:C:332:ILE:HB	1.98	0.45
1:B:29:ILE:HG12	9:B:601:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ALA:O	1:B:52:THR:OG1	2.25	0.45
1:A:226:GLN:O	1:A:230:VAL:HG23	2.17	0.44
1:C:296:GLY:HA2	1:C:301:CYS:SG	2.57	0.44
1:A:53:GLU:CG	1:A:367:PRO:HG3	2.47	0.44
1:C:277:ALA:HB2	1:C:319:GLU:HG2	1.98	0.44
1:A:29:ILE:HG22	1:A:438:MET:HE1	2.00	0.43
1:A:48:MET:SD	2:A:500:IMP:H8	2.58	0.43
1:A:44:ILE:O	1:A:355:MET:HA	2.18	0.43
1:A:301:CYS:SG	2:A:500:IMP:C2	3.07	0.43
1:B:34:THR:HB	1:B:289:ASP:HB3	1.99	0.43
1:B:31:THR:HG21	1:B:42:PRO:HB3	2.00	0.43
1:B:41:MET:CE	1:B:65:GLY:HA3	2.49	0.43
1:A:31:THR:HG21	1:A:42:PRO:HB3	2.01	0.43
1:C:386:SER:O	1:C:390:MET:HG3	2.18	0.43
1:C:217:ARG:HD3	1:C:239:ASP:CG	2.39	0.42
1:A:447:GLU:O	1:A:451:LYS:HG3	2.18	0.42
1:C:321:VAL:HG11	1:C:350:GLY:HA3	2.00	0.42
1:A:27:VAL:HG21	1:A:438:MET:HE3	2.02	0.42
1:C:360:LEU:HD22	1:C:423:ILE:CD1	2.49	0.42
1:C:365:GLU:OE1	1:C:365:GLU:N	2.46	0.42
1:A:253:ILE:HA	1:A:253:ILE:HD13	1.92	0.42
1:C:222:ILE:HG12	1:C:241:VAL:CG1	2.49	0.42
1:C:60:MET:CE	1:C:423:ILE:HD12	2.50	0.42
1:B:41:MET:HE2	1:B:65:GLY:HA3	2.00	0.42
1:C:62:ARG:HD3	1:C:205:TYR:CE2	2.55	0.42
1:C:14:LEU:HD12	1:C:458:ILE:HG21	2.02	0.42
1:A:416:ARG:NH2	6:A:509:EDO:O1	2.45	0.42
1:C:295:ILE:C	1:C:297:PRO:HD3	2.41	0.42
1:B:41:MET:HE2	1:B:65:GLY:CA	2.50	0.41
1:B:261:LYS:HA	1:B:261:LYS:HD2	1.81	0.41
1:A:300:ILE:C	1:A:300:ILE:CD1	2.88	0.41
1:C:41:MET:HG2	1:C:43:LEU:H	1.85	0.41
1:C:261:LYS:HD2	1:C:261:LYS:HA	1.90	0.41
1:A:271:ALA:HB3	1:A:283:LEU:HD13	2.03	0.41
1:C:82:VAL:HG13	1:C:218:VAL:HG11	2.03	0.41
1:A:356:ILE:CG2	1:A:359:LEU:HB2	2.50	0.41
1:C:300:ILE:HD13	1:C:383:GLY:HA2	2.01	0.41
1:A:356:ILE:HG21	1:A:359:LEU:HB2	2.02	0.40
1:B:272:GLY:HA3	1:B:273:ASN:HA	1.97	0.40
1:B:441:VAL:HG13	6:B:509:EDO:H12	2.02	0.40
1:A:46:ALA:HB1	1:A:48:MET:HE2	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	348/406 (86%)	342 (98%)	6 (2%)	0	100	100
1	B	349/406 (86%)	342 (98%)	7 (2%)	0	100	100
1	C	350/406 (86%)	344 (98%)	6 (2%)	0	100	100
All	All	1047/1218 (86%)	1028 (98%)	19 (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	278/323 (86%)	275 (99%)	3 (1%)	73	84
1	B	279/323 (86%)	272 (98%)	7 (2%)	47	67
1	C	280/323 (87%)	275 (98%)	5 (2%)	59	75
All	All	837/969 (86%)	822 (98%)	15 (2%)	59	75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	52	THR

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Mol	Chain	Res	Type
1	A	444	LYS
1	B	5	LYS
1	B	41	MET
1	B	50	THR
1	B	52	THR
1	B	322	GLU
1	B	438	MET
1	B	464	LYS
1	C	52	THR
1	C	66	LEU
1	C	203	LYS
1	C	235	GLU
1	C	424	ARG

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

Mol	Chain	Res	Type
1	B	72	ASN
1	B	391	GLN
1	C	70	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 5 are monoatomic - leaving 24 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	$\# Z > 2$
5	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.12	0
6	EDO	A	509	-	3,3,3	0.38	0	2,2,2	0.65	0
3	8KY	C	502	-	26,29,29	1.14	4 (15%)	37,41,41	1.24	4 (10%)
6	EDO	A	506	-	3,3,3	0.56	0	2,2,2	0.32	0
5	SO4	A	505	-	4,4,4	0.13	0	6,6,6	0.08	0
6	EDO	A	508	-	3,3,3	0.50	0	2,2,2	0.32	0
2	IMP	B	500	-	21,25,25	0.93	0	23,38,38	1.55	5 (21%)
2	IMP	A	500	-	21,25,25	0.89	0	23,38,38	1.64	5 (21%)
7	GOL	C	506	-	5,5,5	0.42	0	5,5,5	0.70	0
7	GOL	B	508	-	5,5,5	0.35	0	5,5,5	0.36	0
5	SO4	A	504	-	4,4,4	0.15	0	6,6,6	0.09	0
5	SO4	B	504	-	4,4,4	0.11	0	6,6,6	0.44	0
6	EDO	B	509	-	3,3,3	0.51	0	2,2,2	0.24	0
5	SO4	B	507	-	4,4,4	0.14	0	6,6,6	0.11	0
3	8KY	A	501	-	26,29,29	1.18	3 (11%)	37,41,41	1.30	7 (18%)
6	EDO	B	510	-	3,3,3	0.58	0	2,2,2	0.24	0
5	SO4	B	506	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	C	505	-	4,4,4	0.17	0	6,6,6	0.16	0
5	SO4	B	505	-	4,4,4	0.15	0	6,6,6	0.24	0
6	EDO	A	507	-	3,3,3	0.50	0	2,2,2	0.32	0
3	8KY	B	501	-	26,29,29	1.43	5 (19%)	37,41,41	0.83	1 (2%)
5	SO4	A	503	-	4,4,4	0.15	0	6,6,6	0.12	0
5	SO4	C	504	-	4,4,4	0.13	0	6,6,6	0.11	0
2	IMP	C	501	-	21,25,25	0.91	0	23,38,38	1.54	5 (21%)

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	B	500	-	-	0/6/26/26	0/3/3/3
6	EDO	B	509	-	-	0/1/1/1	-
6	EDO	A	509	-	-	0/1/1/1	-
3	8KY	B	501	-	-	6/22/24/24	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	8KY	A	501	-	-	5/22/24/24	0/2/2/2
6	EDO	B	510	-	-	0/1/1/1	-
7	GOL	C	506	-	-	4/4/4/4	-
7	GOL	B	508	-	-	3/4/4/4	-
2	IMP	A	500	-	-	0/6/26/26	0/3/3/3
3	8KY	C	502	-	-	6/22/24/24	0/2/2/2
6	EDO	A	507	-	-	1/1/1/1	-
6	EDO	A	506	-	-	0/1/1/1	-
6	EDO	A	508	-	-	0/1/1/1	-
2	IMP	C	501	-	-	5/6/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	8KY	C17-N4	-3.24	1.35	1.41
3	B	501	8KY	C8-C7	-2.97	1.31	1.46
3	A	501	8KY	C20-CL	2.96	1.80	1.73
3	B	501	8KY	C11-C1	-2.89	1.50	1.53
3	C	502	8KY	C8-C7	-2.73	1.33	1.46
3	A	501	8KY	C8-C7	-2.69	1.33	1.46
3	B	501	8KY	C11-N3	-2.69	1.44	1.47
3	C	502	8KY	C20-CL	2.58	1.79	1.73
3	C	502	8KY	C17-N4	-2.47	1.36	1.41
3	C	502	8KY	C11-C1	-2.43	1.50	1.53
3	A	501	8KY	C17-N4	-2.40	1.36	1.41
3	B	501	8KY	C20-CL	2.07	1.78	1.73

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	IMP	N3-C2-N1	-4.93	120.98	128.68
2	B	500	IMP	N3-C2-N1	-4.70	121.34	128.68
2	C	501	IMP	N3-C2-N1	-4.66	121.40	128.68
2	A	500	IMP	C3'-C2'-C1'	3.08	105.61	100.98
3	C	502	8KY	O1-C19-C20	3.00	120.10	116.40
2	A	500	IMP	C2-N1-C6	2.87	120.69	115.88
3	B	501	8KY	O1-C19-C20	2.84	119.90	116.40
2	C	501	IMP	C3'-C2'-C1'	2.83	105.24	100.98
2	B	500	IMP	C2-N1-C6	2.81	120.58	115.88
2	B	500	IMP	C3'-C2'-C1'	2.80	105.20	100.98
3	C	502	8KY	C12-C11-N3	2.80	115.40	107.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	IMP	C2-N1-C6	2.79	120.55	115.88
3	C	502	8KY	C11-N3-C10	2.45	129.36	124.17
3	A	501	8KY	C21-C20-CL	2.42	123.25	118.41
3	A	501	8KY	C12-C11-N3	2.33	114.15	107.89
3	A	501	8KY	O1-C19-C20	2.32	119.27	116.40
2	A	500	IMP	C6-C5-C4	-2.32	118.58	120.80
3	A	501	8KY	C12-C11-C13	-2.30	106.79	109.55
2	A	500	IMP	C4-C5-N7	-2.28	107.02	109.40
3	A	501	8KY	O4-C10-N3	-2.17	119.89	123.84
2	C	501	IMP	C4-C5-N7	-2.08	107.23	109.40
2	B	500	IMP	C6-C5-C4	-2.06	118.83	120.80
3	A	501	8KY	C1-C11-N3	-2.04	107.84	110.82
2	B	500	IMP	C4-C5-N7	-2.03	107.28	109.40
3	A	501	8KY	C19-C20-CL	-2.03	117.05	119.43
2	C	501	IMP	C6-C5-C4	-2.02	118.87	120.80
3	C	502	8KY	C21-C20-CL	2.02	122.45	118.41

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502	8KY	C20-C19-O1-C28
7	C	506	GOL	O1-C1-C2-C3
2	C	501	IMP	C5'-O5'-P-O2P
2	C	501	IMP	C5'-O5'-P-O3P
2	C	501	IMP	C3'-C4'-C5'-O5'
3	A	501	8KY	C20-C19-O1-C28
3	B	501	8KY	C20-C19-O1-C28
7	C	506	GOL	C1-C2-C3-O3
3	B	501	8KY	C24-C28-O1-C19
2	C	501	IMP	O4'-C4'-C5'-O5'
2	C	501	IMP	C5'-O5'-P-O1P
7	B	508	GOL	O1-C1-C2-O2
7	C	506	GOL	O1-C1-C2-O2
3	B	501	8KY	C18-C19-O1-C28
3	A	501	8KY	C18-C19-O1-C28
3	B	501	8KY	C4-C5-C7-C8
3	C	502	8KY	C18-C19-O1-C28
3	B	501	8KY	C12-C11-N3-C10
3	C	502	8KY	C4-C5-C7-C8
3	A	501	8KY	C4-C5-C7-C8
3	B	501	8KY	C6-C5-C7-C8

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Mol	Chain	Res	Type	Atoms
7	B	508	GOL	O1-C1-C2-C3
3	A	501	8KY	C6-C5-C7-C8
6	A	507	EDO	O1-C1-C2-O2
3	C	502	8KY	C6-C5-C7-C8
7	C	506	GOL	O2-C2-C3-O3
7	B	508	GOL	O2-C2-C3-O3
3	A	501	8KY	C24-C28-O1-C19
3	C	502	8KY	C4-C5-C7-C9
3	C	502	8KY	C6-C5-C7-C9

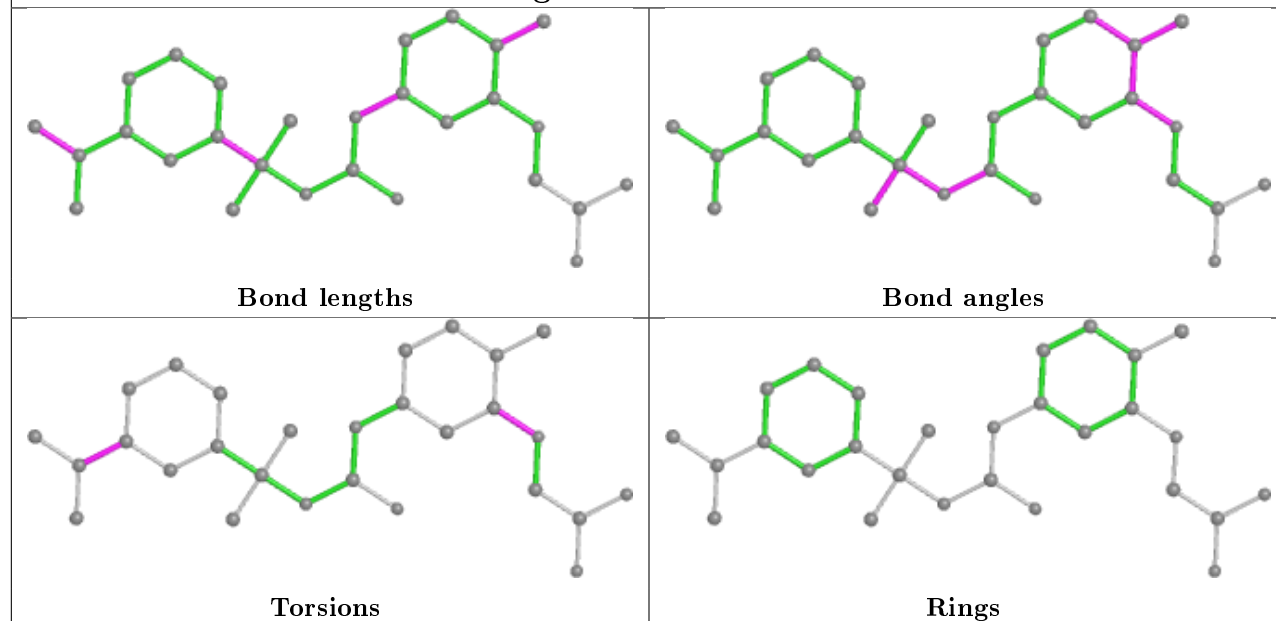
There are no ring outliers.

6 monomers are involved in 12 short contacts:

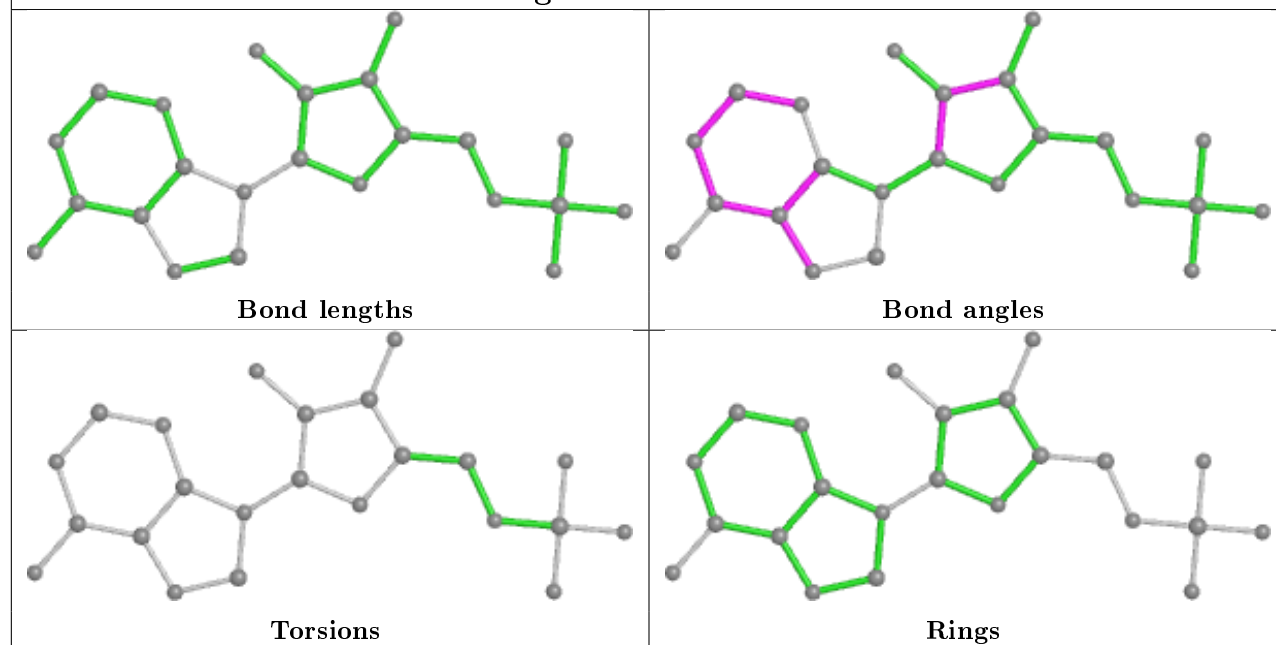
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	509	EDO	1	0
6	A	508	EDO	1	0
2	B	500	IMP	1	0
2	A	500	IMP	6	0
6	B	509	EDO	1	0
2	C	501	IMP	2	0

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.

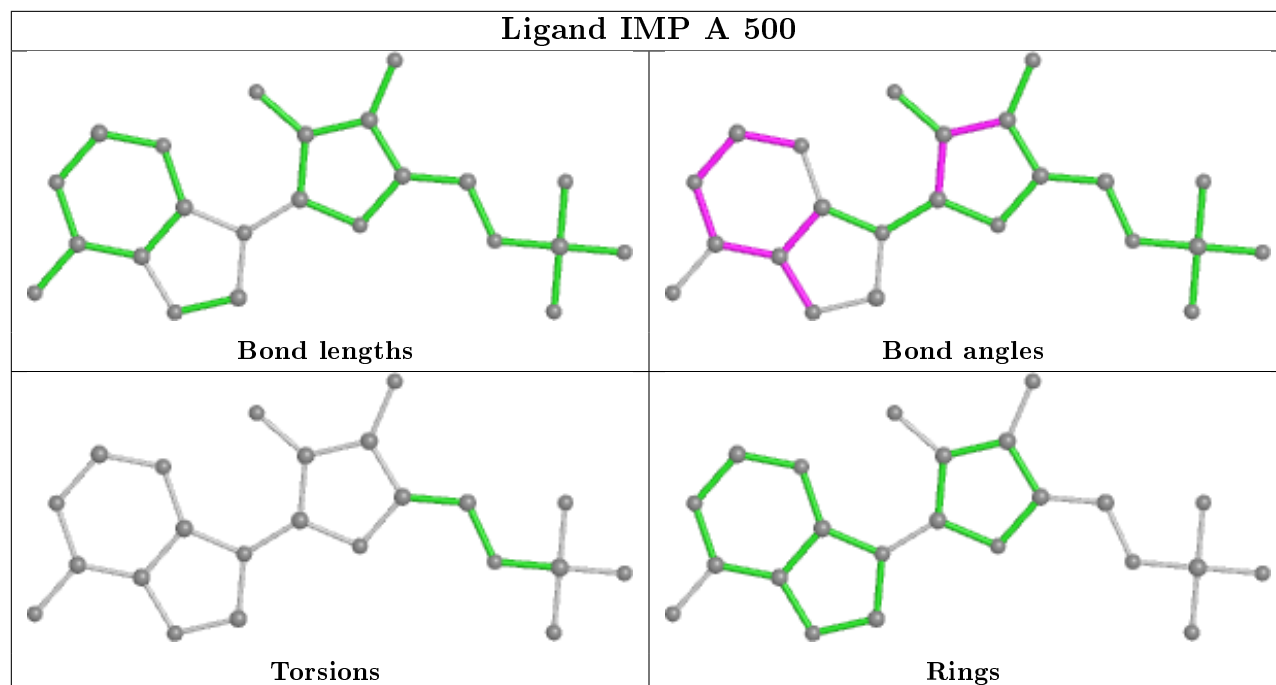
Ligand 8KY C 502



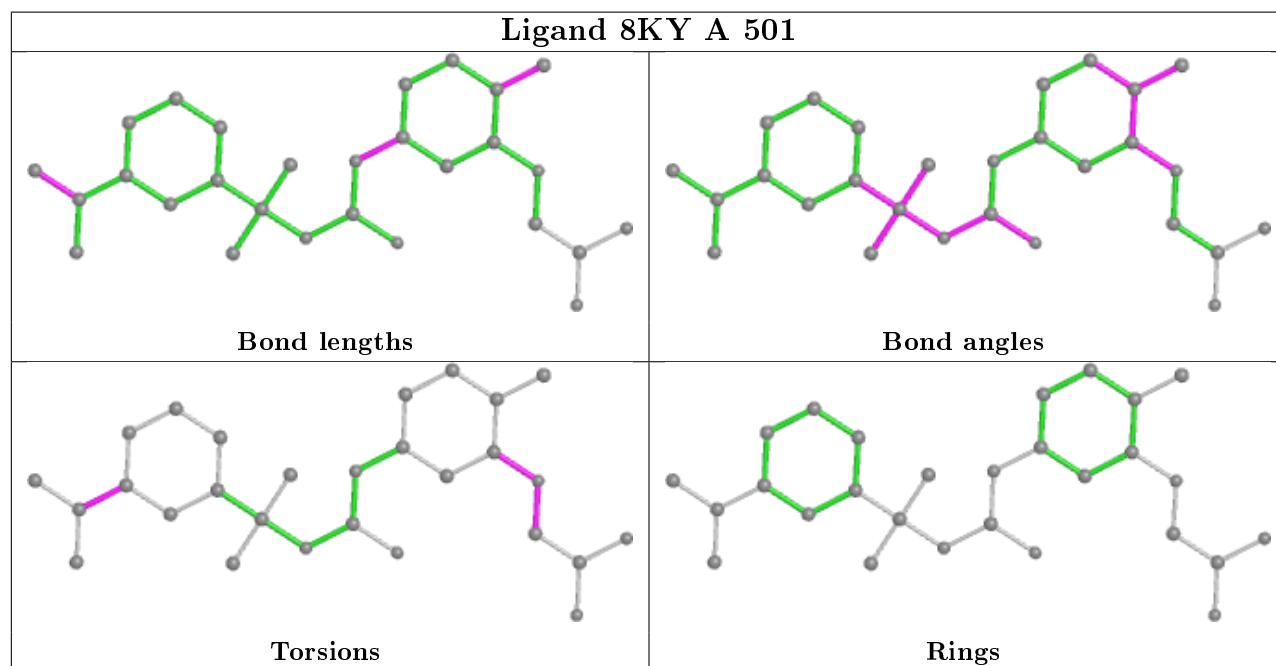
Ligand IMP B 500

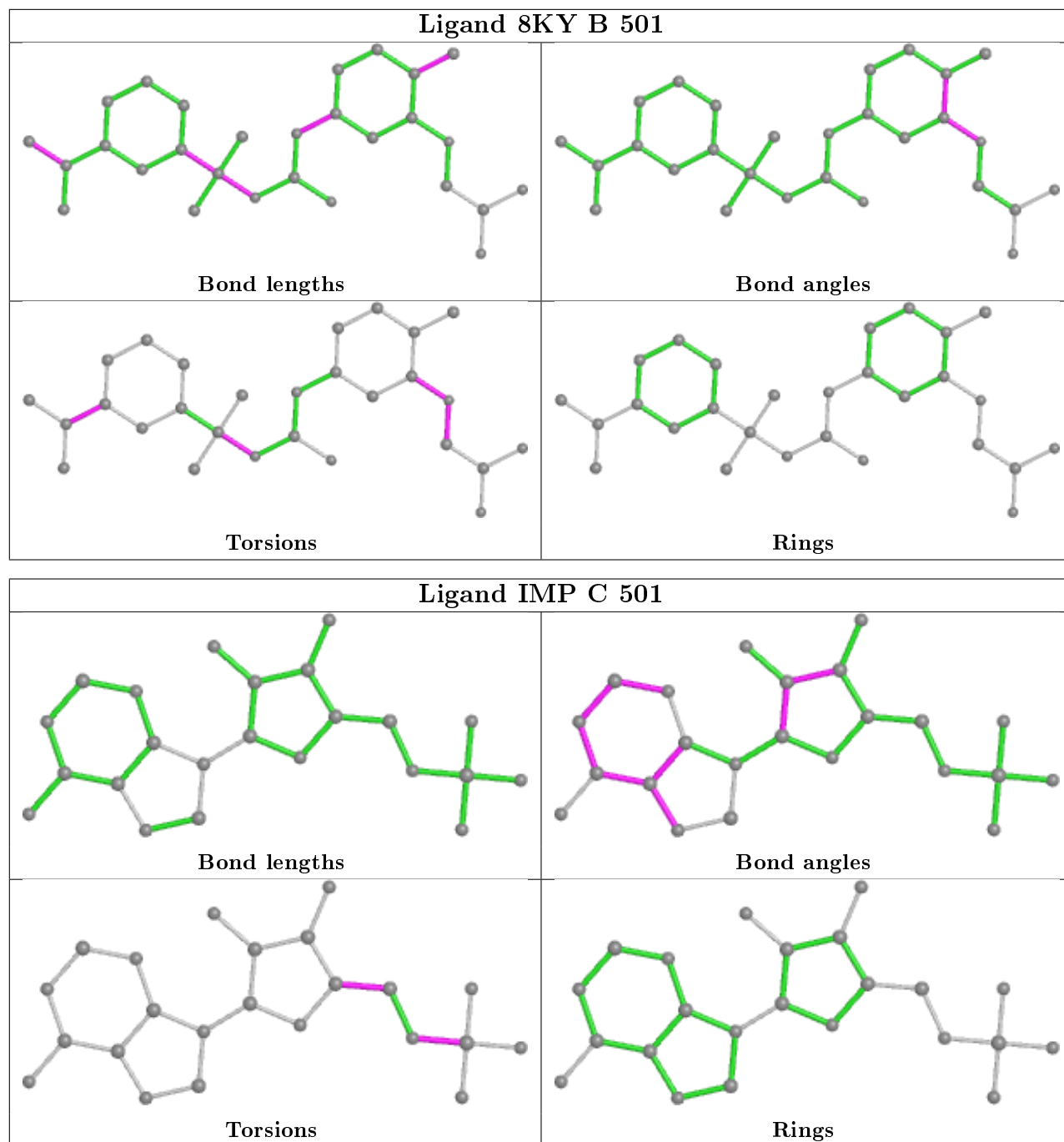


Ligand IMP A 500



Ligand 8KY A 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	354/406 (87%)	-0.19	4 (1%) 80 85	30, 42, 67, 111	0
1	B	355/406 (87%)	-0.19	2 (0%) 89 91	27, 39, 61, 99	0
1	C	355/406 (87%)	-0.18	1 (0%) 94 96	28, 42, 69, 99	0
All	All	1064/1218 (87%)	-0.19	7 (0%) 87 90	27, 41, 67, 111	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	LEU	2.8
1	A	87	LYS	2.7
1	B	408	LEU	2.4
1	A	80	ARG	2.2
1	B	482	VAL	2.1
1	C	0	ALA	2.1
1	A	235	GLU	2.1

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,

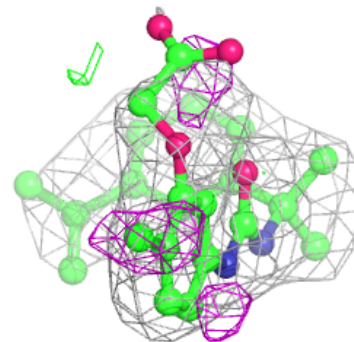
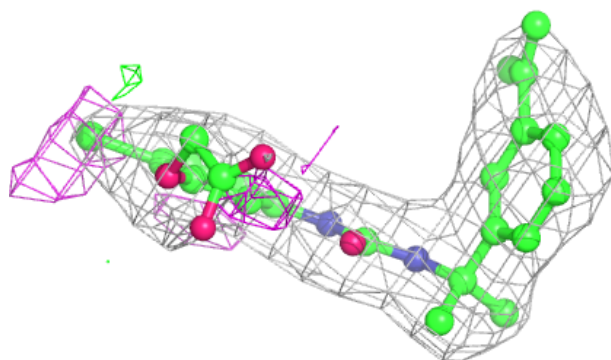
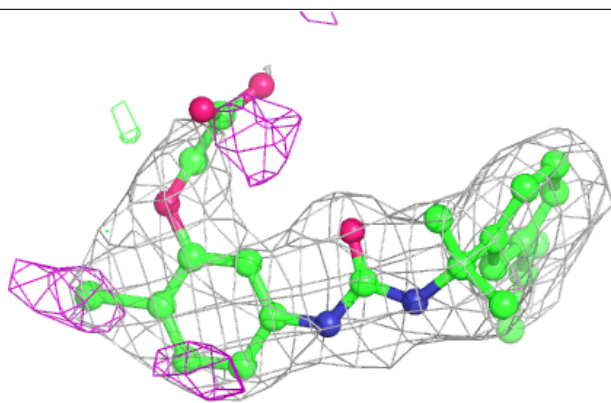
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	A	506	4/4	0.69	0.48	61,62,64,66	0
8	CL	C	507	1/1	0.75	0.08	89,89,89,89	0
5	SO4	B	506	5/5	0.78	0.31	147,147,148,148	0
8	CL	C	508	1/1	0.81	0.10	72,72,72,72	0
6	EDO	B	510	4/4	0.83	0.36	62,72,76,78	0
5	SO4	A	505	5/5	0.84	0.27	118,118,121,123	0
6	EDO	A	509	4/4	0.84	0.21	54,55,60,62	0
7	GOL	C	506	6/6	0.85	0.44	64,67,69,70	0
6	EDO	A	508	4/4	0.85	0.14	59,63,67,68	0
5	SO4	C	504	5/5	0.85	0.32	117,120,121,122	0
7	GOL	B	508	6/6	0.86	0.16	73,76,78,78	0
6	EDO	B	509	4/4	0.90	0.23	46,52,54,54	0
3	8KY	B	501	28/28	0.90	0.21	28,43,89,96	0
5	SO4	B	505	5/5	0.91	0.14	89,94,99,101	0
6	EDO	A	507	4/4	0.92	0.42	69,69,69,69	0
5	SO4	A	504	5/5	0.92	0.18	128,128,128,128	0
5	SO4	B	503	5/5	0.93	0.32	109,112,115,116	0
5	SO4	B	507	5/5	0.94	0.40	109,109,113,114	0
3	8KY	A	501	28/28	0.94	0.20	30,44,86,93	0
5	SO4	C	505	5/5	0.94	0.26	98,100,102,103	0
5	SO4	A	503	5/5	0.94	0.13	79,79,81,81	5
4	K	A	502	1/1	0.94	0.18	49,49,49,49	0
2	IMP	C	501	23/23	0.94	0.14	25,42,48,49	0
5	SO4	B	504	5/5	0.95	0.13	74,77,79,85	0
2	IMP	A	500	23/23	0.96	0.14	31,38,46,50	0
4	K	B	502	1/1	0.96	0.20	50,50,50,50	0
3	8KY	C	502	28/28	0.96	0.26	25,44,76,77	0
2	IMP	B	500	23/23	0.96	0.18	28,36,39,42	0
4	K	C	503	1/1	0.96	0.08	54,54,54,54	0

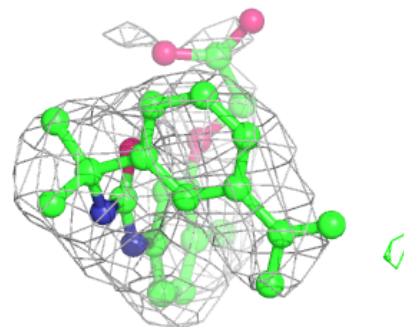
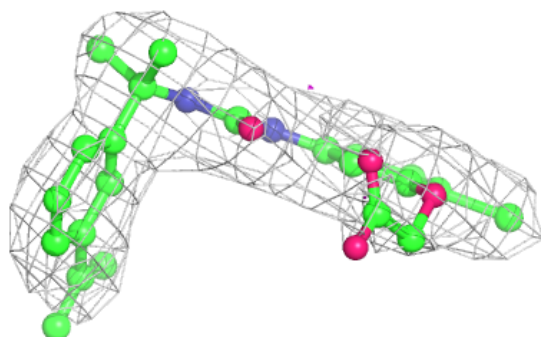
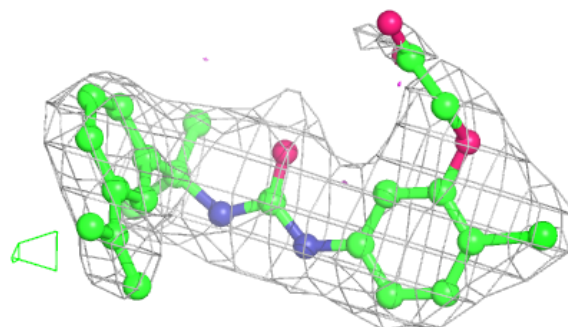
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8KY 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)

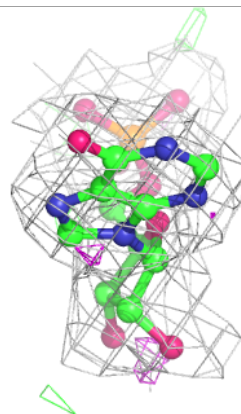
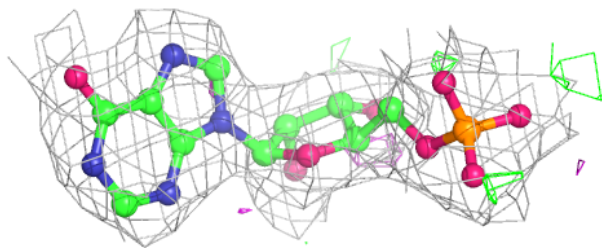
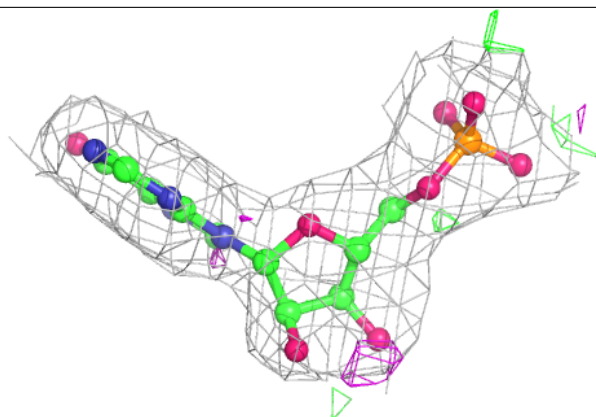
**Electron density around 8KY A 501:**

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

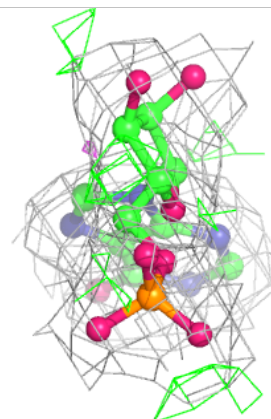
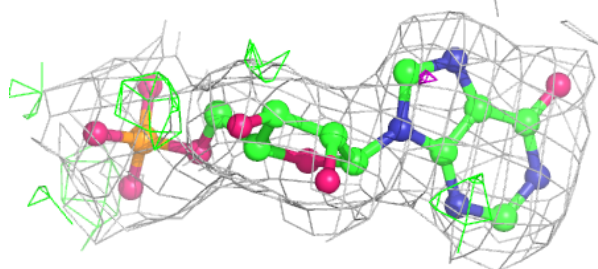
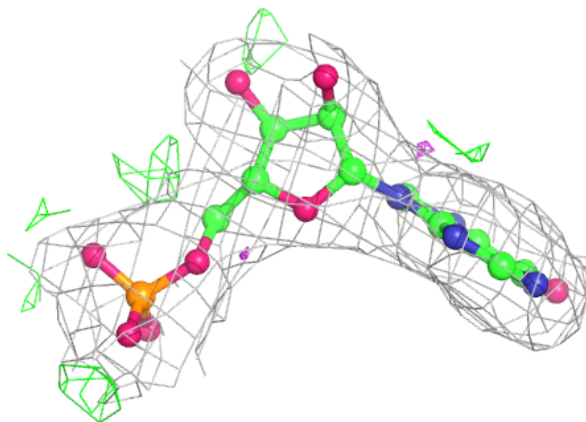


Electron density around IMP C 501:

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

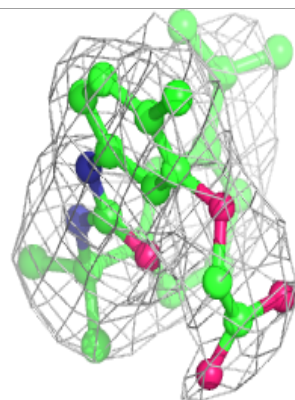
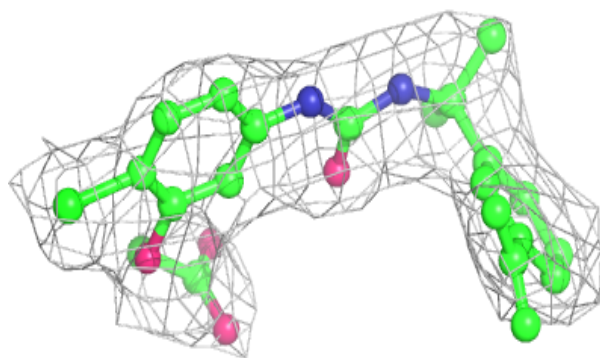
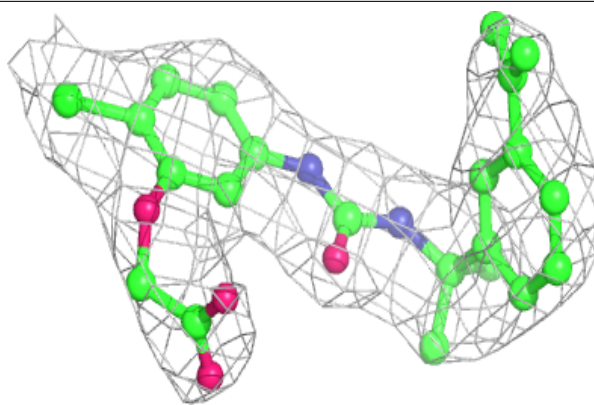
**Electron density around IMP A 500:**

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

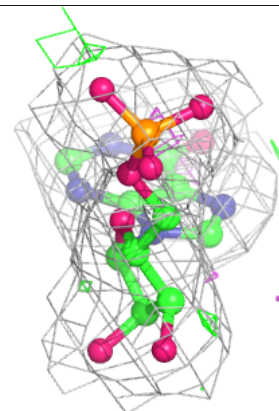
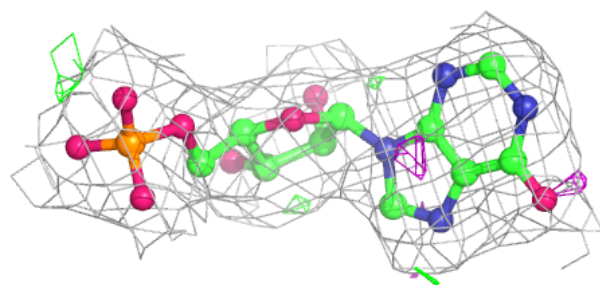
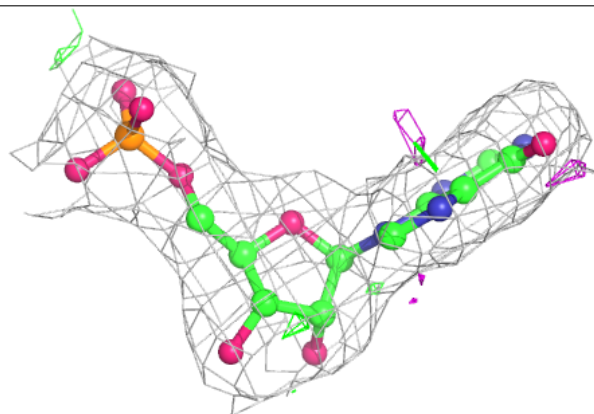


Electron density around 8KY C 502:

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

**Electron density around IMP B 500:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.