Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 07:51 AM BST

PDB ID	:	3USB
Title	:	Crystal Structure of Bacillus anthracis Inosine Monophosphate Dehydrogenase in the complex with IMP
Authors	:	Kim, Y.; Zhang, R.; Wu, R.; Gu, M.; Anderson, W.F.; Joachimiak, A.; CSGID; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2011-11-23
Resolution	:	2.38 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:

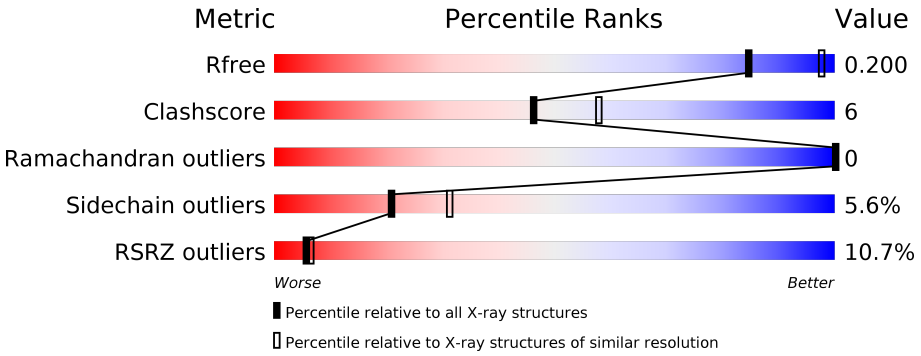
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	511	6% 76% 9% • 14%
1	B	511	11% 64% 12% • 22%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6903 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	442	Total	C	N	O	S	Se	0	4	0
			3354	2124	575	638	3	14			
1	B	401	Total	C	N	O	S	Se	0	7	0
			3052	1933	520	582	3	14			

There are 48 discrepancies between the modelled and reference sequences:

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

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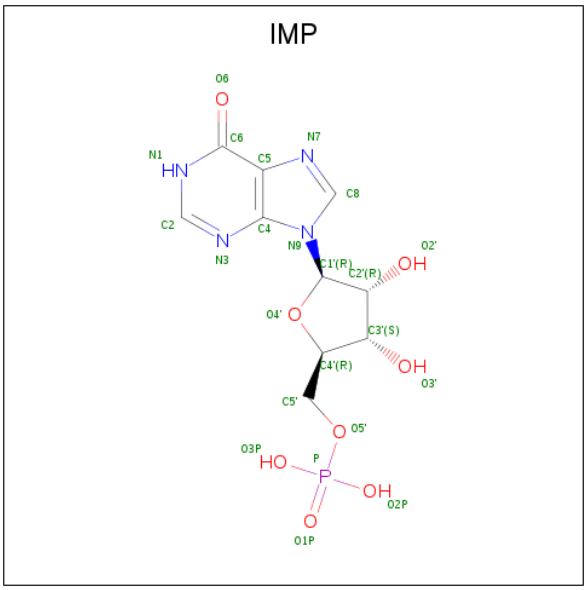
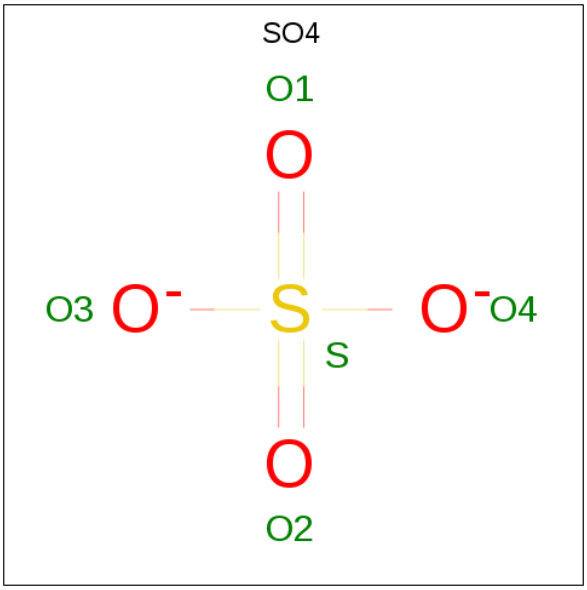
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-21	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-20	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-19	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-18	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-17	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-16	SER	-	EXPRESSION TAG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

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



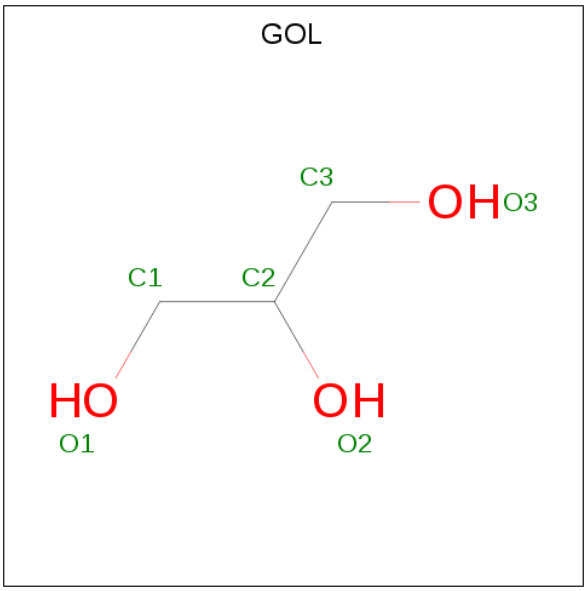
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0

- Molecule 6 is water.

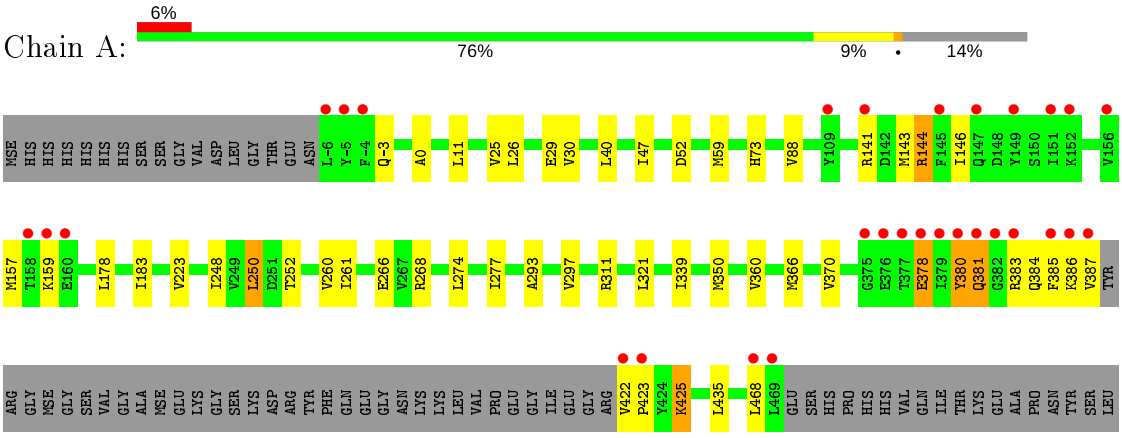
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	257	Total O 257 257	0	0
6	B	159	Total O 159 159	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

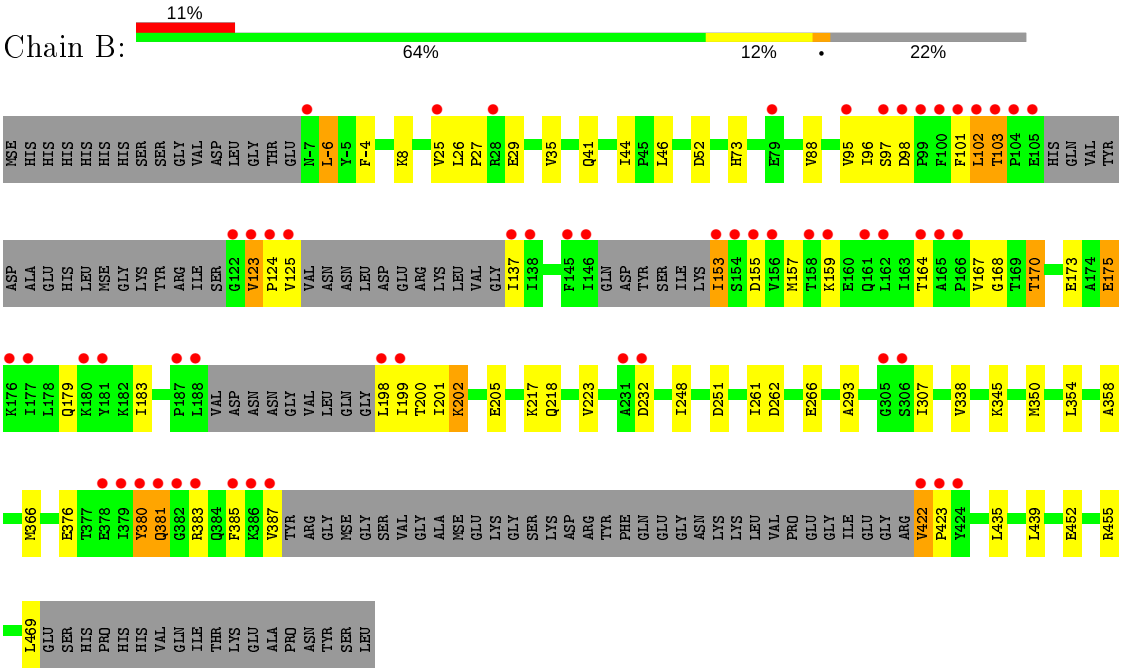
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain A:



- Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	122.52Å 122.52Å 140.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.74 – 2.38 38.74 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.74-2.38) 98.3 (38.74-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.06 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_851), REFMAC	Depositor
R, R_{free}	0.170 , 0.201 0.166 , 0.200	Depositor DCC
R_{free} test set	2058 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6903	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: GOL, CL, SO4, IMP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.56	0/3385	0.67	1/4552 (0.0%)
1	B	0.53	0/3074	0.67	0/4126
All	All	0.55	0/6459	0.67	1/8678 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	40	LEU	CA-CB-CG	5.11	127.06	115.30

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	3354	0	3456	45	0
1	B	3052	0	3145	37	0
2	A	23	0	11	0	0
2	B	23	0	11	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	12	0	16	1	0
4	B	12	0	16	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	257	0	0	2	0
6	B	159	0	0	1	0
All	All	6903	0	6655	83	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 (83) 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:380:TYR:HD2	1:A:381:GLN:N	1.43	1.17
1:A:380:TYR:CE2	1:A:381:GLN:HG2	1.90	1.07
1:A:380:TYR:CD2	1:A:381:GLN:N	2.30	0.98
1:A:380:TYR:HE2	1:A:381:GLN:HG2	1.23	0.96
1:A:380:TYR:CE2	1:A:381:GLN:CG	2.56	0.89
1:A:380:TYR:HE2	1:A:381:GLN:CG	1.89	0.84
1:A:381:GLN:HA	1:A:381:GLN:OE1	1.88	0.73
1:A:378:GLU:OE1	1:A:387:VAL:HG11	1.88	0.73
1:A:380:TYR:CD2	1:A:380:TYR:C	2.61	0.72
1:A:380:TYR:CE2	1:A:381:GLN:HB2	2.25	0.71
1:A:380:TYR:HD2	1:A:381:GLN:H	1.35	0.71
1:A:380:TYR:CE2	1:A:381:GLN:CB	2.76	0.68
1:B:167:VAL:HG12	1:B:168:GLY:H	1.61	0.65
1:B:-6:LEU:CD2	1:B:-4:PHE:O	2.49	0.61
1:B:125:VAL:HG11	1:B:157:MSE:SE	2.51	0.61
1:A:380:TYR:HE2	1:A:381:GLN:CB	2.12	0.60
1:B:97:SER:HG	1:B:198:LEU:N	1.98	0.60
1:A:386:LYS:HB2	1:A:422:VAL:HG13	1.85	0.59
1:A:47:ILE:HG13	1:A:360[A]:VAL:HG11	1.82	0.59
1:A:252:THR:HG21	1:A:260:VAL:HG21	1.84	0.59
1:B:-6:LEU:HD23	1:B:-4:PHE:O	2.04	0.58
1:A:157:MSE:HE3	1:A:159:LYS:HE3	1.85	0.58
1:A:380:TYR:HE2	1:A:381:GLN:HB2	1.67	0.57
1:B:52:ASP:HA	1:B:73:HIS:CD2	2.41	0.56
1:B:96:ILE:HD12	1:B:218:GLN:HG3	1.89	0.55
1:A:143:MSE:HA	1:A:146:ILE:HD12	1.90	0.54
1:A:141:ARG:HA	1:A:144:ARG:HD3	1.88	0.54
1:B:366:MSE:HE2	1:B:435:LEU:HD21	1.89	0.53
1:A:59:MSE:HE1	1:A:370:VAL:HG22	1.92	0.52
1:A:380:TYR:CD2	1:A:381:GLN:HB2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:VAL:HG11	1:A:223:VAL:HB	1.90	0.52
1:A:383:ARG:HB3	1:A:385:PHE:CE2	2.45	0.52
1:A:52:ASP:HA	1:A:73:HIS:CD2	2.45	0.52
1:B:95:VAL:HG23	1:B:96:ILE:HG13	1.91	0.52
1:B:102:LEU:HD23	1:B:103:THR:H	1.74	0.51
1:A:178:LEU:HD23	1:A:183:ILE:HG13	1.93	0.51
1:A:380:TYR:CD2	1:A:381:GLN:CB	2.94	0.51
1:B:170:THR:HG22	1:B:173:GLU:H	1.77	0.50
1:B:27:PRO:HD3	4:B:501:GOL:H11	1.94	0.50
1:A:422:VAL:HG23	1:A:423:PRO:HD2	1.94	0.49
1:B:44:ILE:HD12	1:B:46:LEU:HD12	1.93	0.49
1:B:26:LEU:O	1:B:29[A]:GLU:HG2	2.12	0.49
1:A:26:LEU:O	1:A:29:GLU:HG2	2.13	0.49
1:B:88:VAL:HG11	1:B:223:VAL:HB	1.96	0.48
1:B:-6:LEU:HD21	1:B:-4:PHE:O	2.13	0.48
1:B:200:THR:OG1	1:B:202:LYS:HG2	2.14	0.48
1:B:350:MSE:HE1	1:B:435:LEU:O	2.13	0.48
1:B:102:LEU:HD22	1:B:153:ILE:HD12	1.96	0.47
1:B:422:VAL:HG23	1:B:423:PRO:HD2	1.96	0.47
1:A:261:ILE:HG23	1:A:293:ALA:HB2	1.97	0.47
1:A:248:ILE:HD12	1:A:250:LEU:HD13	1.97	0.46
1:B:175:GLU:O	1:B:179:GLN:HG2	2.16	0.45
1:B:338:VAL:HG22	1:B:358:ALA:HA	1.98	0.45
1:A:25:VAL:HG23	1:A:29:GLU:HG3	1.99	0.45
1:B:27:PRO:HG3	4:B:501:GOL:H32	1.99	0.44
1:A:366:MSE:O	1:A:425[A]:LYS:HE3	2.18	0.44
1:B:26:LEU:HB2	1:B:29[A]:GLU:HG2	2.00	0.44
1:A:366:MSE:HE1	1:A:435:LEU:HD21	1.99	0.44
1:A:157:MSE:HE2	1:A:157:MSE:HB3	1.84	0.44
1:A:47:ILE:HG13	1:A:360[A]:VAL:CG1	2.48	0.43
1:B:123:VAL:HA	1:B:124:PRO:HD3	1.75	0.43
1:B:380:TYR:HB2	1:B:385:PHE:CD2	2.53	0.43
1:A:277:ILE:HG12	1:A:297:VAL:HB	2.00	0.43
1:A:11:LEU:O	1:A:321[B]:LEU:HB3	2.19	0.43
1:A:266:GLU:OE1	6:A:729:HOH:O	2.21	0.42
1:A:-3:GLN:HB3	1:A:0:ALA:HB2	2.02	0.42
1:B:261:ILE:HG23	1:B:293:ALA:HB2	2.01	0.42
1:A:59:MSE:HE1	1:A:370:VAL:CG2	2.49	0.42
1:B:201:ILE:O	1:B:205:GLU:HG3	2.19	0.42
1:B:350:MSE:HE3	1:B:439:LEU:HB2	2.01	0.42
1:B:8:LYS:HD3	4:B:502:GOL:O2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:LEU:O	1:B:455:ARG:HG2	2.20	0.42
1:A:339:ILE:HG12	1:A:360[B]:VAL:CG2	2.50	0.41
1:A:350:MSE:HE1	1:A:435:LEU:HD13	2.02	0.41
1:B:25:VAL:HG22	1:B:29[A]:GLU:HG3	2.02	0.41
1:B:380:TYR:HB3	1:B:381:GLN:H	1.76	0.41
1:B:262:ASP:O	1:B:266:GLU:HG3	2.21	0.41
4:A:503:GOL:H2	6:A:601:HOH:O	2.20	0.41
1:A:380:TYR:CD2	1:A:381:GLN:CA	3.04	0.41
1:A:268:ARG:NH1	1:A:274:LEU:O	2.35	0.41
1:B:248:ILE:HG13	1:B:248:ILE:O	2.20	0.40
1:B:217:LYS:HG2	6:B:617:HOH:O	2.21	0.40
1:B:35:VAL:HG22	1:B:41:GLN:HG2	2.04	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	442/511 (86%)	433 (98%)	9 (2%)	0	100	100
1	B	396/511 (78%)	389 (98%)	7 (2%)	0	100	100
All	All	838/1022 (82%)	822 (98%)	16 (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	361/398 (91%)	350 (97%)	11 (3%)	41 59
1	B	328/398 (82%)	300 (92%)	28 (8%)	10 14
All	All	689/796 (87%)	650 (94%)	39 (6%)	21 30

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	144	ARG
1	A	250	LEU
1	A	311	ARG
1	A	378	GLU
1	A	380	TYR
1	A	381	GLN
1	A	384	GLN
1	A	425[A]	LYS
1	A	425[B]	LYS
1	A	468	LEU
1	B	-6	LEU
1	B	98	ASP
1	B	101	PHE
1	B	102	LEU
1	B	103	THR
1	B	123	VAL
1	B	137	ILE
1	B	153	ILE
1	B	155	ASP
1	B	159	LYS
1	B	164	THR
1	B	170	THR
1	B	175	GLU
1	B	183	ILE
1	B	199	ILE
1	B	202	LYS
1	B	232	ASP
1	B	251	ASP
1	B	307	ILE
1	B	345	LYS
1	B	376	GLU
1	B	380	TYR
1	B	381	GLN

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Mol	Chain	Res	Type
1	B	383	ARG
1	B	387	VAL
1	B	422	VAL
1	B	452	GLU
1	B	469	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	GOL	A	502	-	5,5,5	0.32	0	5,5,5	0.45	0
4	GOL	A	503	-	5,5,5	0.39	0	5,5,5	0.51	0
3	SO4	A	501	-	4,4,4	0.18	0	6,6,6	0.19	0
4	GOL	B	502	-	5,5,5	0.50	0	5,5,5	0.42	0
2	IMP	B	500	-	21,25,25	1.39	3 (14%)	23,38,38	1.56	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	B	501	-	5,5,5	0.31	0	5,5,5	0.45	0
3	SO4	B	503	-	4,4,4	0.18	0	6,6,6	0.24	0
2	IMP	A	500	-	21,25,25	1.39	3 (14%)	23,38,38	1.63	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
4	GOL	A	502	-	-	4/4/4/4	-
4	GOL	A	503	-	-	4/4/4/4	-
4	GOL	B	502	-	-	0/4/4/4	-
2	IMP	B	500	-	-	5/6/26/26	0/3/3/3
4	GOL	B	501	-	-	4/4/4/4	-
2	IMP	A	500	-	-	5/6/26/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	IMP	C2-N3	4.10	1.38	1.32
2	A	500	IMP	C2-N3	4.06	1.38	1.32
2	A	500	IMP	C6-N1	3.61	1.39	1.33
2	B	500	IMP	C6-N1	3.59	1.39	1.33
2	A	500	IMP	C2-N1	2.71	1.38	1.33
2	B	500	IMP	C2-N1	2.70	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	IMP	N3-C2-N1	-5.84	119.54	128.68
2	B	500	IMP	N3-C2-N1	-5.44	120.18	128.68
2	A	500	IMP	C2-N1-C6	3.04	120.97	115.88
2	B	500	IMP	C2-N1-C6	2.88	120.70	115.88
2	B	500	IMP	O2P-P-O1P	2.06	118.76	110.68

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	GOL	O1-C1-C2-C3
4	A	502	GOL	C1-C2-C3-O3
4	A	502	GOL	O2-C2-C3-O3
2	B	500	IMP	C5'-O5'-P-O1P
2	B	500	IMP	C5'-O5'-P-O2P
2	B	500	IMP	C5'-O5'-P-O3P
4	B	501	GOL	O1-C1-C2-C3
4	B	501	GOL	C1-C2-C3-O3
2	A	500	IMP	C5'-O5'-P-O1P
2	A	500	IMP	C5'-O5'-P-O2P
2	A	500	IMP	C5'-O5'-P-O3P
2	A	500	IMP	C3'-C4'-C5'-O5'
4	A	503	GOL	O1-C1-C2-O2
2	B	500	IMP	C3'-C4'-C5'-O5'
4	A	503	GOL	O1-C1-C2-C3
4	A	503	GOL	C1-C2-C3-O3
4	A	502	GOL	O1-C1-C2-O2
4	B	501	GOL	O1-C1-C2-O2
2	A	500	IMP	O4'-C4'-C5'-O5'
4	B	501	GOL	O2-C2-C3-O3
2	B	500	IMP	O4'-C4'-C5'-O5'
4	A	503	GOL	O2-C2-C3-O3

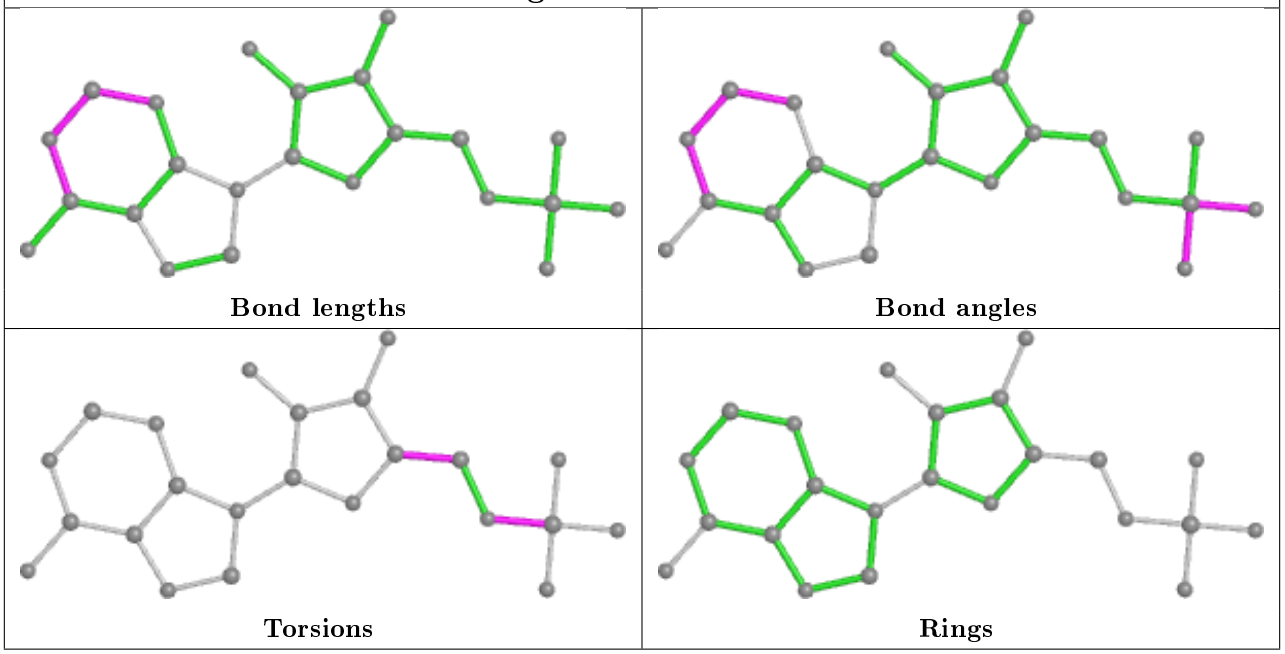
There are no ring outliers.

3 monomers are involved in 4 short contacts:

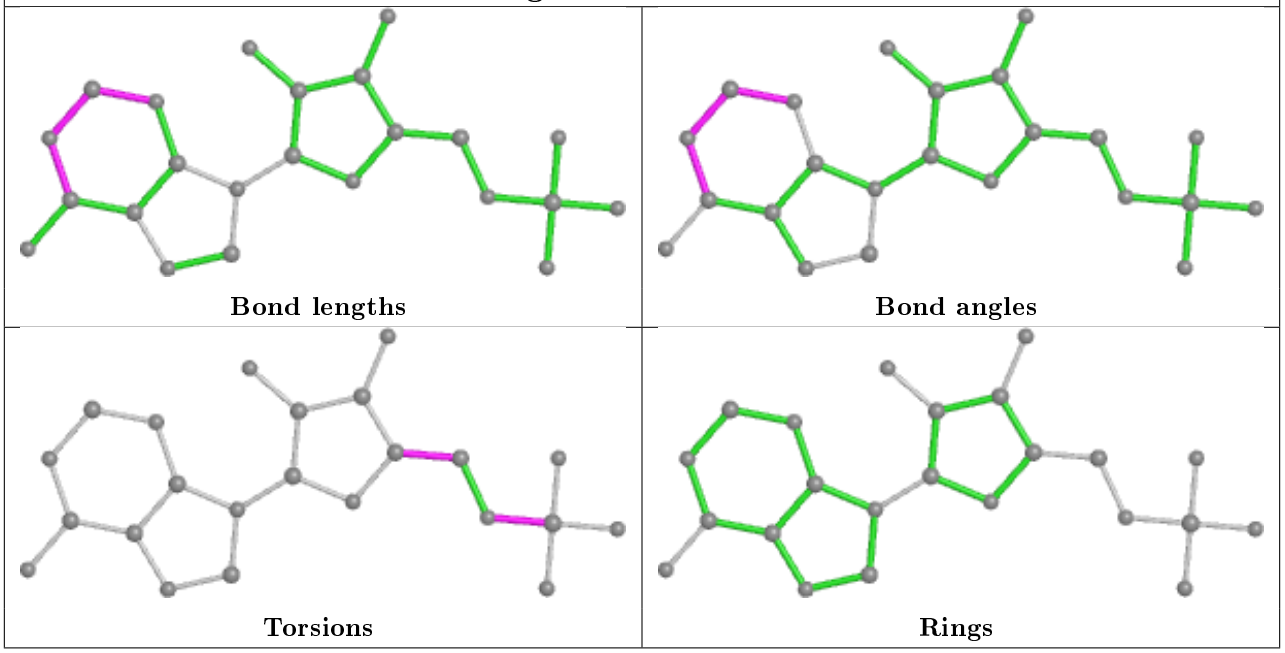
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	GOL	1	0
4	B	502	GOL	1	0
4	B	501	GOL	2	0

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 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 B 500



Ligand IMP A 500



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	428/511 (83%)	-0.01	30 (7%) 16 17	10, 29, 77, 128	0
1	B	388/511 (75%)	0.48	57 (14%) 2 2	12, 39, 101, 127	3 (0%)
All	All	816/1022 (79%)	0.22	87 (10%) 6 6	10, 33, 92, 128	3 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	PHE	10.7
1	B	101	PHE	8.8
1	B	102	LEU	8.8
1	B	188	LEU	7.5
1	B	380	TYR	6.5
1	A	-5	TYR	5.9
1	B	137	ILE	5.9
1	B	138	ILE	5.8
1	B	-7	ASN	5.1
1	B	383	ARG	5.1
1	B	99	PRO	5.1
1	B	231	ALA	5.1
1	A	380	TYR	5.0
1	B	166	PRO	5.0
1	B	156	VAL	4.9
1	A	383	ARG	4.8
1	A	159	LYS	4.8
1	B	153	ILE	4.7
1	A	147	GLN	4.6
1	A	381	GLN	4.5
1	B	146	ILE	4.5
1	A	-4	PHE	4.4
1	B	422	VAL	4.4
1	A	385	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	162	LEU	4.3
1	A	-6	LEU	4.3
1	B	98	ASP	4.2
1	B	123	VAL	4.0
1	B	423	PRO	4.0
1	A	387	VAL	3.9
1	A	469	LEU	3.9
1	B	104	PRO	3.8
1	B	181	TYR	3.8
1	B	124	PRO	3.7
1	B	103	THR	3.7
1	B	387	VAL	3.7
1	A	377	THR	3.6
1	A	379	ILE	3.6
1	B	385	PHE	3.6
1	B	122	GLY	3.5
1	B	378	GLU	3.5
1	B	97	SER	3.5
1	B	145	PHE	3.4
1	B	379	ILE	3.4
1	B	159	LYS	3.4
1	B	125	VAL	3.4
1	B	381	GLN	3.3
1	A	145	PHE	3.3
1	B	187	PRO	3.2
1	A	378	GLU	3.2
1	A	156	VAL	3.2
1	B	105	GLU	3.2
1	B	198	LEU	3.0
1	B	165	ALA	3.0
1	B	28	ARG	3.0
1	B	180	LYS	3.0
1	B	232	ASP	3.0
1	B	382	GLY	2.9
1	B	199	ILE	2.8
1	A	376	GLU	2.8
1	A	375	GLY	2.8
1	B	158	THR	2.7
1	A	423	PRO	2.6
1	A	158	THR	2.6
1	B	164	THR	2.6
1	A	382	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	160	GLU	2.5
1	A	109	TYR	2.5
1	A	141	ARG	2.4
1	A	149	TYR	2.4
1	B	176	LYS	2.3
1	B	25	VAL	2.3
1	A	151	ILE	2.3
1	B	177	ILE	2.3
1	B	161	GLN	2.3
1	A	468	LEU	2.2
1	B	424	TYR	2.2
1	B	154	SER	2.2
1	B	95	VAL	2.2
1	A	152	LYS	2.2
1	B	79	GLU	2.2
1	B	306	SER	2.2
1	A	386	LYS	2.1
1	B	386	LYS	2.1
1	B	305	GLY	2.1
1	B	155	ASP	2.1
1	A	422	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	503	6/6	0.76	0.26	43,54,57,58	0
4	GOL	A	502	6/6	0.84	0.24	53,60,61,62	0

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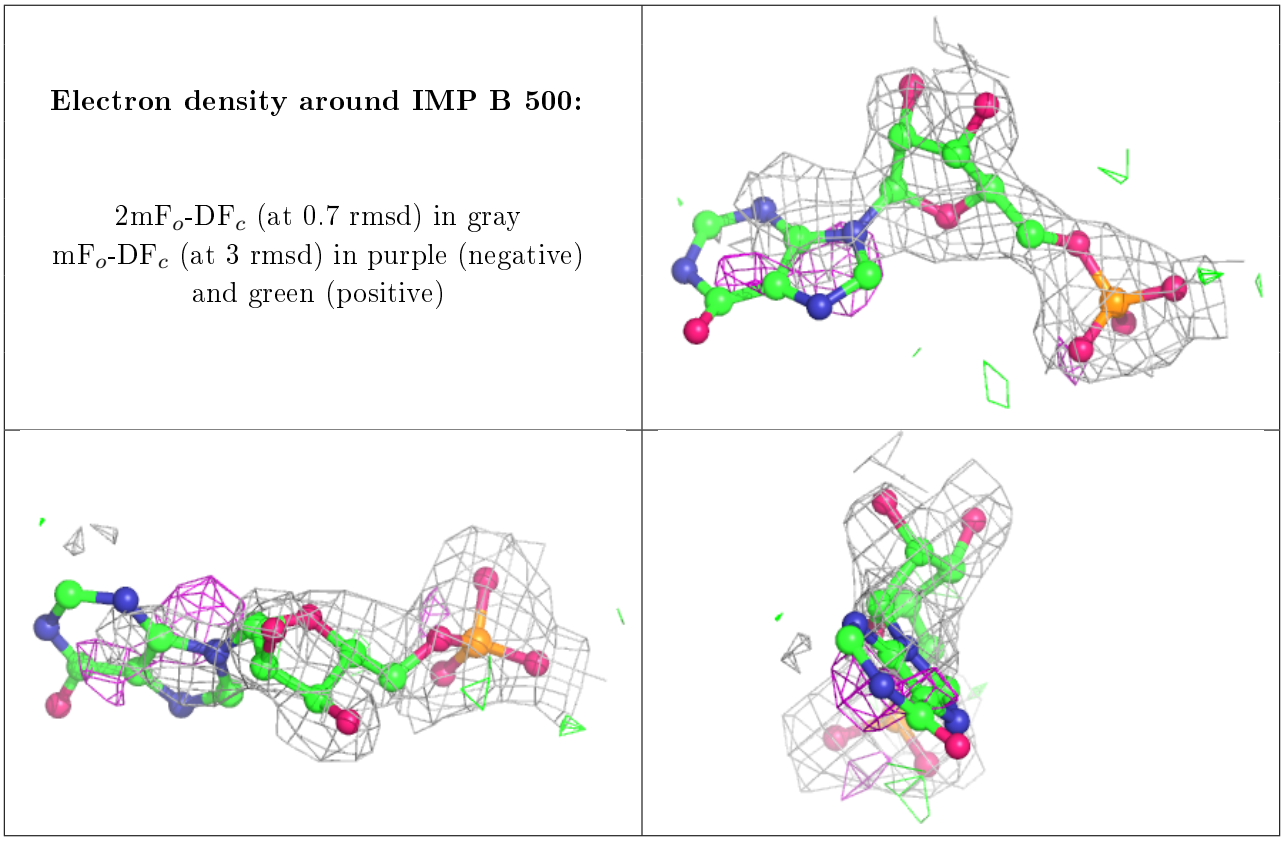
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	501	6/6	0.84	0.29	68,69,71,73	0
4	GOL	B	502	6/6	0.89	0.26	32,43,50,52	0
2	IMP	B	500	23/23	0.90	0.23	44,96,121,121	0
5	CL	B	504	1/1	0.93	0.12	59,59,59,59	0
2	IMP	A	500	23/23	0.93	0.19	33,75,103,104	0
3	SO4	A	501	5/5	0.95	0.11	85,87,88,88	0
3	SO4	B	503	5/5	0.95	0.30	89,89,90,90	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.

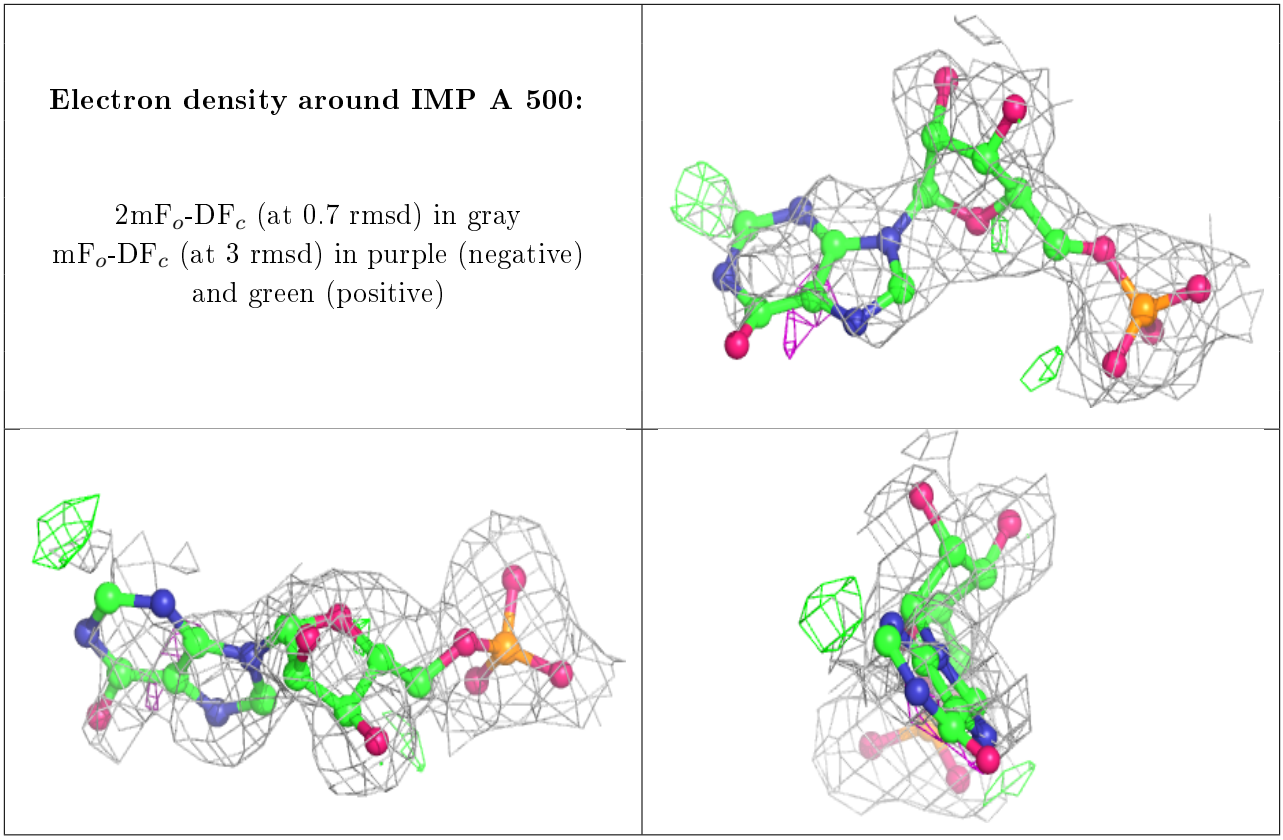
Electron density around IMP B 500:

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



Electron density around IMP 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)



6.5 Other polymers (i)

There are no such residues in this entry.