



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:58 pm BST

PDB ID : 3TSD  
Title : Crystal Structure of Inosine-5'-monophosphate Dehydrogenase from *Bacillus anthracis* str. Ames complexed with XMP  
Authors : Kim, Y.; Makowska-Grzyska, M.; Hasseman, J.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2011-09-13  
Resolution : 2.65 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

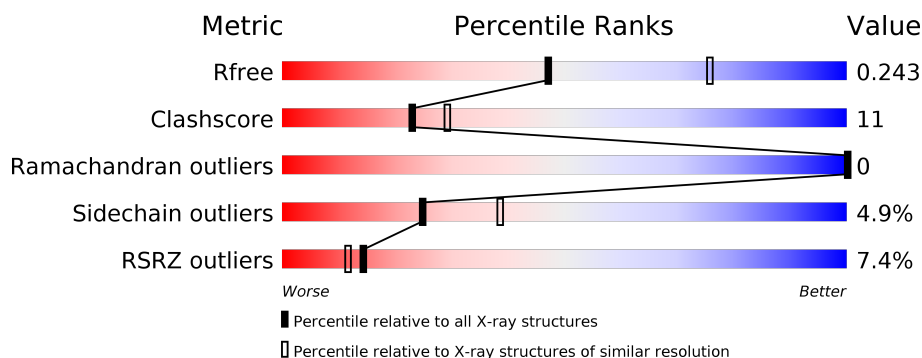
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	511	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>16%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	511	<div> <div>9%</div> <div> <div></div> <div>65%</div> <div>16%</div> <div>•</div> <div>17%</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
3	TAR	B	501	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6667 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	0	0	0
			3318	2093	576	632	17			
1	B	426	Total	C	N	O	S	1	0	0
			3191	2013	557	603	18			

There are 48 discrepancies between the modelled and reference sequences:

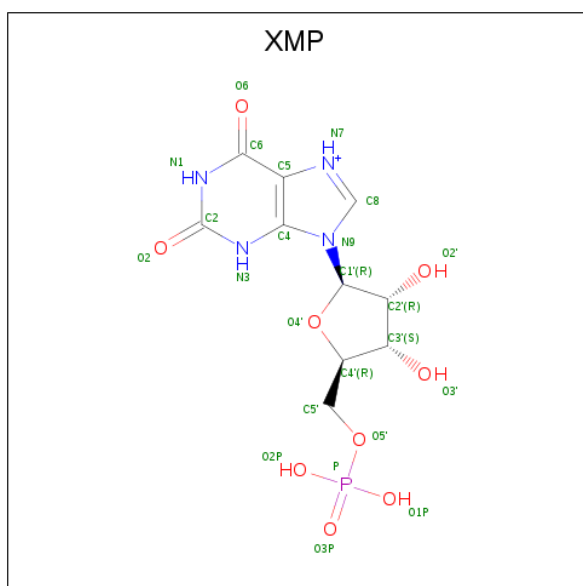
Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	EXPRESSION TAG	UNP Q81W29
A	-22	HIS	-	EXPRESSION TAG	UNP Q81W29
A	-21	HIS	-	EXPRESSION TAG	UNP Q81W29
A	-20	HIS	-	EXPRESSION TAG	UNP Q81W29
A	-19	HIS	-	EXPRESSION TAG	UNP Q81W29
A	-18	HIS	-	EXPRESSION TAG	UNP Q81W29
A	-17	HIS	-	EXPRESSION TAG	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	MET	-	EXPRESSION TAG	UNP Q81W29

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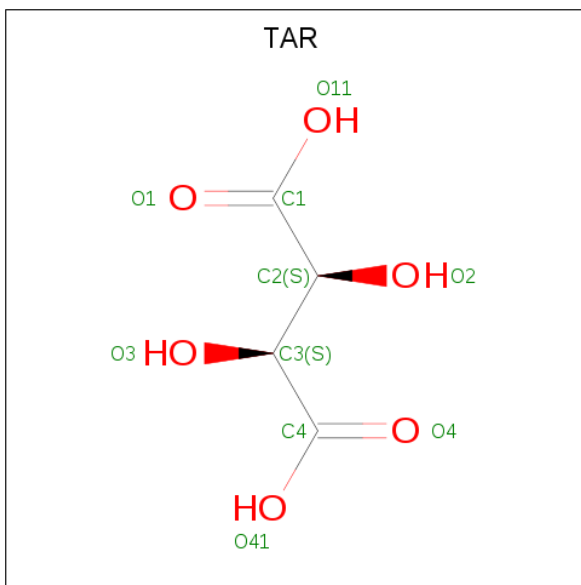
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-21	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-20	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-19	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-18	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-17	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-16	SER	-	EXPRESSION TAG	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 XANTHOSINE-5'-MONOPHOSPHATE (three-letter code: XMP) (formula:  $C_{10}H_{14}N_4O_9P$ ).



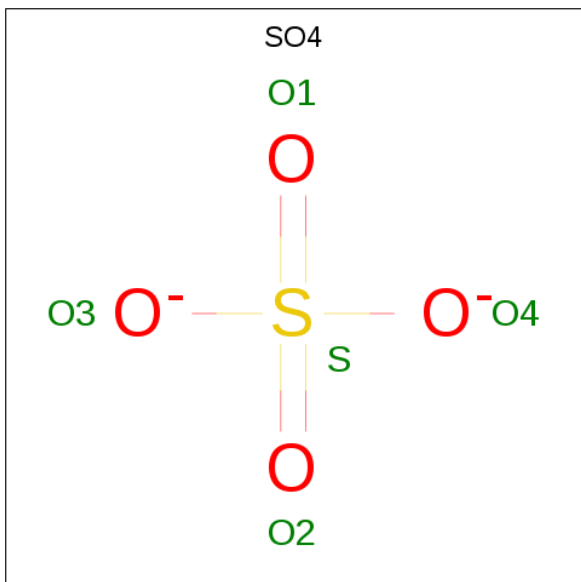
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	10	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			24	10	4	9	1		

- Molecule 3 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

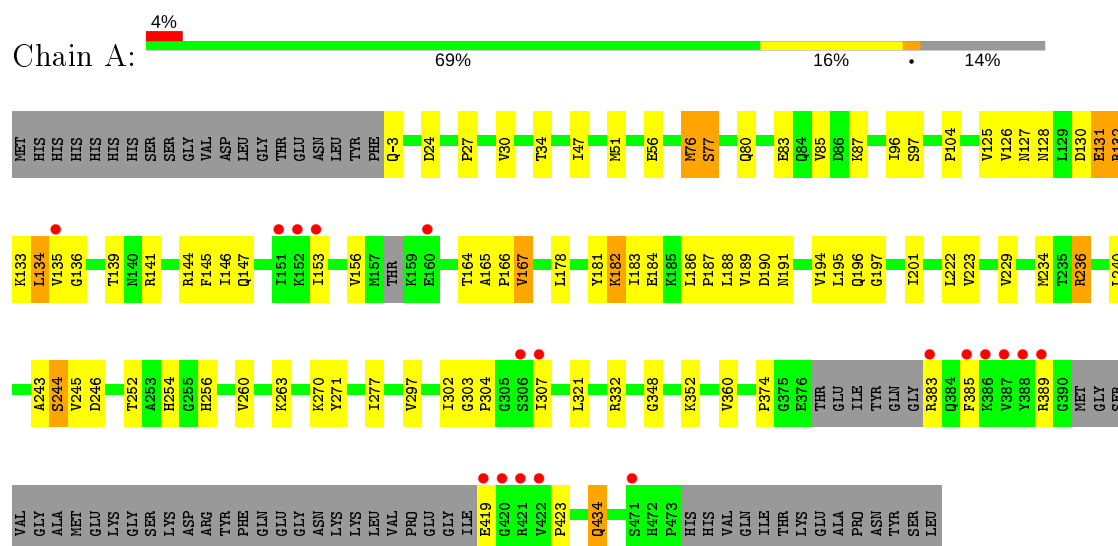
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		
5	B	46	Total	O	0	0
			46	46		

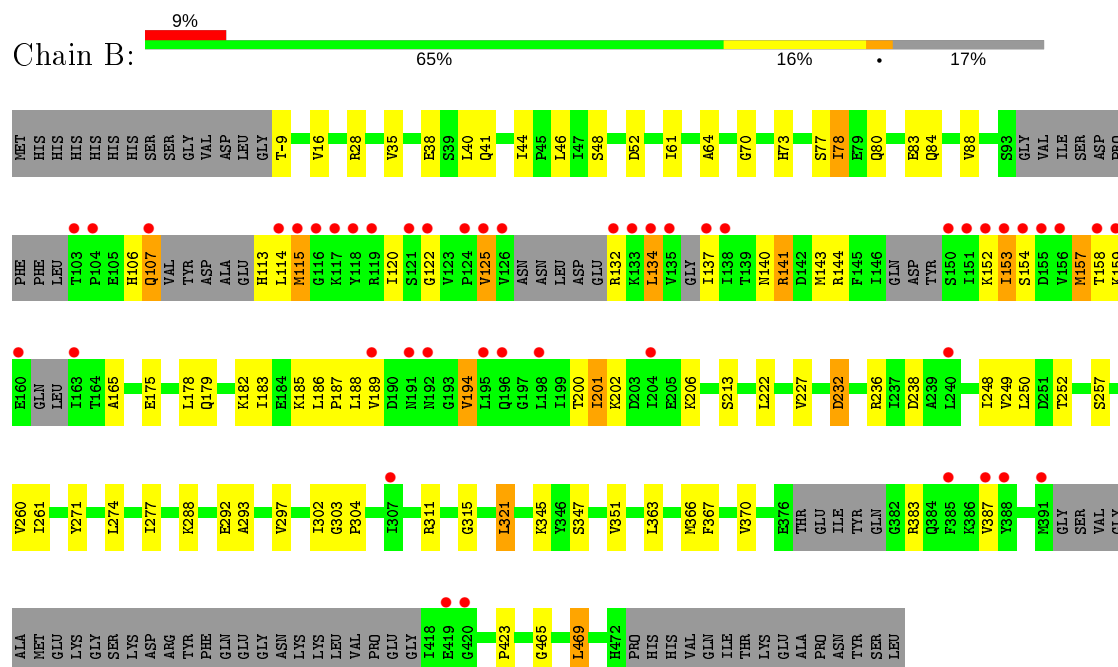
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.25Å 123.25Å 141.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.98 – 2.65 44.09 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.0 (38.98-2.65) 94.7 (44.09-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_851)	Depositor
R, $R_{free}$	0.192 , 0.245 0.185 , 0.243	Depositor DCC
$R_{free}$ test set	1549 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.6	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.033 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6667	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XMP, SO4, TAR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.43	0/3362	0.62	0/4540
1	B	0.45	0/3226	0.64	0/4344
All	All	0.44	0/6588	0.63	0/8884

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

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	3318	0	3411	83	0
1	B	3191	0	3300	80	0
2	A	24	0	12	0	0
2	B	24	0	12	0	0
3	B	10	0	4	13	0
4	B	5	0	0	1	0
5	A	49	0	0	3	0
5	B	46	0	0	1	0
All	All	6667	0	6739	152	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 11.

All (152) 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:B:137:ILE:HD11	3:B:501:TAR:C2	1.43	1.46
1:B:137:ILE:CD1	3:B:501:TAR:C2	2.24	1.15
1:A:223:VAL:CG1	1:A:245:VAL:HG23	1.89	1.01
1:B:137:ILE:HD11	3:B:501:TAR:H2	0.98	0.96
1:A:223:VAL:HG13	1:A:245:VAL:CG2	1.95	0.96
1:A:223:VAL:HG13	1:A:245:VAL:HG23	0.99	0.95
1:B:137:ILE:HD11	3:B:501:TAR:C1	1.96	0.95
1:A:125:VAL:HB	1:A:136:GLY:O	1.68	0.93
1:B:137:ILE:CD1	3:B:501:TAR:H2	1.93	0.91
1:A:240:LEU:O	1:A:243:ALA:HB3	1.71	0.88
1:B:137:ILE:CD1	3:B:501:TAR:C1	2.52	0.86
1:B:137:ILE:CD1	3:B:501:TAR:O2	2.23	0.86
1:B:154:SER:HA	1:B:157:MET:HE3	1.58	0.84
1:A:77:SER:HB3	1:A:80:GLN:OE1	1.78	0.83
1:B:137:ILE:HD12	3:B:501:TAR:O2	1.81	0.81
1:A:125:VAL:CB	1:A:136:GLY:O	2.28	0.81
1:A:85:VAL:HG11	1:A:245:VAL:HB	1.69	0.74
1:A:132:ARG:CZ	1:A:132:ARG:HB2	2.16	0.74
1:A:252:THR:HG21	1:A:260:VAL:HG21	1.69	0.73
1:B:252:THR:HG21	1:B:260:VAL:HG21	1.72	0.71
1:A:128:ASN:OD1	1:A:131:GLU:HB2	1.90	0.70
1:A:222:LEU:CD2	1:A:246:ASP:OD1	2.40	0.69
1:A:389:ARG:HG2	1:A:419:GLU:HA	1.75	0.69
1:B:183:ILE:HD12	3:B:501:TAR:O3	1.93	0.68
1:A:181:TYR:O	1:B:144:ARG:NH2	2.26	0.67
1:A:243:ALA:O	1:A:244:SER:HB2	1.93	0.67
1:A:127:ASN:ND2	1:A:133:LYS:HB3	2.12	0.64
1:A:125:VAL:CG2	1:A:136:GLY:O	2.46	0.64
1:A:178:LEU:HD23	1:A:183:ILE:HG13	1.78	0.64
1:B:132:ARG:HB3	1:B:194:VAL:HG22	1.80	0.62
1:B:303:GLY:HA3	1:B:311:ARG:HE	1.64	0.62
1:A:127:ASN:HD21	1:A:133:LYS:HB3	1.65	0.62
1:A:243:ALA:O	1:A:244:SER:CB	2.48	0.61
1:B:232:ASP:N	1:B:232:ASP:OD1	2.34	0.61
1:A:128:ASN:CG	1:A:131:GLU:HB2	2.21	0.61
1:A:254:HIS:CE1	1:A:256:HIS:HB3	2.36	0.61
1:B:113:HIS:CG	1:B:114:LEU:H	2.19	0.60
1:A:47:ILE:HG13	1:A:360:VAL:HG11	1.83	0.60
1:A:383:ARG:HB3	1:B:423:PRO:HB2	1.82	0.60
1:B:44:ILE:HD12	1:B:46:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASN:OD1	1:A:131:GLU:N	2.26	0.59
1:B:277:ILE:HG12	1:B:297:VAL:HB	1.85	0.59
1:A:182:LYS:NZ	1:B:143:MET:HB2	2.18	0.58
1:A:126:VAL:HA	1:A:134:LEU:HA	1.86	0.58
1:A:128:ASN:ND2	1:A:131:GLU:HB2	2.19	0.57
1:A:85:VAL:CG1	1:A:245:VAL:HB	2.34	0.57
1:B:52:ASP:HA	1:B:73:HIS:CD2	2.40	0.57
1:A:125:VAL:HG23	1:A:136:GLY:O	2.04	0.57
1:A:184:GLU:HB3	1:A:201:ILE:HG12	1.86	0.57
1:A:383:ARG:HG2	1:A:385:PHE:CE1	2.41	0.56
1:B:78:ILE:HD12	1:B:236:ARG:HA	1.87	0.56
1:B:106:HIS:O	1:B:153:ILE:HG22	2.05	0.56
1:A:303:GLY:HA3	5:A:531:HOH:O	2.06	0.56
1:B:238:ASP:OD1	1:B:271:TYR:OH	2.22	0.56
1:B:80:GLN:HA	1:B:83:GLU:OE1	2.06	0.56
1:A:164:THR:HG22	1:A:187:PRO:HG2	1.89	0.55
1:A:383:ARG:NH1	1:B:383:ARG:HD3	2.21	0.55
1:A:222:LEU:HD23	1:A:246:ASP:OD1	2.06	0.55
1:A:165:ALA:HB1	1:A:166:PRO:HD2	1.87	0.55
1:B:366:MET:HG3	5:B:527:HOH:O	2.06	0.55
1:A:182:LYS:HZ1	1:B:143:MET:HB2	1.73	0.54
1:B:347:SER:O	1:B:351:VAL:HG23	2.08	0.54
1:B:257:SER:HB2	1:B:260:VAL:HG23	1.90	0.53
1:A:229:VAL:HG21	1:A:260:VAL:HG22	1.90	0.53
1:A:56:GLU:HG3	1:A:374:PRO:HG3	1.90	0.53
1:B:125:VAL:HG11	1:B:157:MET:HG3	1.91	0.52
1:A:222:LEU:CD2	1:A:246:ASP:CG	2.77	0.52
1:A:96:ILE:O	1:A:197:GLY:HA3	2.10	0.52
1:B:137:ILE:HD13	3:B:501:TAR:C1	2.37	0.52
1:A:182:LYS:HB3	1:B:140:ASN:HD21	1.75	0.51
1:B:153:ILE:O	1:B:153:ILE:HG12	2.10	0.51
1:B:227:VAL:HB	1:B:250:LEU:HD23	1.92	0.51
1:A:222:LEU:HD22	1:A:246:ASP:CG	2.31	0.51
1:A:190:ASP:HB3	1:A:196:GLN:HE21	1.74	0.51
1:B:261:ILE:HG23	1:B:293:ALA:HB2	1.93	0.50
1:B:227:VAL:O	1:B:250:LEU:HA	2.11	0.50
1:B:302:ILE:C	1:B:304:PRO:HD3	2.32	0.50
1:A:-3:GLN:HB2	5:A:534:HOH:O	2.12	0.50
1:A:222:LEU:HA	1:A:246:ASP:OD2	2.12	0.50
1:A:147:GLN:HE21	1:B:179:GLN:NE2	2.09	0.50
1:A:130:ASP:O	1:A:132:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLU:O	1:B:179:GLN:HB2	2.11	0.50
1:A:132:ARG:HB3	1:A:194:VAL:HG13	1.94	0.49
1:A:434:GLN:NE2	5:A:507:HOH:O	2.46	0.49
1:B:132:ARG:HH21	1:B:194:VAL:HG13	1.77	0.49
1:A:167:VAL:HG11	1:A:196:GLN:HG2	1.95	0.48
1:A:134:LEU:HD22	1:A:189:VAL:HG11	1.96	0.48
1:A:104:PRO:HA	1:A:153:ILE:HB	1.95	0.48
1:B:122:GLY:HA3	1:B:185:LYS:HE3	1.95	0.48
1:B:185:LYS:HG2	1:B:200:THR:HG22	1.96	0.48
1:A:144:ARG:HH12	1:B:202:LYS:HE3	1.79	0.48
1:B:183:ILE:CD1	3:B:501:TAR:O3	2.60	0.48
1:B:40:LEU:HD12	1:B:222:LEU:HD13	1.94	0.48
1:B:107:GLN:HA	1:B:152:LYS:HA	1.95	0.47
1:A:146:ILE:HG12	1:A:156:VAL:HG11	1.97	0.47
1:A:165:ALA:O	1:A:188:LEU:HA	2.14	0.46
1:A:191:ASN:N	1:A:191:ASN:OD1	2.45	0.46
1:A:383:ARG:HH11	1:B:383:ARG:HD3	1.80	0.46
1:A:302:ILE:C	1:A:304:PRO:HD3	2.36	0.46
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.80	0.46
1:B:120:ILE:HG22	1:B:185:LYS:HD3	1.99	0.45
1:B:465:GLY:O	1:B:469:LEU:HD22	2.15	0.45
1:A:223:VAL:O	1:A:245:VAL:HG22	2.15	0.45
1:A:348:GLY:O	1:A:352:LYS:HG3	2.16	0.45
1:B:35:VAL:HG22	1:B:41:GLN:HG2	1.97	0.45
1:A:24:ASP:OD1	1:A:24:ASP:N	2.43	0.45
1:B:311:ARG:O	1:B:315:GLY:HA2	2.17	0.45
1:A:189:VAL:HG12	1:A:195:LEU:HA	1.99	0.45
1:A:145:PHE:CD2	1:B:182:LYS:HA	2.52	0.45
1:B:113:HIS:CG	1:B:114:LEU:N	2.85	0.45
1:B:345:LYS:HD2	1:B:345:LYS:HA	1.70	0.44
1:A:277:ILE:HG12	1:A:297:VAL:HB	1.99	0.44
1:B:137:ILE:HD13	3:B:501:TAR:O11	2.17	0.44
1:A:236:ARG:O	1:A:240:LEU:HG	2.18	0.44
1:B:201:ILE:HD12	1:B:202:LYS:H	1.83	0.43
1:B:248:ILE:HG12	1:B:274:LEU:HD21	2.00	0.43
1:B:80:GLN:O	1:B:84:GLN:HB2	2.18	0.43
1:B:137:ILE:CD1	3:B:501:TAR:O11	2.67	0.43
1:B:64:ALA:O	1:B:213:SER:HA	2.18	0.43
1:B:363:LEU:HB2	1:B:367:PHE:CE1	2.54	0.43
1:A:222:LEU:HD22	1:A:246:ASP:OD1	2.16	0.43
1:B:113:HIS:CD2	1:B:114:LEU:H	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:O	1:A:87:LYS:HG3	2.19	0.43
1:B:141:ARG:CG	1:B:141:ARG:HH21	2.31	0.43
1:B:134:LEU:HD21	1:B:189:VAL:HG11	2.00	0.43
1:B:178:LEU:HB2	1:B:183:ILE:O	2.19	0.43
1:B:141:ARG:HB2	4:B:502:SO4:S	2.59	0.42
1:A:27:PRO:O	1:A:30:VAL:HG22	2.19	0.42
1:B:165:ALA:HB3	1:B:188:LEU:HD23	2.00	0.42
1:A:139:THR:OG1	1:A:141:ARG:HG3	2.19	0.42
1:A:423:PRO:HB3	1:B:383:ARG:HG3	2.02	0.42
1:B:61:ILE:HG13	1:B:88:VAL:HG22	2.00	0.42
1:B:367:PHE:O	1:B:370:VAL:HG22	2.19	0.42
1:B:48:SER:OG	1:B:70:GLY:HA2	2.19	0.42
1:A:222:LEU:HD23	1:A:246:ASP:CG	2.40	0.41
1:A:270:LYS:HG2	1:A:271:TYR:CE2	2.54	0.41
1:B:157:MET:HG2	1:B:158:THR:N	2.34	0.41
1:A:76:MET:O	1:A:236:ARG:NH2	2.52	0.41
1:A:240:LEU:O	1:A:243:ALA:CB	2.56	0.41
1:B:206:LYS:HA	1:B:206:LYS:HD3	1.84	0.41
1:A:128:ASN:HD21	1:A:131:GLU:HB2	1.85	0.41
1:B:288:LYS:O	1:B:292:GLU:HG2	2.21	0.41
1:A:234:MET:CE	1:A:270:LYS:HD3	2.51	0.41
1:A:178:LEU:HD21	1:A:186:LEU:HB2	2.02	0.41
1:B:227:VAL:N	1:B:249:VAL:O	2.36	0.41
1:B:38:GLU:OE1	1:B:38:GLU:N	2.39	0.41
1:B:186:LEU:HA	1:B:187:PRO:HD2	1.99	0.40
1:A:223:VAL:O	1:A:245:VAL:CG2	2.68	0.40
1:B:115:MET:HE2	1:B:115:MET:HB2	1.91	0.40
1:A:182:LYS:HE3	1:A:182:LYS:HB2	1.88	0.40
1:A:51:MET:HE1	1:A:307:ILE:HD11	2.04	0.40
1:B:321:LEU:HD22	1:B:321:LEU:HA	1.74	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	434/511 (85%)	430 (99%)	4 (1%)	0	100	100
1	B	408/511 (80%)	406 (100%)	2 (0%)	0	100	100
All	All	842/1022 (82%)	836 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	356/415 (86%)	341 (96%)	15 (4%)	30	45
1	B	342/415 (82%)	323 (94%)	19 (6%)	21	33
All	All	698/830 (84%)	664 (95%)	34 (5%)	25	38

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	76	MET
1	A	77	SER
1	A	97	SER
1	A	131	GLU
1	A	132	ARG
1	A	134	LEU
1	A	135	VAL
1	A	167	VAL
1	A	182	LYS
1	A	236	ARG
1	A	244	SER
1	A	263	LYS
1	A	332	ARG
1	A	434	GLN

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Mol	Chain	Res	Type
1	B	-9	THR
1	B	16	VAL
1	B	28	ARG
1	B	77	SER
1	B	78	ILE
1	B	107	GLN
1	B	115	MET
1	B	125	VAL
1	B	134	LEU
1	B	141	ARG
1	B	153	ILE
1	B	157	MET
1	B	159	LYS
1	B	194	VAL
1	B	201	ILE
1	B	232	ASP
1	B	321	LEU
1	B	387	VAL
1	B	469	LEU

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	147	GLN
1	A	196	GLN
1	A	254	HIS
1	B	106	HIS
1	B	107	GLN
1	B	113	HIS
1	B	140	ASN
1	B	254	HIS
1	B	472	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	TAR	B	501	-	3,9,9	1.88	2 (66%)	6,12,12	0.66	0
2	XMP	B	500	-	21,26,26	1.79	1 (4%)	23,40,40	1.91	3 (13%)
4	SO4	B	502	-	4,4,4	0.32	0	6,6,6	0.05	0
2	XMP	A	500	-	21,26,26	1.74	1 (4%)	23,40,40	1.83	3 (13%)

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	TAR	B	501	-	-	0/4/12/12	-
2	XMP	B	500	-	-	5/6/26/26	0/3/3/3
2	XMP	A	500	-	-	0/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	XMP	O6-C6	7.33	1.43	1.24
2	A	500	XMP	O6-C6	7.15	1.42	1.24
3	B	501	TAR	O3-C3	-2.30	1.38	1.42
3	B	501	TAR	O2-C2	-2.14	1.38	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	XMP	C6-N1-C2	6.42	120.56	115.14
2	A	500	XMP	C6-N1-C2	6.08	120.28	115.14
2	A	500	XMP	O2P-P-O1P	3.12	119.55	107.64
2	B	500	XMP	O2P-P-O1P	3.08	119.40	107.64
2	B	500	XMP	C5-C6-N1	-2.96	119.39	123.43
2	A	500	XMP	C5-C6-N1	-2.89	119.48	123.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

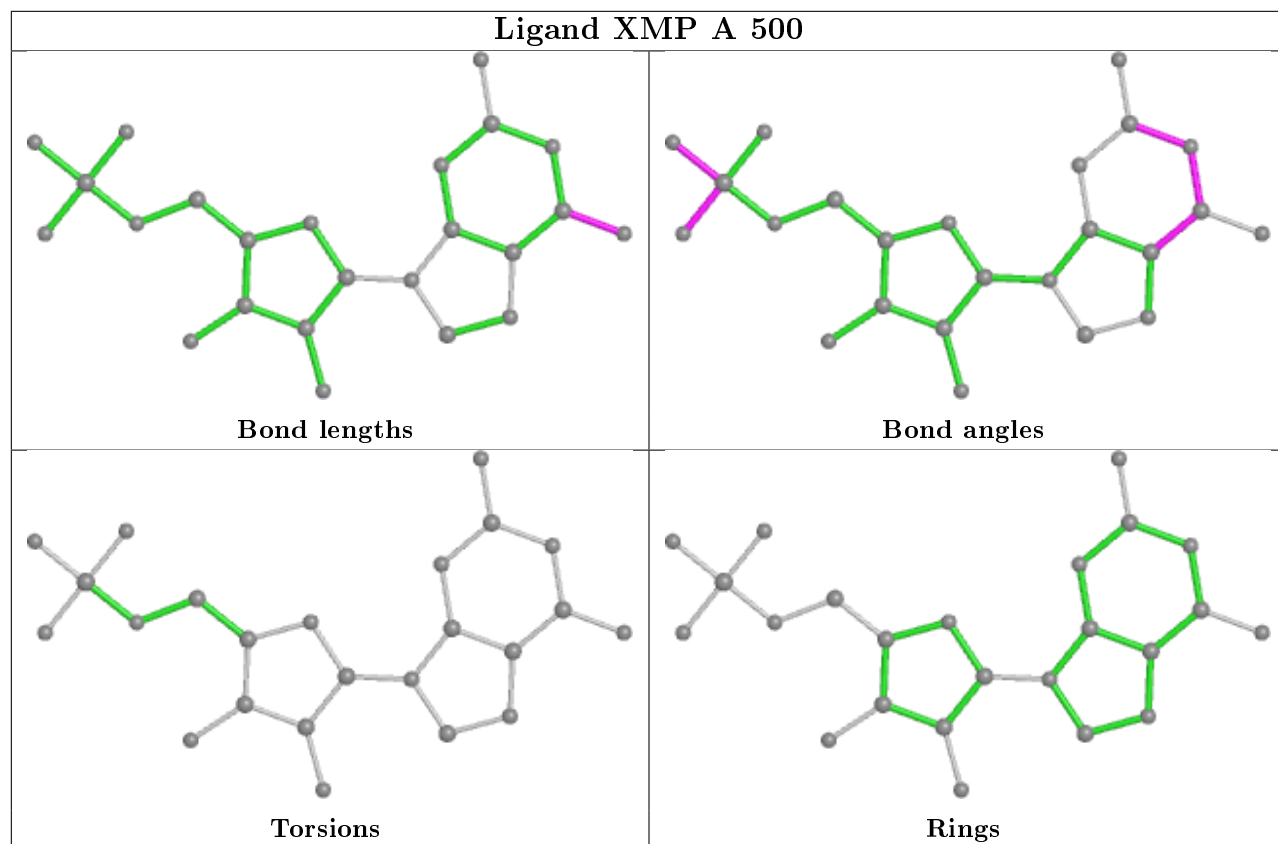
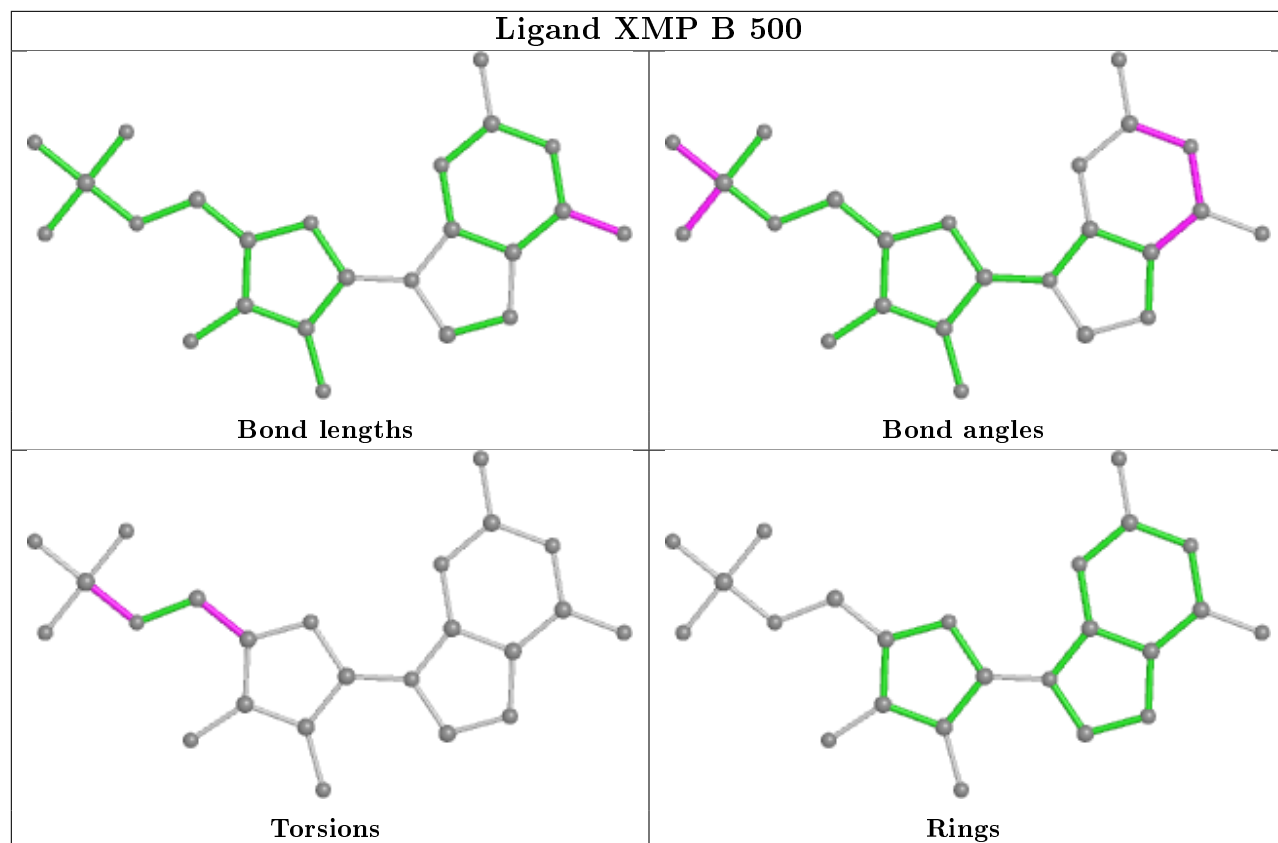
Mol	Chain	Res	Type	Atoms
2	B	500	XMP	C5'-O5'-P-O1P
2	B	500	XMP	C5'-O5'-P-O2P
2	B	500	XMP	C5'-O5'-P-O3P
2	B	500	XMP	C3'-C4'-C5'-O5'
2	B	500	XMP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	TAR	13	0
4	B	502	SO4	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.



## 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	442/511 (86%)	0.03	18 (4%) 37 33	41, 69, 121, 166	1 (0%)
1	B	426/511 (83%)	0.33	46 (10%) 5 4	42, 77, 145, 191	5 (1%)
All	All	868/1022 (84%)	0.18	64 (7%) 14 12	41, 72, 137, 191	6 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	387	VAL	8.4
1	B	195	LEU	6.7
1	A	153	ILE	6.1
1	A	420	GLY	6.0
1	B	134	LEU	5.5
1	B	135	VAL	5.4
1	A	421	ARG	5.3
1	B	156	VAL	5.1
1	B	117	LYS	5.0
1	B	388	TYR	5.0
1	A	388	TYR	4.5
1	B	387	VAL	4.4
1	B	152	LYS	4.4
1	A	389	ARG	4.0
1	B	122	GLY	4.0
1	B	391	MET	3.9
1	B	137	ILE	3.9
1	A	307	ILE	3.8
1	B	150	SER	3.8
1	B	163	ILE	3.7
1	A	422	VAL	3.7
1	B	191	ASN	3.6
1	B	118	TYR	3.5
1	B	138	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	192	ASN	3.3
1	B	124	PRO	3.3
1	B	151	ILE	3.2
1	B	159	LYS	3.2
1	B	114	LEU	3.2
1	A	471	SER	3.1
1	A	385	PHE	3.1
1	B	189	VAL	3.1
1	B	125	VAL	3.1
1	B	154	SER	3.0
1	B	126	VAL	3.0
1	B	103	THR	3.0
1	B	115	MET	3.0
1	A	419	GLU	2.9
1	A	383	ARG	2.9
1	B	133	LYS	2.9
1	B	198	LEU	2.9
1	B	160	GLU	2.8
1	B	158	THR	2.8
1	B	116	GLY	2.7
1	A	160	GLU	2.7
1	B	153	ILE	2.6
1	B	196	GLN	2.6
1	B	107	GLN	2.5
1	B	419	GLU	2.5
1	B	420	GLY	2.4
1	B	104	PRO	2.4
1	A	151	ILE	2.4
1	B	119	ARG	2.3
1	A	386	LYS	2.2
1	B	307	ILE	2.2
1	A	306	SER	2.1
1	B	121	SER	2.1
1	A	135	VAL	2.1
1	B	132	ARG	2.1
1	A	152	LYS	2.1
1	B	385	PHE	2.1
1	B	155	ASP	2.0
1	B	240	LEU	2.0
1	B	204	ILE	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](#)

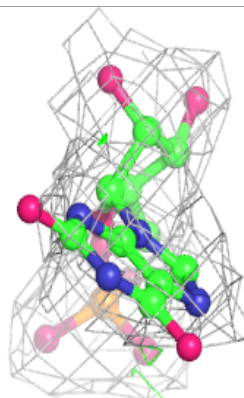
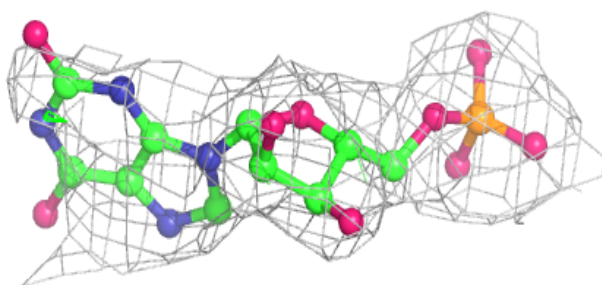
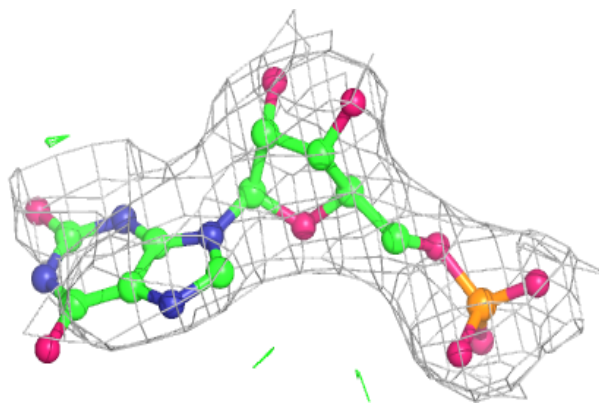
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	TAR	B	501	10/10	0.79	0.31	108,117,128,128	0
4	SO4	B	502	5/5	0.85	0.10	143,146,149,150	0
2	XMP	B	500	24/24	0.95	0.16	74,99,146,151	0
2	XMP	A	500	24/24	0.96	0.15	69,96,134,135	0

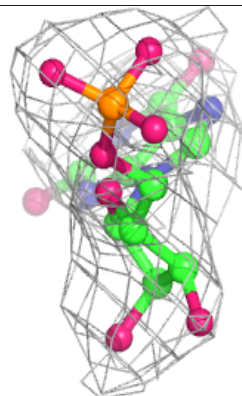
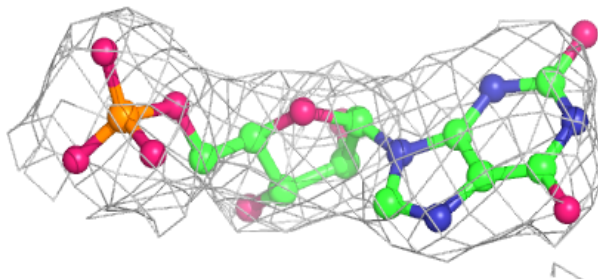
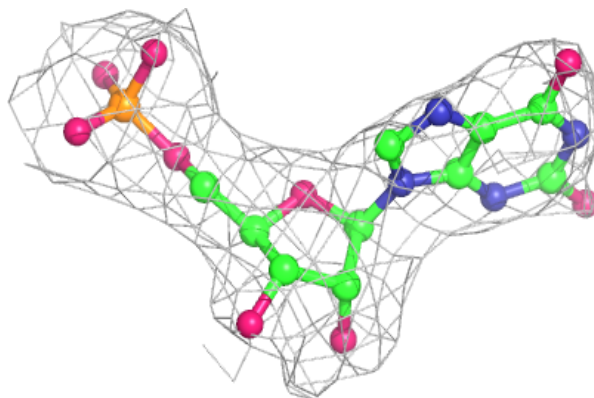
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around XMP 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 XMP 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.