



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 08:29 AM EST

PDB ID : 1M9N  
Title : CRYSTAL STRUCTURE OF THE HOMODIMERIC BIFUNCTIONAL TRANSFORMYLASE AND CYCLOHYDROLASE ENZYME AVIAN ATIC IN COMPLEX WITH AICAR AND XMP AT 1.93 ANGSTROMS.  
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Deposited on : 2002-07-29  
Resolution : 1.93 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

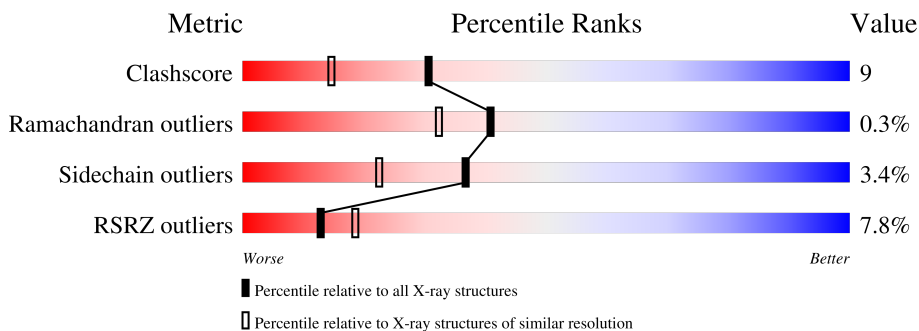
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

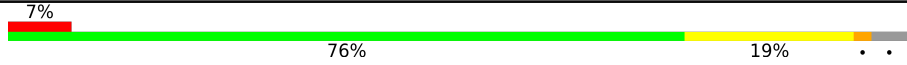
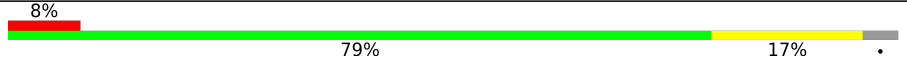
The reported resolution of this entry is 1.93 Å.

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))
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	613	
1	B	613	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 9625 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 AICAR TRANSFORMYLASE-IMP CYCLOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	590	4510	2843	800	848	19	0	0	0
1	B	590	4510	2843	800	848	19	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P31335
A	-18	GLY	-	expression tag	UNP P31335
A	-17	SER	-	expression tag	UNP P31335
A	-16	SER	-	expression tag	UNP P31335
A	-15	HIS	-	expression tag	UNP P31335
A	-14	HIS	-	expression tag	UNP P31335
A	-13	HIS	-	expression tag	UNP P31335
A	-12	HIS	-	expression tag	UNP P31335
A	-11	HIS	-	expression tag	UNP P31335
A	-10	HIS	-	expression tag	UNP P31335
A	-9	SER	-	expression tag	UNP P31335
A	-8	SER	-	insertion	UNP P31335
A	-7	GLY	-	expression tag	UNP P31335
A	-6	LEU	-	expression tag	UNP P31335
A	-5	VAL	-	expression tag	UNP P31335
A	-4	PRO	-	expression tag	UNP P31335
A	-3	ARG	-	expression tag	UNP P31335
A	-2	GLY	-	expression tag	UNP P31335
A	-1	SER	-	expression tag	UNP P31335
A	0	HIS	-	expression tag	UNP P31335
B	-19	MET	-	expression tag	UNP P31335
B	-18	GLY	-	expression tag	UNP P31335
B	-17	SER	-	expression tag	UNP P31335
B	-16	SER	-	expression tag	UNP P31335
B	-15	HIS	-	expression tag	UNP P31335

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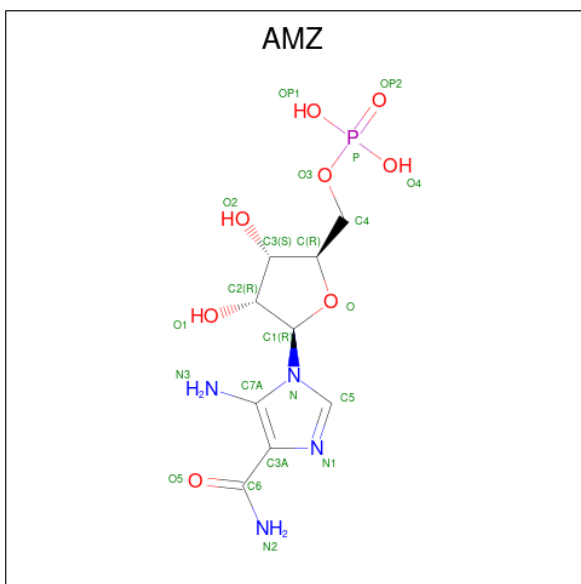
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P31335
B	-13	HIS	-	expression tag	UNP P31335
B	-12	HIS	-	expression tag	UNP P31335
B	-11	HIS	-	expression tag	UNP P31335
B	-10	HIS	-	expression tag	UNP P31335
B	-9	SER	-	expression tag	UNP P31335
B	-8	SER	-	expression tag	UNP P31335
B	-7	GLY	-	expression tag	UNP P31335
B	-6	LEU	-	expression tag	UNP P31335
B	-5	VAL	-	expression tag	UNP P31335
B	-4	PRO	-	expression tag	UNP P31335
B	-3	ARG	-	expression tag	UNP P31335
B	-2	GLY	-	expression tag	UNP P31335
B	-1	SER	-	expression tag	UNP P31335
B	0	HIS	-	expression tag	UNP P31335

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

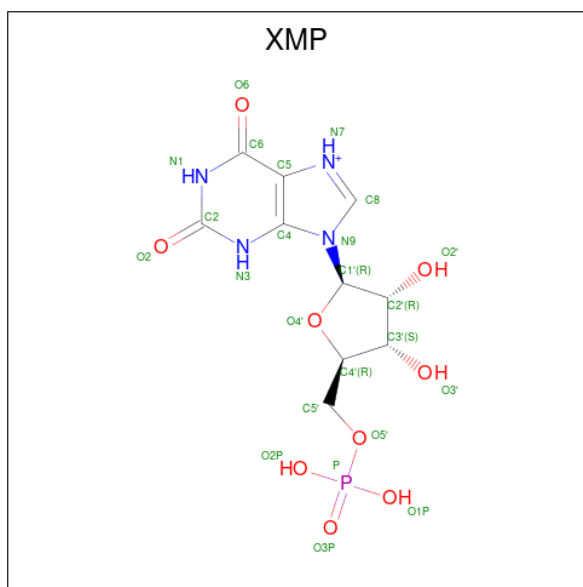
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0

- Molecule 3 is AMINOIMIDAZOLE 4-CARBOXAMIDE RIBONUCLEOTIDE (three-letter code: AMZ) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>4</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	9	4	8	1		
3	B	1	Total	C	N	O	P	0	0
			22	9	4	8	1		

- Molecule 4 is XANTHOSINE-5'-MONOPHOSPHATE (three-letter code: XMP) (formula:  $C_{10}H_{14}N_4O_9P$ ).



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

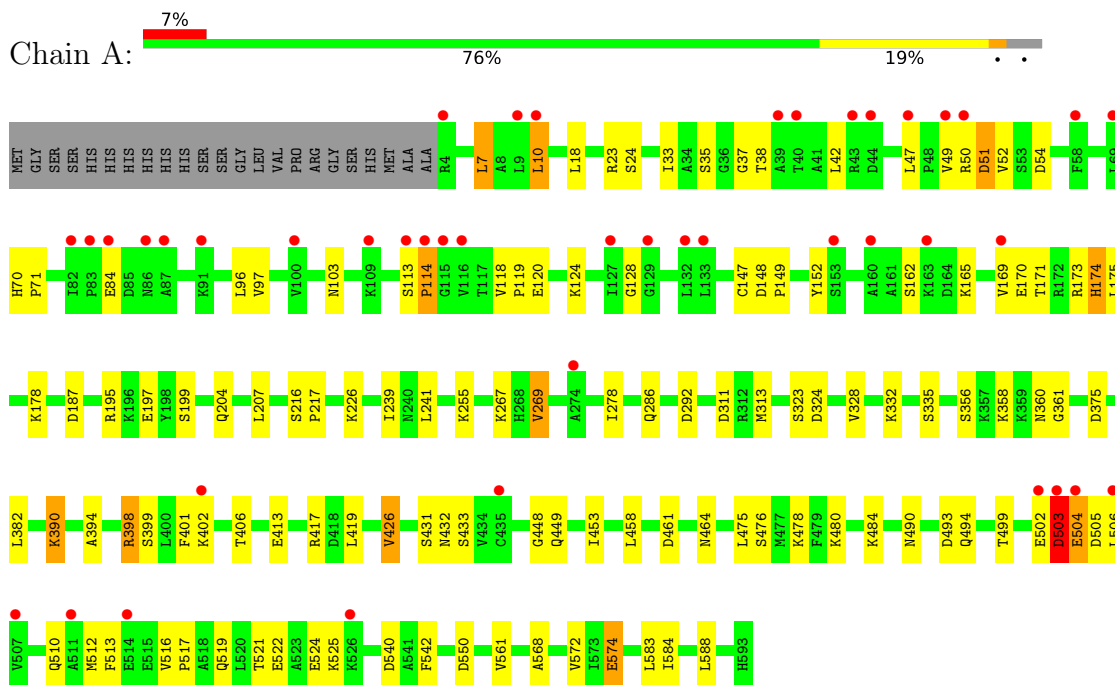
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	295	Total	O	0	0
			295	295		
5	B	216	Total	O	0	0
			216	216		

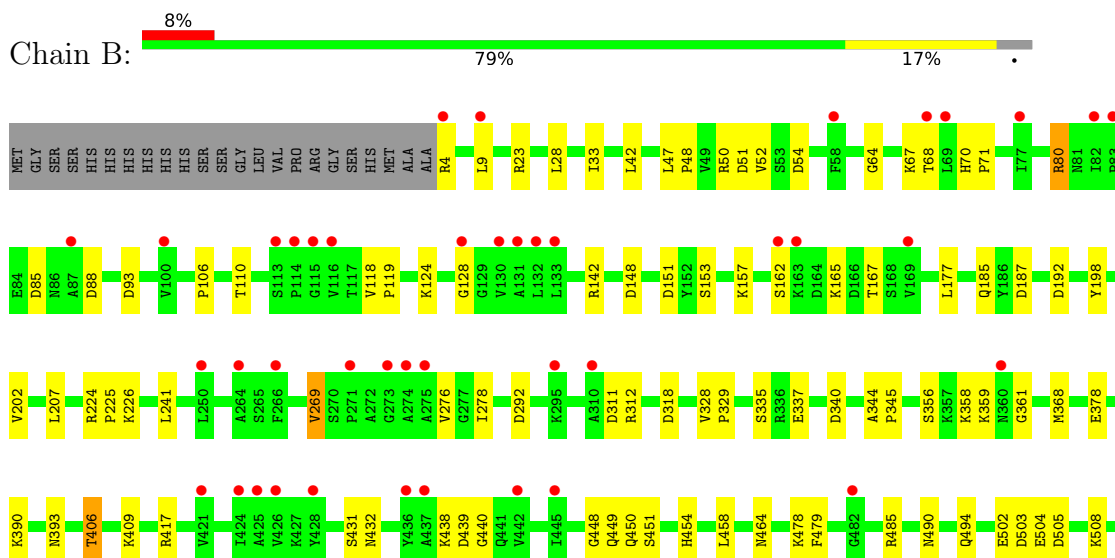
### 3 Residue-property plots i

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: AICAR TRANSFORMYLASE-IMP CYCLOHYDROLASE



#### • Molecule 1: AICAR TRANSFORMYLASE-IMP CYCLOHYDROLASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.48Å 107.88Å 103.86Å 90.00° 91.20° 90.00°	Depositor
Resolution (Å)	29.24 – 1.93 29.24 – 1.93	Depositor EDS
% Data completeness (in resolution range)	90.8 (29.24-1.93) 89.1 (29.24-1.93)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.56 (at 1.93Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.206 , 0.244 0.208 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtrriage
Anisotropy	0.579	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.011 for -h,-l,-k 0.005 for -h,l,k 0.031 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9625	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.49	0/4594	0.77	10/6229 (0.2%)
1	B	0.40	0/4594	0.75	15/6229 (0.2%)
All	All	0.45	0/9188	0.76	25/12458 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ASP	CB-CG-OD2	7.16	124.74	118.30
1	A	550	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	503	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	550	ASP	CB-CG-OD2	6.10	123.79	118.30
1	B	88	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	93	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	505	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	318	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	292	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	493	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	503	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	187	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	311	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	148	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	54	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	311	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	439	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	51	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	192	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	54	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	151	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	324	ASP	CB-CG-OD2	5.08	122.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	505	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	292	ASP	CB-CG-OD2	5.02	122.82	118.30

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	4510	0	4559	99	0
1	B	4510	0	4560	78	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	0	13	1	0
3	B	22	0	13	6	0
4	A	24	0	12	4	0
4	B	24	0	12	2	0
5	A	295	0	0	8	0
5	B	216	0	0	14	0
All	All	9625	0	9169	169	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 9.

All (169) 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:393:ASN:HB3	5:B:1035:HOH:O	1.42	1.15
1:A:390:LYS:HG2	5:A:1230:HOH:O	1.71	0.90
1:A:399:SER:HB3	1:A:402:LYS:HE3	1.55	0.86
1:A:171:THR:O	1:A:175:LEU:HD23	1.77	0.85
1:B:278:ILE:CD1	1:B:440:GLY:HA3	2.09	0.83
1:B:278:ILE:HD11	1:B:417:ARG:HD2	1.60	0.82
1:B:153:SER:O	1:B:157:LYS:HG2	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ILE:CD1	1:A:417:ARG:NH1	2.48	0.77
1:A:197:GLU:HG2	5:A:1107:HOH:O	1.85	0.75
1:A:207:LEU:O	5:A:1206:HOH:O	2.03	0.75
1:A:278:ILE:HD13	1:A:417:ARG:NH1	2.02	0.74
1:B:278:ILE:HD13	1:B:440:GLY:HA3	1.71	0.73
1:A:522:GLU:OE2	1:A:525:LYS:HE3	1.91	0.70
1:A:521:THR:OG1	1:A:524:GLU:HG3	1.92	0.70
1:A:84:GLU:H	1:A:84:GLU:CD	1.95	0.69
1:A:226:LYS:HE3	5:A:1173:HOH:O	1.92	0.69
1:A:568:ALA:O	1:A:572:VAL:HG23	1.93	0.69
3:B:1002:AMZ:N3	5:B:1005:HOH:O	2.26	0.68
1:B:537:LEU:C	1:B:537:LEU:HD23	2.14	0.68
1:A:313:MET:CE	1:B:454:HIS:HE1	2.07	0.68
1:B:23:ARG:NH2	5:B:1176:HOH:O	2.28	0.67
1:B:337:GLU:OE2	1:B:485:ARG:NH2	2.25	0.67
3:B:1002:AMZ:OP2	5:B:1042:HOH:O	2.12	0.66
1:B:378:GLU:OE2	5:B:1007:HOH:O	2.14	0.66
1:A:390:LYS:CG	5:A:1230:HOH:O	2.38	0.65
1:A:458:LEU:C	1:A:458:LEU:HD23	2.15	0.65
1:B:478:LYS:NZ	5:B:1194:HOH:O	2.28	0.65
1:A:71:PRO:HG3	1:B:70:HIS:CE1	2.31	0.65
1:B:513:PHE:CD2	1:B:517:PRO:HD3	2.32	0.64
1:A:35:SER:OG	4:A:1003:XMP:O3P	2.10	0.62
1:A:113:SER:HB2	1:A:114:PRO:HD2	1.80	0.61
1:B:80:ARG:HG2	1:B:85:ASP:OD2	1.99	0.61
1:B:335:SER:HA	1:B:358:LYS:HD2	1.83	0.61
1:A:84:GLU:N	1:A:84:GLU:OE1	2.28	0.60
1:B:431:SER:HB3	1:B:432:ASN:HA	1.83	0.60
1:B:464:ASN:ND2	1:B:555:ILE:HD13	2.17	0.60
1:A:118:VAL:HB	1:A:119:PRO:HD3	1.83	0.60
1:A:574:GLU:OE1	1:A:574:GLU:HA	2.00	0.59
1:B:64:GLY:O	1:B:67:LYS:HD2	2.01	0.59
1:A:71:PRO:CG	1:B:70:HIS:ND1	2.67	0.58
1:A:313:MET:HE2	1:B:454:HIS:HE1	1.69	0.57
1:A:426:VAL:HG13	1:A:540:ASP:HB3	1.87	0.57
1:A:7:LEU:HD13	1:A:97:VAL:HG22	1.87	0.57
1:A:494:GLN:NE2	1:A:499:THR:O	2.32	0.56
1:A:458:LEU:HD23	1:A:458:LEU:O	2.05	0.56
1:A:10:LEU:HD21	1:A:18:LEU:HD13	1.88	0.55
1:A:148:ASP:N	5:A:1090:HOH:O	2.14	0.55
1:A:10:LEU:HD13	1:A:42:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:HIS:CE1	1:A:175:LEU:HD22	2.40	0.55
1:A:406:THR:HG23	1:A:583:LEU:HB3	1.89	0.55
1:A:10:LEU:CD2	1:A:18:LEU:CD1	2.85	0.55
1:A:71:PRO:HG3	1:B:70:HIS:ND1	2.22	0.55
1:A:10:LEU:HD21	1:A:18:LEU:CD1	2.37	0.54
1:B:464:ASN:HD22	1:B:555:ILE:HD13	1.72	0.54
1:B:537:LEU:HD23	1:B:538:SER:N	2.22	0.54
1:A:286:GLN:HG2	1:A:475:LEU:HD22	1.90	0.54
1:A:37:GLY:HA3	4:A:1003:XMP:O2P	2.08	0.53
1:A:431:SER:HB3	1:A:432:ASN:HA	1.89	0.53
1:A:278:ILE:HD11	1:A:417:ARG:NH1	2.24	0.53
1:A:7:LEU:HD12	1:A:96:LEU:O	2.08	0.53
1:A:128:GLY:HA3	4:A:1003:XMP:C6	2.39	0.53
1:B:202:VAL:HG13	1:B:226:LYS:HG2	1.90	0.53
1:B:431:SER:CB	1:B:432:ASN:HA	2.39	0.53
1:B:344:ALA:HB1	1:B:345:PRO:HD2	1.90	0.52
1:A:49:VAL:HG22	1:A:50:ARG:N	2.24	0.52
1:A:313:MET:HE3	1:B:454:HIS:HE1	1.74	0.52
1:A:71:PRO:CG	1:B:70:HIS:CE1	2.93	0.52
1:B:28:LEU:O	1:B:165:LYS:HD3	2.09	0.52
1:B:490:ASN:HB3	5:B:1202:HOH:O	2.10	0.52
1:B:504:GLU:O	1:B:508:LYS:HG3	2.10	0.52
1:A:335:SER:HA	1:A:358:LYS:HD2	1.92	0.51
1:A:432:ASN:OD1	1:A:449:GLN:HB2	2.11	0.51
1:B:431:SER:O	1:B:448:GLY:HA2	2.11	0.51
1:A:267:LYS:HG2	1:B:450:GLN:HB3	1.93	0.51
1:B:185:GLN:NE2	5:B:1204:HOH:O	2.44	0.51
1:B:224:ARG:HB3	1:B:225:PRO:CD	2.41	0.50
1:A:147:CYS:N	5:A:1090:HOH:O	2.37	0.50
1:A:431:SER:O	1:A:448:GLY:HA2	2.11	0.50
1:B:224:ARG:HB3	1:B:225:PRO:HD2	1.94	0.50
1:A:480:LYS:HE3	1:A:513:PHE:O	2.12	0.50
1:B:23:ARG:HG2	1:B:47:LEU:HD21	1.94	0.50
1:A:476:SER:O	1:A:478:LYS:CD	2.60	0.49
1:A:394:ALA:CB	1:A:588:LEU:HD11	2.42	0.49
1:A:103:ASN:O	4:A:1003:XMP:O3'	2.21	0.49
1:A:207:LEU:HD21	1:A:241:LEU:CD1	2.43	0.49
1:A:401:PHE:HA	1:A:584:ILE:HG21	1.94	0.49
1:A:476:SER:O	1:A:478:LYS:HD2	2.12	0.49
1:A:313:MET:CE	1:B:454:HIS:CE1	2.94	0.48
3:B:1002:AMZ:O3	3:B:1002:AMZ:H13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:PHE:CZ	1:B:513:PHE:HE1	2.32	0.48
1:B:9:LEU:HA	1:B:33:ILE:HG13	1.95	0.48
1:A:399:SER:O	1:A:402:LYS:HG3	2.12	0.48
1:A:313:MET:HE3	1:B:454:HIS:CE1	2.48	0.47
1:A:195:ARG:HG2	1:A:204:GLN:HB2	1.96	0.47
1:A:120:GLU:O	1:A:124:LYS:HD3	2.14	0.47
1:B:207:LEU:HD21	1:B:241:LEU:HD11	1.95	0.47
1:B:390:LYS:NZ	1:B:393:ASN:OD1	2.47	0.47
1:A:375:ASP:HB3	5:A:1224:HOH:O	2.14	0.47
1:B:356:SER:O	1:B:361:GLY:HA2	2.15	0.47
1:B:479:PHE:CZ	1:B:513:PHE:CE1	3.03	0.46
1:A:458:LEU:C	1:A:458:LEU:CD2	2.83	0.46
1:A:70:HIS:ND1	1:B:71:PRO:HG3	2.30	0.46
1:A:278:ILE:HD11	1:A:417:ARG:HD2	1.97	0.46
1:B:432:ASN:OD1	1:B:449:GLN:HB2	2.16	0.46
1:A:490:ASN:O	1:A:494:GLN:HG3	2.16	0.45
1:A:173:ARG:HB3	1:B:198:TYR:CD2	2.51	0.45
1:A:356:SER:O	1:A:361:GLY:HA2	2.16	0.45
1:A:516:VAL:HA	1:A:517:PRO:HD3	1.81	0.45
1:B:552:ALA:HB1	1:B:557:VAL:HG21	1.99	0.45
1:B:340:ASP:OD1	1:B:359:LYS:NZ	2.31	0.45
1:A:542:PHE:CE2	3:B:1002:AMZ:N2	2.79	0.45
1:B:555:ILE:O	1:B:555:ILE:HG13	2.16	0.45
3:B:1002:AMZ:N2	5:B:1028:HOH:O	2.36	0.45
1:A:419:LEU:HD22	1:A:561:VAL:HG12	1.98	0.44
1:A:510:GLN:HE21	1:A:516:VAL:HG11	1.82	0.44
1:B:479:PHE:CE2	1:B:513:PHE:CE1	3.05	0.44
1:B:278:ILE:HD12	1:B:440:GLY:HA3	1.95	0.44
1:B:110:THR:HG21	1:B:124:LYS:HG3	1.99	0.44
1:B:128:GLY:HA3	4:B:1004:XMP:C6	2.46	0.44
1:A:10:LEU:CD2	1:A:18:LEU:HD13	2.47	0.44
1:A:149:PRO:HA	1:A:152:TYR:CZ	2.53	0.44
1:B:513:PHE:HB3	1:B:515:GLU:O	2.17	0.44
3:B:1002:AMZ:H13	3:B:1002:AMZ:H4	1.99	0.44
1:A:399:SER:CB	1:A:402:LYS:HE3	2.38	0.44
1:B:33:ILE:HG22	1:B:50:ARG:HB3	1.99	0.44
1:B:52:VAL:HB	5:B:1160:HOH:O	2.17	0.44
1:B:490:ASN:O	1:B:494:GLN:HG3	2.17	0.44
1:B:68:THR:HG23	4:B:1004:XMP:H7	1.83	0.44
1:B:328:VAL:N	1:B:329:PRO:CD	2.81	0.44
1:A:207:LEU:HD21	1:A:241:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ILE:HB	3:A:1001:AMZ:H8	2.01	0.43
1:A:255:LYS:HD3	1:A:323:SER:HB2	2.00	0.43
1:B:276:VAL:HG23	1:B:278:ILE:HD12	2.00	0.43
1:B:458:LEU:HG	5:B:1138:HOH:O	2.17	0.43
1:A:278:ILE:CD1	1:A:417:ARG:CZ	2.96	0.43
1:A:461:ASP:O	1:A:464:ASN:HB2	2.18	0.43
1:A:118:VAL:N	1:A:119:PRO:CD	2.82	0.43
1:A:398:ARG:NH2	1:A:413:GLU:OE1	2.48	0.43
1:A:149:PRO:HA	1:A:152:TYR:CE1	2.54	0.43
1:B:328:VAL:HB	1:B:329:PRO:HD3	2.00	0.43
1:A:174:HIS:ND1	1:A:175:LEU:HD22	2.34	0.43
1:B:47:LEU:HA	1:B:48:PRO:HD3	1.90	0.43
1:B:345:PRO:HA	1:B:368:MET:O	2.19	0.43
1:A:506:LEU:O	1:A:510:GLN:HG3	2.19	0.42
1:A:71:PRO:HG2	1:B:70:HIS:ND1	2.33	0.42
1:A:426:VAL:CG1	1:A:540:ASP:HB3	2.50	0.42
1:B:479:PHE:CE1	1:B:513:PHE:HE1	2.37	0.42
1:B:432:ASN:OD1	1:B:432:ASN:C	2.58	0.42
1:A:216:SER:HB2	1:A:217:PRO:HA	2.00	0.42
1:A:10:LEU:HD22	1:A:38:THR:HG21	2.02	0.42
1:A:328:VAL:O	1:A:332:LYS:HG3	2.20	0.42
1:B:438:LYS:HD2	1:B:532:LEU:HD11	2.00	0.42
1:A:33:ILE:HA	1:A:50:ARG:O	2.20	0.42
1:B:118:VAL:N	1:B:119:PRO:CD	2.82	0.42
1:B:494:GLN:NE2	5:B:1153:HOH:O	2.42	0.42
1:A:169:VAL:CG2	1:A:170:GLU:N	2.83	0.42
1:B:142:ARG:NH1	5:B:1110:HOH:O	2.18	0.41
1:B:406:THR:HG23	1:B:583:LEU:HB3	2.02	0.41
1:A:10:LEU:CD2	1:A:18:LEU:HD11	2.51	0.41
1:A:503:ASP:HB2	1:A:504:GLU:H	1.74	0.41
1:A:49:VAL:CG2	1:A:50:ARG:N	2.82	0.41
1:B:4:ARG:O	5:B:1195:HOH:O	2.22	0.41
1:B:42:LEU:HD22	1:B:47:LEU:HD12	2.02	0.41
1:A:278:ILE:HD11	1:A:417:ARG:CD	2.51	0.40
1:B:516:VAL:HA	1:B:517:PRO:HD3	1.83	0.40
1:B:537:LEU:C	1:B:537:LEU:CD2	2.87	0.40
1:A:23:ARG:HG2	1:A:47:LEU:HD21	2.02	0.40
1:A:174:HIS:CE1	1:A:175:LEU:CD2	3.04	0.40
1:A:162:SER:OG	1:A:165:LYS:N	2.55	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	588/613 (96%)	571 (97%)	14 (2%)	3 (0%)	29	17
1	B	588/613 (96%)	576 (98%)	11 (2%)	1 (0%)	47	39
All	All	1176/1226 (96%)	1147 (98%)	25 (2%)	4 (0%)	41	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
1	A	502	GLU
1	A	269	VAL
1	B	269	VAL

### 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	484/502 (96%)	462 (96%)	22 (4%)	27	12
1	B	484/502 (96%)	473 (98%)	11 (2%)	50	38
All	All	968/1004 (96%)	935 (97%)	33 (3%)	37	22

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	10	LEU

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Mol	Chain	Res	Type
1	A	24	SER
1	A	51	ASP
1	A	52	VAL
1	A	174	HIS
1	A	178	LYS
1	A	199	SER
1	A	269	VAL
1	A	360	ASN
1	A	382	LEU
1	A	390	LYS
1	A	398	ARG
1	A	426	VAL
1	A	433	SER
1	A	453	ILE
1	A	484	LYS
1	A	503	ASP
1	A	504	GLU
1	A	512	MET
1	A	519	GLN
1	A	574	GLU
1	B	80	ARG
1	B	106	PRO
1	B	162	SER
1	B	167	THR
1	B	177	LEU
1	B	269	VAL
1	B	312	ARG
1	B	406	THR
1	B	409	LYS
1	B	451	SER
1	B	502	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	185	GLN
1	A	464	ASN
1	A	510	GLN
1	B	90	ASN
1	B	464	ASN
1	B	490	ASN



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AMZ	A	1001	-	18,23,23	1.25	2 (11%)	22,35,35	2.23	6 (27%)
4	XMP	B	1004	-	20,26,26	1.33	2 (10%)	27,40,40	4.29	7 (25%)
4	XMP	A	1003	-	20,26,26	1.79	4 (20%)	27,40,40	4.37	6 (22%)
3	AMZ	B	1002	-	18,23,23	1.38	2 (11%)	22,35,35	2.07	5 (22%)

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	AMZ	A	1001	-	-	0/6/30/30	0/2/2/2
4	XMP	B	1004	-	-	0/6/26/26	0/3/3/3
4	XMP	A	1003	-	-	3/6/26/26	0/3/3/3
3	AMZ	B	1002	-	-	0/6/30/30	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	XMP	C5-C6	4.39	1.56	1.47
3	B	1002	AMZ	C7A-N3	3.47	1.44	1.33
3	B	1002	AMZ	P-OP2	3.32	1.61	1.50
4	A	1003	XMP	P-O3P	3.29	1.61	1.50
4	A	1003	XMP	C8-N7	3.12	1.40	1.35
4	B	1004	XMP	C5-C6	3.12	1.53	1.47
3	A	1001	AMZ	C7A-N3	3.11	1.43	1.33
4	B	1004	XMP	P-O3P	2.94	1.60	1.50
3	A	1001	AMZ	P-OP2	2.84	1.59	1.50
4	A	1003	XMP	C2-N1	2.75	1.42	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1004	XMP	N3-C2-N1	16.77	125.65	115.90
4	A	1003	XMP	N3-C2-N1	14.89	124.55	115.90
4	A	1003	XMP	C6-N1-C2	-11.75	117.61	126.88
4	A	1003	XMP	C4-N3-C2	-10.24	112.11	128.11
4	B	1004	XMP	C6-N1-C2	-8.98	119.80	126.88
4	B	1004	XMP	C4-N3-C2	-8.11	115.44	128.11
3	A	1001	AMZ	O-C1-C2	6.92	117.04	106.93
3	B	1002	AMZ	O-C1-C2	6.49	116.41	106.93
4	B	1004	XMP	O2-C2-N3	-5.29	114.44	122.08
4	A	1003	XMP	O2-C2-N3	-3.67	116.79	122.08
4	A	1003	XMP	C3'-C2'-C1'	3.62	106.43	100.98
3	B	1002	AMZ	O5-C6-N2	-3.56	117.52	122.58
3	A	1001	AMZ	C3A-C6-N2	3.41	121.14	115.75
4	B	1004	XMP	C8-N7-C5	-3.24	96.82	102.99
3	A	1001	AMZ	O5-C6-N2	-3.21	118.01	122.58
3	B	1002	AMZ	O-C-C3	2.99	111.02	105.11
4	A	1003	XMP	C8-N7-C5	-2.98	97.31	102.99
3	A	1001	AMZ	O-C-C3	2.65	110.36	105.11
3	A	1001	AMZ	C3-C2-C1	-2.64	97.01	100.98
4	B	1004	XMP	C5-C6-N1	2.60	118.54	113.95
3	A	1001	AMZ	O4-P-O3	2.53	113.47	106.73
3	B	1002	AMZ	C3-C2-C1	-2.46	97.28	100.98
3	B	1002	AMZ	O5-C6-C3A	2.28	125.37	119.89
4	B	1004	XMP	C3'-C2'-C1'	2.06	104.09	100.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

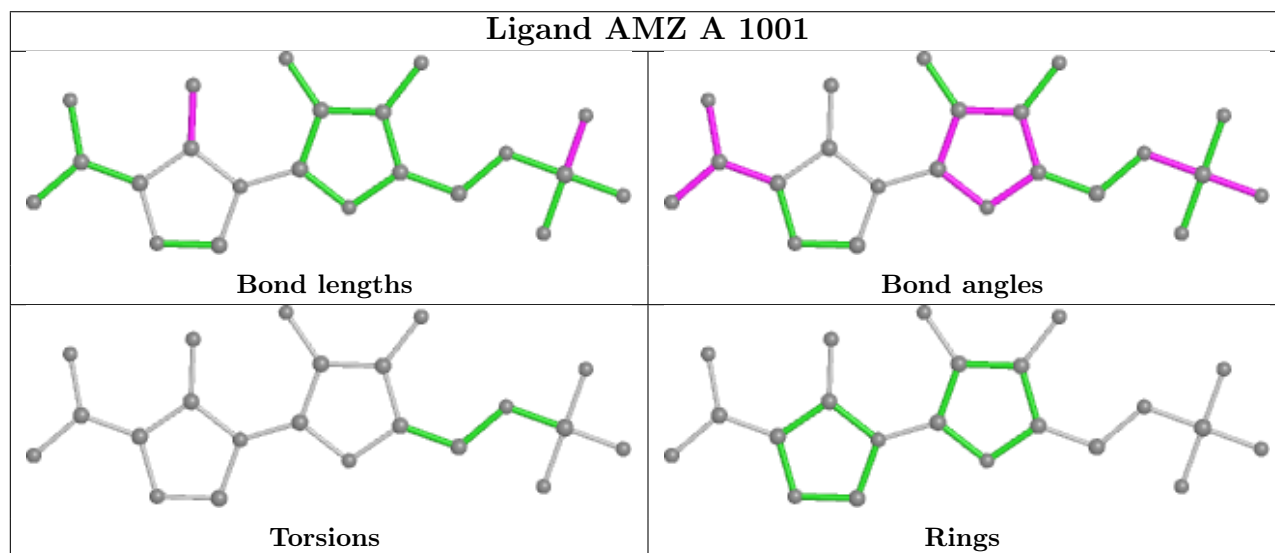
Mol	Chain	Res	Type	Atoms
4	A	1003	XMP	C5'-O5'-P-O1P
4	A	1003	XMP	C5'-O5'-P-O2P
4	A	1003	XMP	C5'-O5'-P-O3P

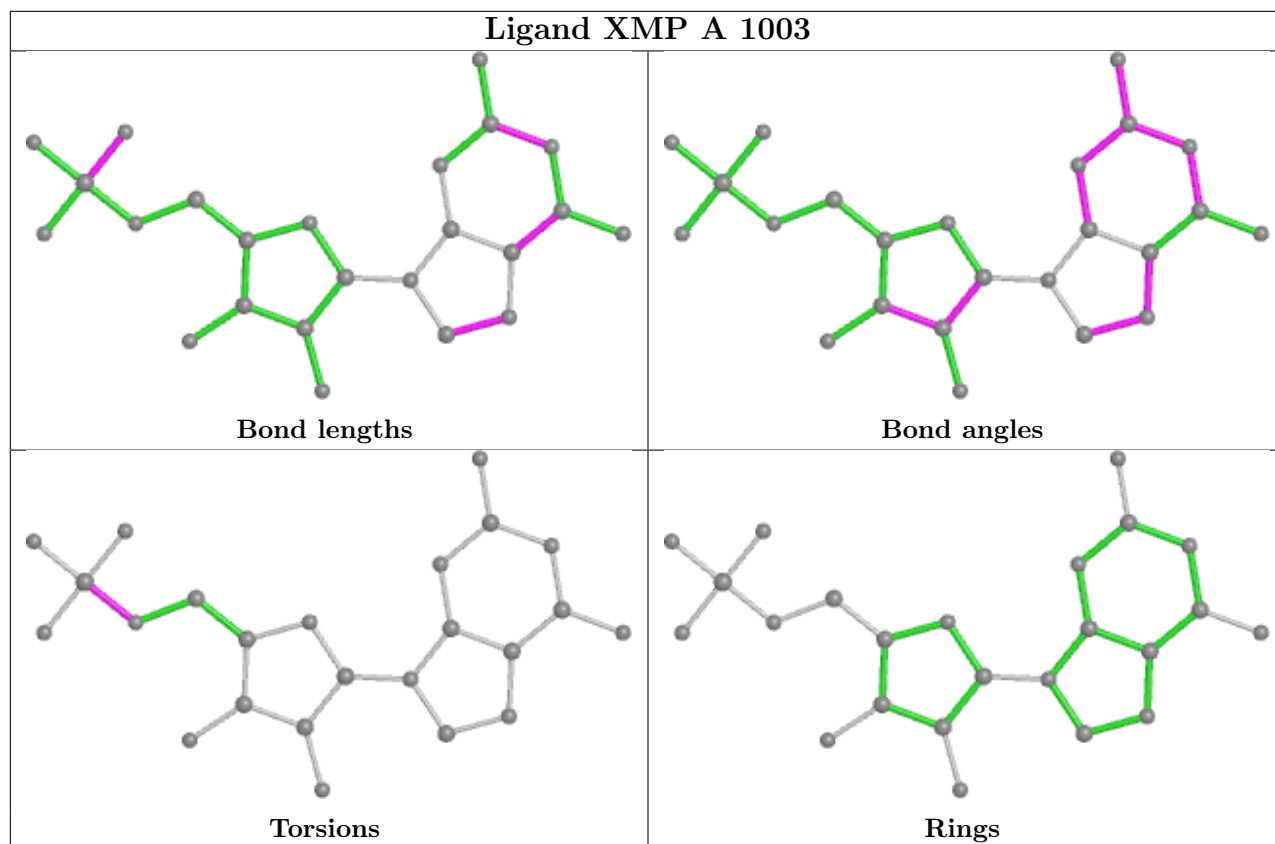
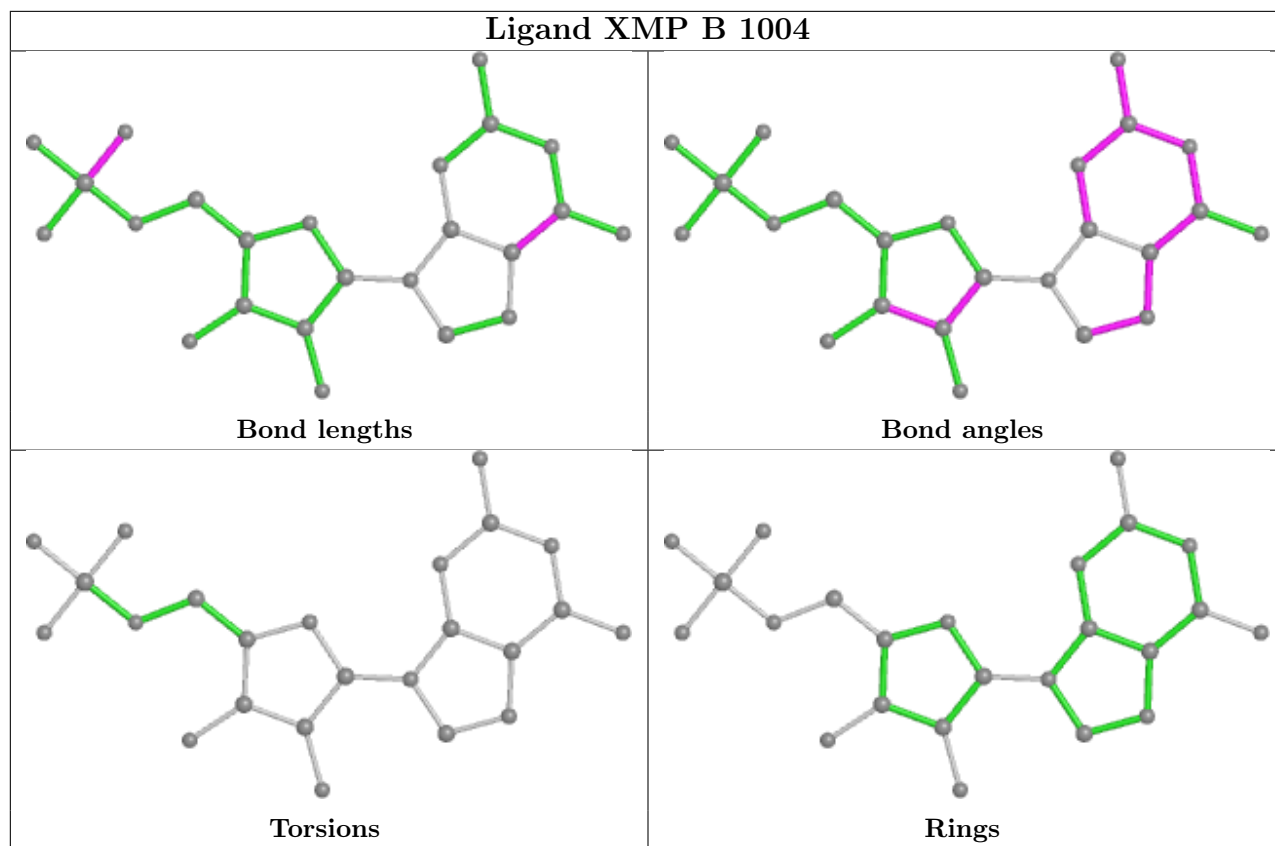
There are no ring outliers.

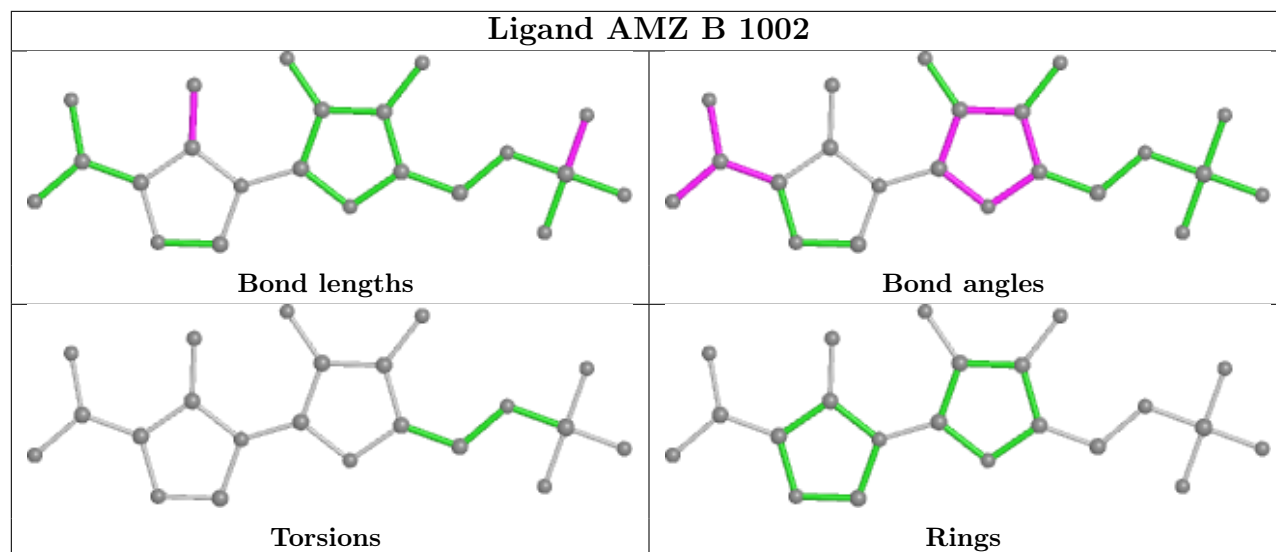
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	AMZ	1	0
4	B	1004	XMP	2	0
4	A	1003	XMP	4	0
3	B	1002	AMZ	6	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 [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<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	590/613 (96%)	0.39	43 (7%) 15 21	3, 9, 19, 26	0
1	B	590/613 (96%)	0.43	49 (8%) 11 16	3, 9, 18, 25	0
All	All	1180/1226 (96%)	0.41	92 (7%) 13 18	3, 9, 19, 26	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	ALA	6.4
1	A	114	PRO	5.1
1	A	502	GLU	4.7
1	B	114	PRO	4.6
1	A	504	GLU	4.6
1	B	4	ARG	4.4
1	B	163	LYS	4.2
1	B	82	ILE	4.2
1	B	274	ALA	4.1
1	A	163	LYS	4.0
1	B	132	LEU	3.9
1	A	49	VAL	3.8
1	B	250	LEU	3.7
1	B	513	PHE	3.6
1	B	69	LEU	3.6
1	A	4	ARG	3.6
1	B	360	ASN	3.5
1	B	295	LYS	3.4
1	B	424	ILE	3.3
1	A	160	ALA	3.3
1	A	83	PRO	3.3
1	A	69	LEU	3.3
1	B	115	GLY	3.2
1	B	83	PRO	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	507	VAL	3.2
1	B	273	GLY	3.2
1	B	116	VAL	3.1
1	B	421	VAL	3.1
1	A	113	SER	3.1
1	B	9	LEU	3.1
1	B	482	GLY	3.1
1	A	84	GLU	2.9
1	B	275	ALA	2.9
1	B	113	SER	2.9
1	B	133	LEU	2.9
1	B	515	GLU	2.8
1	B	567	ALA	2.8
1	B	521	THR	2.8
1	B	100	VAL	2.8
1	B	169	VAL	2.8
1	A	87	ALA	2.7
1	A	91	LYS	2.7
1	B	264	ALA	2.7
1	B	128	GLY	2.6
1	A	503	ASP	2.5
1	A	169	VAL	2.5
1	A	274	ALA	2.5
1	B	520	LEU	2.5
1	A	9	LEU	2.5
1	B	131	ALA	2.5
1	B	518	ALA	2.4
1	A	40	THR	2.4
1	B	445	ILE	2.4
1	A	132	LEU	2.4
1	A	153	SER	2.4
1	B	425	ALA	2.4
1	A	86	ASN	2.4
1	A	127	ILE	2.4
1	B	130	VAL	2.4
1	A	47	LEU	2.3
1	B	310	ALA	2.3
1	A	100	VAL	2.3
1	B	87	ALA	2.3
1	B	442	VAL	2.3
1	A	82	ILE	2.3
1	B	266	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	436	TYR	2.2
1	A	44	ASP	2.2
1	B	511	ALA	2.2
1	A	10	LEU	2.2
1	A	129	GLY	2.1
1	B	437	ALA	2.1
1	B	426	VAL	2.1
1	A	109	LYS	2.1
1	A	115	GLY	2.1
1	A	514	GLU	2.1
1	B	162	SER	2.1
1	B	271	PRO	2.1
1	A	435	CYS	2.1
1	A	133	LEU	2.1
1	A	506	LEU	2.1
1	A	58	PHE	2.1
1	A	402	LYS	2.1
1	A	43	ARG	2.0
1	B	428	TYR	2.0
1	A	116	VAL	2.0
1	A	526	LYS	2.0
1	A	50	ARG	2.0
1	A	511	ALA	2.0
1	B	58	PHE	2.0
1	B	77	ILE	2.0
1	B	68	THR	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 monosaccharides in this entry.

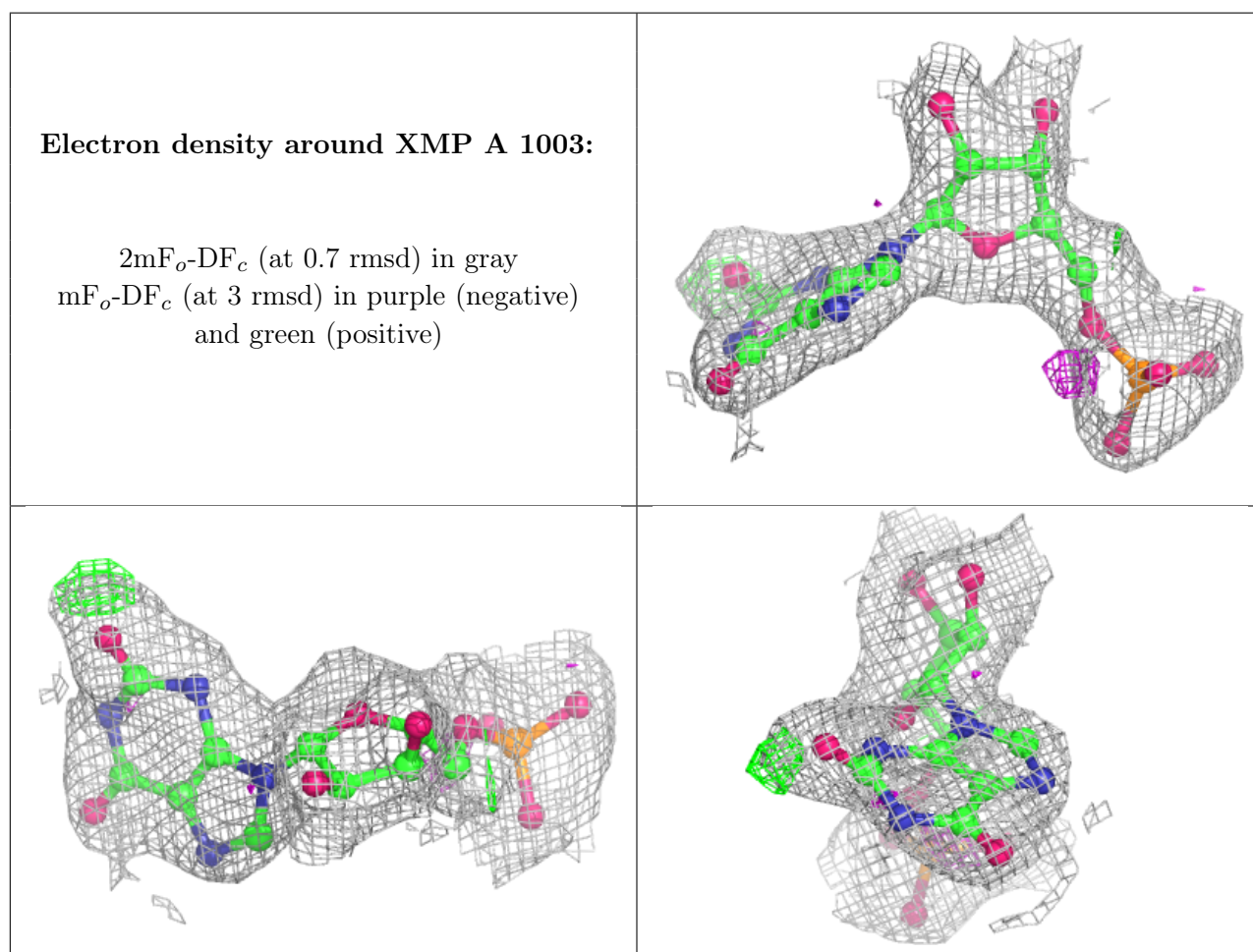
## 6.4 Ligands [\(i\)](#)

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<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.



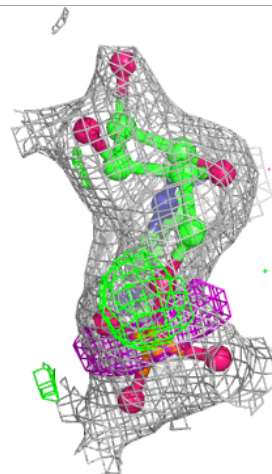
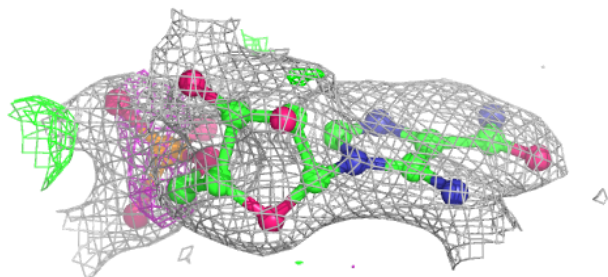
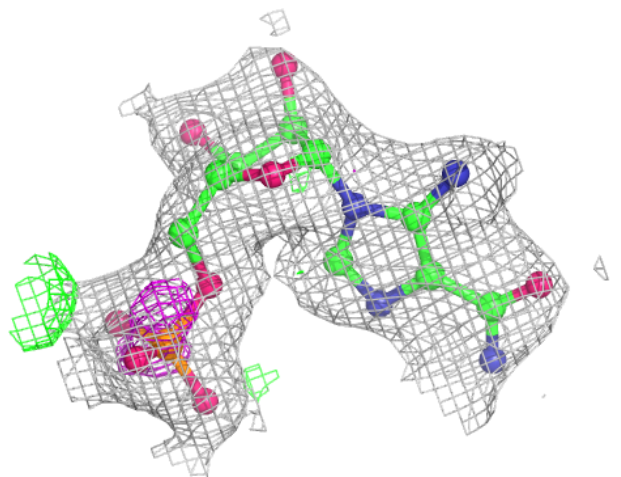
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	XMP	A	1003	24/24	0.89	0.13	61,62,63,64	0
3	AMZ	B	1002	22/22	0.93	0.14	47,57,63,64	0
3	AMZ	A	1001	22/22	0.94	0.14	42,49,53,56	0
4	XMP	B	1004	24/24	0.95	0.11	39,43,45,46	0
2	K	A	594	1/1	0.99	0.07	32,32,32,32	0
2	K	B	594	1/1	0.99	0.07	37,37,37,37	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.



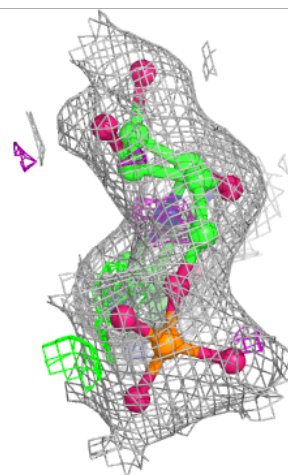
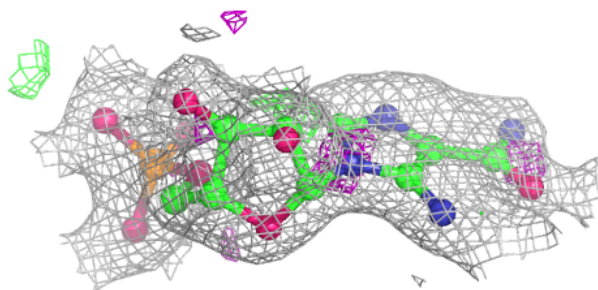
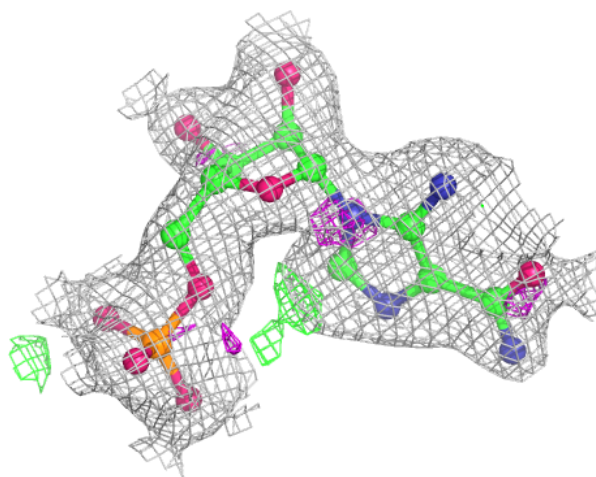
**Electron density around AMZ B 1002:**

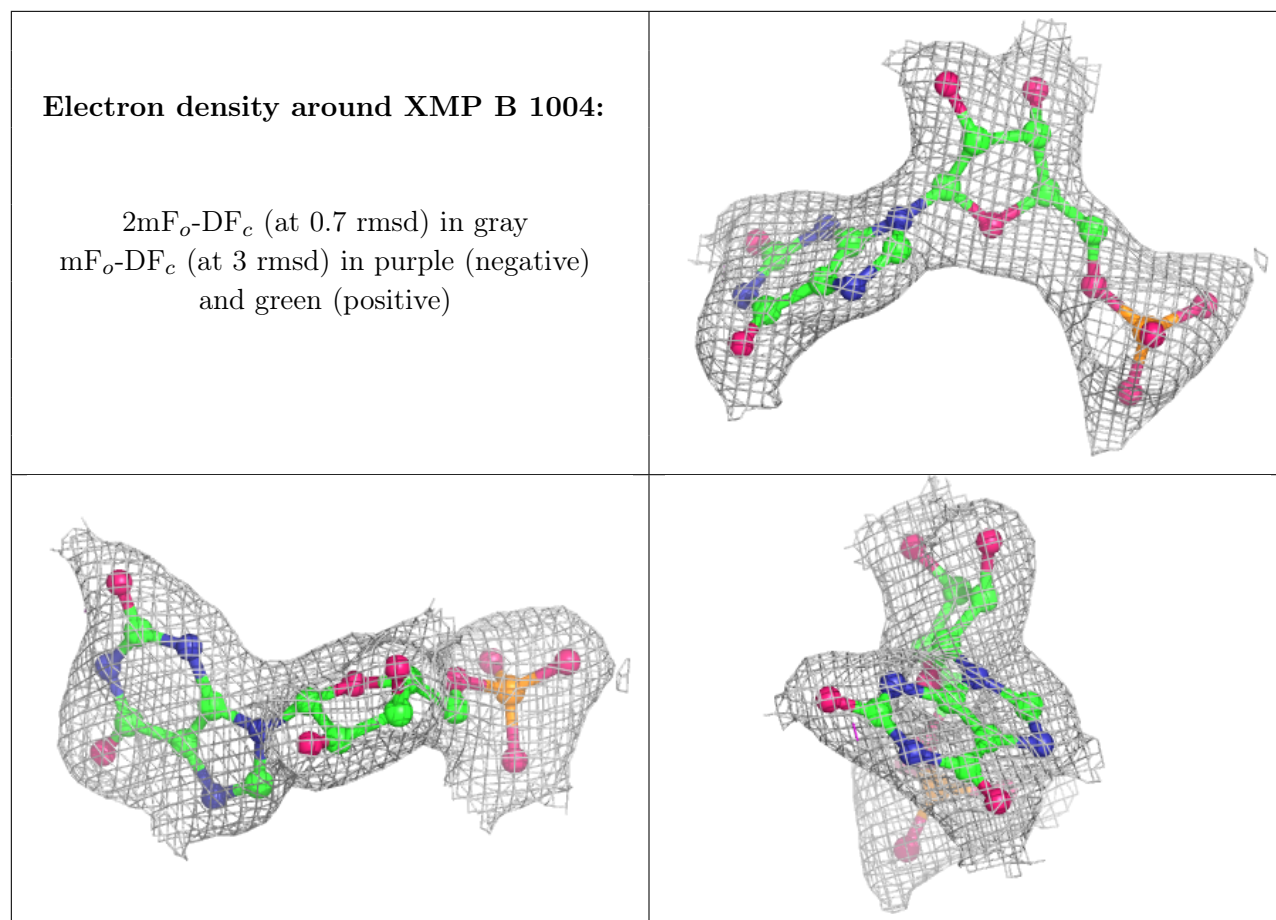
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around AMZ A 1001:**

$2mF_o-DF_c$  (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.