



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:47 PM UTC

PDB ID : 7ZH9 / pdb_00007zh9
Title : Uba1 in complex with ATP
Authors : Misra, M.; Schindelin, H.
Deposited on : 2022-04-05
Resolution : 1.72 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 types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

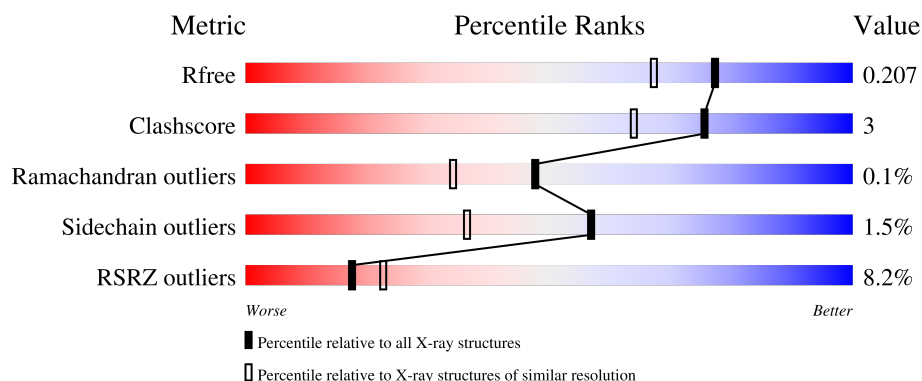
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

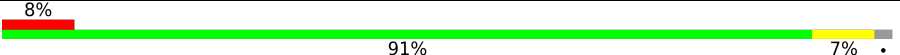
The reported resolution of this entry is 1.72 Å.

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}	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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

Mol	Chain	Length	Quality of chain
1	A	1024	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 17115 atoms, of which 8103 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 Ubiquitin-activating enzyme E1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1005	Total	C	H	N	O	S	0	26	0
			16075	5145	8017	1324	1564	25			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Mg	0	0
			3	3		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			13	3	7	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			12	3	6	3		
6	A	1	Total	C	H	O	0	0
			13	3	7	3		
6	A	1	Total	C	H	O	0	0
			12	3	6	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			11	3	5	3		

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total K 1 1	0	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

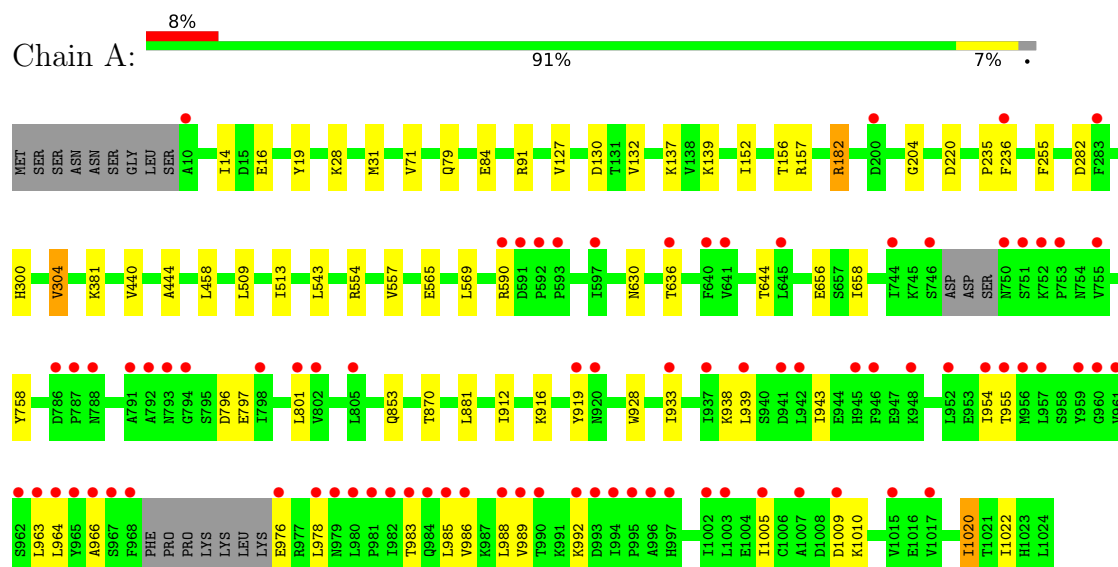
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	823	Total O 849 849	0	26

3 Residue-property plots

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: Ubiquitin-activating enzyme E1 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.72Å 118.06Å 196.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.24 – 1.72 47.24 – 1.72	Depositor EDS
% Data completeness (in resolution range)	69.3 (47.24-1.72) 64.8 (47.24-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.72Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660)	Depositor
R, R_{free}	0.165 , 0.206 0.167 , 0.207	Depositor DCC
R_{free} test set	4617 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17115	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ACT, K, CL, GOL, ATP, MG

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	0.48	0/8299	0.52	0/11228

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	919	TYR	Peptide

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	8058	8017	8018	46	0
2	A	31	12	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	1	0
4	A	4	3	3	0	0
5	A	3	0	0	0	0
6	A	60	71	80	1	0
7	A	1	0	0	0	0
8	A	1	0	0	1	0
9	A	849	0	0	9	0
All	All	9012	8103	8113	48	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 3.

All (48) 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:139:LYS:NZ	9:A:1206:HOH:O	2.18	0.70
1:A:1005:ILE:CG1	1:A:1020:ILE:HD11	2.22	0.70
1:A:84[A]:GLU:OE1	9:A:1201:HOH:O	2.11	0.69
1:A:758:TYR:OH	9:A:1202[A]:HOH:O	2.13	0.67
1:A:963:LEU:HD13	1:A:966:ALA:HB2	1.76	0.66
1:A:130:ASP:OD1	9:A:1203:HOH:O	2.13	0.65
1:A:282:ASP:O	9:A:1204:HOH:O	2.16	0.62
1:A:963:LEU:HD12	1:A:963:LEU:O	1.99	0.62
1:A:130:ASP:OD2	9:A:1205:HOH:O	2.16	0.60
8:A:1118:CL:CL	9:A:1577:HOH:O	2.55	0.55
1:A:71:VAL:HG22	1:A:91:ARG:HG2	1.88	0.54
1:A:954:ILE:CD1	1:A:1005:ILE:HD12	2.38	0.54
1:A:1005:ILE:HD11	1:A:1020:ILE:HD11	1.89	0.54
1:A:954:ILE:HD11	1:A:1005:ILE:HD12	1.92	0.52
1:A:796:ASP:OD1	1:A:797:GLU:N	2.43	0.51
6:A:1109:GOL:H12	9:A:1673:HOH:O	2.11	0.51
1:A:955:THR:O	1:A:955:THR:HG22	2.11	0.51
1:A:988:LEU:HD12	1:A:992:LYS:NZ	2.26	0.50
1:A:440:VAL:HG12	1:A:543:LEU:HD21	1.95	0.49
1:A:1005:ILE:CD1	1:A:1020:ILE:HD11	2.43	0.48
1:A:444:ALA:HB1	1:A:870:THR:HG21	1.97	0.47
1:A:939:LEU:HD23	1:A:978:LEU:HB2	1.95	0.47
1:A:978:LEU:HD13	1:A:985:LEU:HD13	1.98	0.46
1:A:989:VAL:HG12	1:A:989:VAL:O	2.16	0.46
1:A:127:VAL:HA	1:A:152:ILE:O	2.17	0.45
1:A:881:LEU:C	1:A:881:LEU:HD23	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:GLU:HG3	1:A:801:LEU:HD21	1.99	0.44
1:A:300:HIS:O	1:A:304:VAL:HG13	2.17	0.44
1:A:458:LEU:O	1:A:509[A]:LEU:HD11	2.18	0.43
1:A:1005:ILE:HG13	1:A:1020:ILE:HD11	1.99	0.43
1:A:16:GLU:OE2	1:A:853:GLN:HG2	2.19	0.43
1:A:933:ILE:HB	1:A:1022:ILE:HD13	1.99	0.43
1:A:1009:ASP:OD1	1:A:1010:LYS:N	2.41	0.43
1:A:235:PRO:HG2	1:A:236:PHE:CE2	2.54	0.43
1:A:912:ILE:HD12	1:A:912:ILE:N	2.34	0.42
1:A:554:ARG:NH2	9:A:1253:HOH:O	2.52	0.42
1:A:644:THR:O	1:A:644:THR:HG22	2.19	0.42
1:A:182[B]:ARG:CD	1:A:204:GLY:O	2.68	0.42
1:A:14:ILE:HD12	1:A:28:LYS:HG3	2.02	0.42
1:A:19:TYR:CG	1:A:31:MET:HE1	2.55	0.42
1:A:509[B]:LEU:HD23	1:A:513:ILE:HD11	2.02	0.42
1:A:557:VAL:HA	1:A:928:TRP:CZ3	2.54	0.41
1:A:381:LYS:CE	3:A:1102:SO4:O1	2.69	0.41
1:A:255:PHE:CD1	1:A:255:PHE:C	2.98	0.41
1:A:132:VAL:O	1:A:137:LYS:NZ	2.53	0.41
1:A:630:ASN:HB3	1:A:658:ILE:HD11	2.02	0.41
1:A:156:THR:O	1:A:157:ARG:HD3	2.22	0.40
1:A:964:LEU:HD11	1:A:986:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1025/1024 (100%)	988 (96%)	36 (4%)	1 (0%)	48 34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ASP

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	908/900 (101%)	893 (98%)	15 (2%)	53 31

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

Mol	Chain	Res	Type
1	A	79	GLN
1	A	182[A]	ARG
1	A	182[B]	ARG
1	A	304	VAL
1	A	565[A]	GLU
1	A	565[B]	GLU
1	A	569	LEU
1	A	590	ARG
1	A	636	THR
1	A	916	LYS
1	A	938	LYS
1	A	943	ILE
1	A	976	GLU
1	A	983	THR
1	A	1020	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	A	320	ASN
1	A	333	GLN
1	A	411	GLN
1	A	643	GLN
1	A	844	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 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	ACT	A	1103	-	3,3,3	1.19	0	3,3,3	1.44	0
6	GOL	A	1114	-	5,5,5	0.76	0	5,5,5	1.03	0
2	ATP	A	1101	5	32,33,33	1.74	8 (25%)	48,52,52	1.89	13 (27%)
6	GOL	A	1111	-	5,5,5	0.86	0	5,5,5	1.23	1 (20%)
6	GOL	A	1112	-	5,5,5	1.06	0	5,5,5	1.09	0
6	GOL	A	1108	-	5,5,5	0.83	0	5,5,5	1.17	1 (20%)
6	GOL	A	1116	-	5,5,5	1.03	0	5,5,5	1.41	1 (20%)
6	GOL	A	1109	-	5,5,5	1.05	0	5,5,5	1.07	0
6	GOL	A	1113	-	5,5,5	0.90	0	5,5,5	1.34	1 (20%)
6	GOL	A	1115	-	5,5,5	0.93	0	5,5,5	0.91	0
6	GOL	A	1110	-	5,5,5	0.60	0	5,5,5	0.83	0
6	GOL	A	1107	-	5,5,5	1.19	0	5,5,5	1.02	0
3	SO4	A	1102	-	4,4,4	0.23	0	6,6,6	0.11	0

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
6	GOL	A	1114	-	-	2/4/4/4	-
2	ATP	A	1101	5	-	6/22/38/38	0/3/3/3
6	GOL	A	1111	-	-	2/4/4/4	-
6	GOL	A	1112	-	-	2/4/4/4	-
6	GOL	A	1108	-	-	0/4/4/4	-
6	GOL	A	1116	-	-	0/4/4/4	-
6	GOL	A	1109	-	-	2/4/4/4	-
6	GOL	A	1113	-	-	2/4/4/4	-
6	GOL	A	1115	-	-	2/4/4/4	-
6	GOL	A	1110	-	-	0/4/4/4	-
6	GOL	A	1107	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	ATP	PB-O3A	-4.63	1.54	1.59
2	A	1101	ATP	C5-C4	4.10	1.46	1.39
2	A	1101	ATP	PA-O3A	3.47	1.63	1.59
2	A	1101	ATP	C8-N7	2.87	1.37	1.31
2	A	1101	ATP	PB-O3B	2.57	1.62	1.59
2	A	1101	ATP	PG-O2G	-2.40	1.45	1.54
2	A	1101	ATP	C5-C6	2.22	1.47	1.41
2	A	1101	ATP	O4'-C1'	2.19	1.47	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	ATP	C5-C4-N3	-4.60	120.39	126.72
2	A	1101	ATP	N3-C4-N9	4.41	134.66	127.17
2	A	1101	ATP	C4-N9-C8	4.05	109.99	105.74
2	A	1101	ATP	N3-C2-N1	-3.53	123.23	128.58
2	A	1101	ATP	O2B-PB-O3A	3.24	116.03	107.27
2	A	1101	ATP	C2-N3-C4	3.16	119.56	111.83
2	A	1101	ATP	O2A-PA-O1A	2.99	126.36	112.44
2	A	1101	ATP	O3B-PB-O1B	-2.77	102.39	110.70
6	A	1116	GOL	C3-C2-C1	-2.60	102.24	111.80
6	A	1113	GOL	C3-C2-C1	-2.51	102.58	111.80
2	A	1101	ATP	O4'-C1'-N9	2.22	112.35	108.09
6	A	1111	GOL	C3-C2-C1	-2.21	103.69	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	ATP	O2B-PB-O3B	2.14	113.06	107.27
2	A	1101	ATP	O3A-PA-O1A	-2.14	104.28	110.70
2	A	1101	ATP	N9-C8-N7	-2.12	110.93	113.94
6	A	1108	GOL	C3-C2-C1	-2.11	104.07	111.80
2	A	1101	ATP	O3G-PG-O3B	-2.03	97.84	104.64

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	ATP	C5'-O5'-PA-O2A
2	A	1101	ATP	C5'-O5'-PA-O3A
6	A	1109	GOL	C1-C2-C3-O3
6	A	1111	GOL	O1-C1-C2-C3
6	A	1112	GOL	O1-C1-C2-C3
6	A	1113	GOL	O1-C1-C2-C3
6	A	1114	GOL	C1-C2-C3-O3
6	A	1115	GOL	O1-C1-C2-C3
6	A	1109	GOL	O2-C2-C3-O3
6	A	1111	GOL	O1-C1-C2-O2
6	A	1115	GOL	O1-C1-C2-O2
6	A	1112	GOL	O1-C1-C2-O2
6	A	1113	GOL	O1-C1-C2-O2
6	A	1114	GOL	O2-C2-C3-O3
2	A	1101	ATP	PB-O3A-PA-O2A
2	A	1101	ATP	C5'-O5'-PA-O1A
2	A	1101	ATP	PB-O3A-PA-O1A
2	A	1101	ATP	PG-O3B-PB-O2B

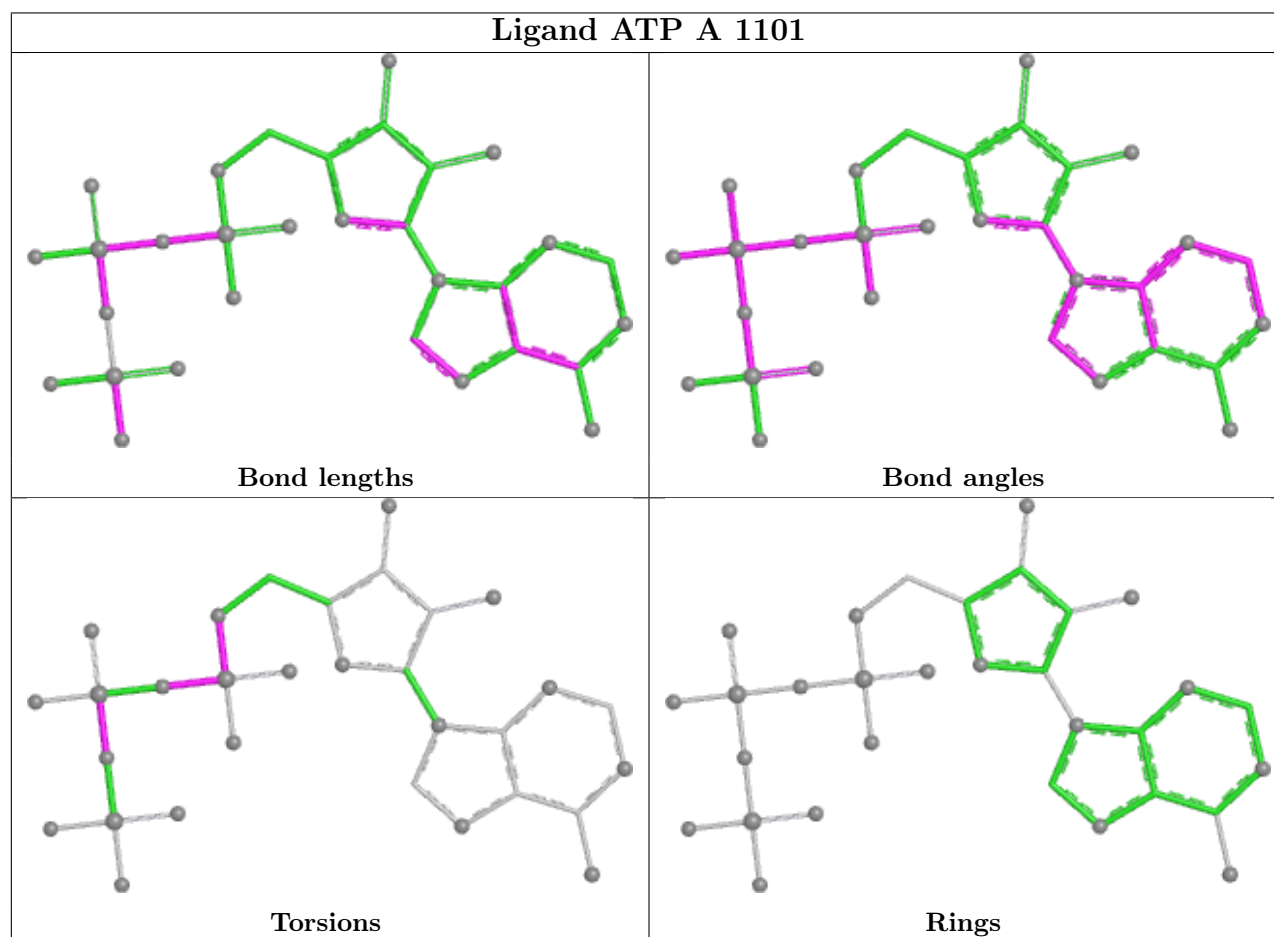
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1109	GOL	1	0
3	A	1102	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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	1005/1024 (98%)	0.15	82 (8%)	17 23	10, 37, 122, 181	26 (2%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	994	ILE	7.2
1	A	964	LEU	6.6
1	A	957	LEU	5.7
1	A	968	PHE	5.7
1	A	980	LEU	5.2
1	A	995	PRO	4.8
1	A	946	PHE	4.6
1	A	986	VAL	4.2
1	A	988	LEU	4.0
1	A	798	ILE	3.9
1	A	982	ILE	3.9
1	A	792	ALA	3.9
1	A	954	ILE	3.9
1	A	983	THR	3.8
1	A	746	SER	3.8
1	A	961	VAL	3.8
1	A	990	THR	3.7
1	A	960	GLY	3.6
1	A	989	VAL	3.6
1	A	952	LEU	3.6
1	A	1003	LEU	3.6
1	A	645	LEU	3.6
1	A	1005	ILE	3.5
1	A	996	ALA	3.5
1	A	755	VAL	3.4
1	A	1017	VAL	3.4
1	A	592	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	750	ASN	3.4
1	A	966	ALA	3.3
1	A	283[A]	PHE	3.3
1	A	751	SER	3.3
1	A	985	LEU	3.3
1	A	787	PRO	3.0
1	A	919	TYR	3.0
1	A	1002	ILE	3.0
1	A	801	LEU	3.0
1	A	636	THR	2.9
1	A	593	PRO	2.9
1	A	791	ALA	2.9
1	A	1015	VAL	2.8
1	A	939	LEU	2.8
1	A	942	LEU	2.7
1	A	963	LEU	2.7
1	A	933	ILE	2.6
1	A	1009	ASP	2.6
1	A	978	LEU	2.6
1	A	802	VAL	2.5
1	A	948	LYS	2.4
1	A	959	TYR	2.4
1	A	945	HIS	2.4
1	A	793	ASN	2.4
1	A	979	ASN	2.4
1	A	786	ASP	2.4
1	A	992	LYS	2.4
1	A	794	GLY	2.4
1	A	788	ASN	2.4
1	A	955	THR	2.3
1	A	993	ASP	2.3
1	A	640	PHE	2.3
1	A	753	PRO	2.3
1	A	805	LEU	2.3
1	A	962	SER	2.3
1	A	941	ASP	2.3
1	A	967	SER	2.3
1	A	597	ILE	2.3
1	A	965	TYR	2.2
1	A	997	HIS	2.2
1	A	752	LYS	2.2
1	A	937	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	641	VAL	2.2
1	A	591	ASP	2.2
1	A	590	ARG	2.2
1	A	920	ASN	2.2
1	A	984	GLN	2.1
1	A	10	ALA	2.1
1	A	1007	ALA	2.1
1	A	744	ILE	2.1
1	A	956	MET	2.1
1	A	976	GLU	2.1
1	A	200	ASP	2.1
1	A	981	PRO	2.1
1	A	236	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1102	5/5	0.83	0.24	119,119,140,166	0
6	GOL	A	1114	6/6	0.85	0.19	66,79,90,90	0
6	GOL	A	1115	6/6	0.86	0.28	87,104,112,112	0
6	GOL	A	1109	6/6	0.88	0.16	44,57,79,89	0
6	GOL	A	1113	6/6	0.89	0.12	43,57,94,113	0
4	ACT	A	1103	4/4	0.89	0.38	90,106,127,127	0
6	GOL	A	1111	6/6	0.89	0.13	50,61,84,89	0
6	GOL	A	1116	6/6	0.90	0.20	65,73,87,87	0
6	GOL	A	1110	6/6	0.92	0.12	35,55,76,91	0
6	GOL	A	1112	6/6	0.92	0.12	42,53,63,70	0

Continued on next page...

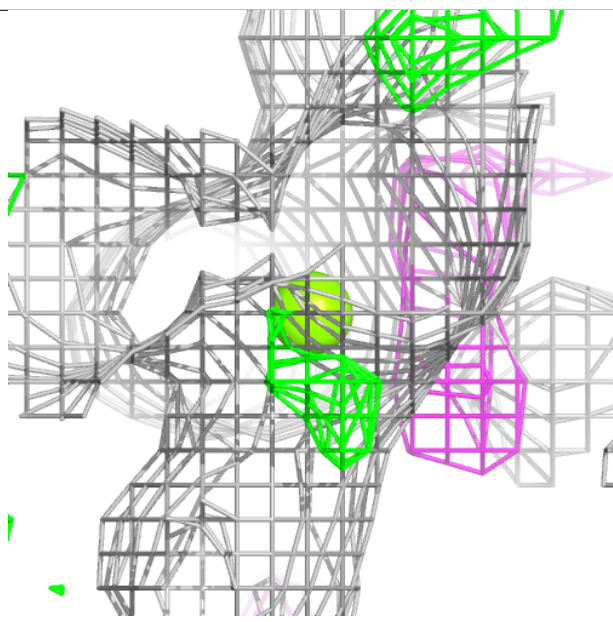
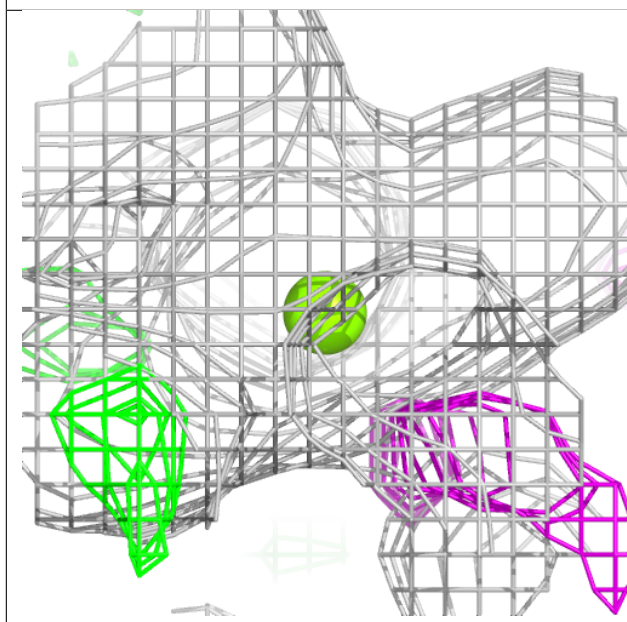
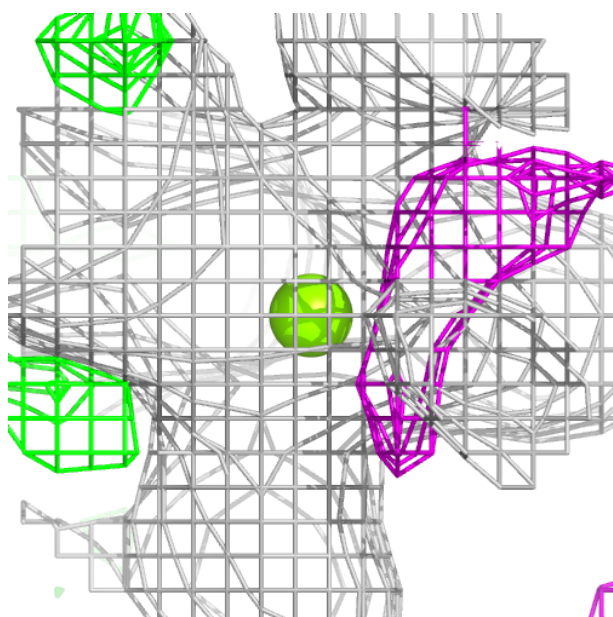
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	A	1106	1/1	0.94	0.06	41,41,41,41	0
5	MG	A	1105	1/1	0.95	0.13	36,36,36,36	0
6	GOL	A	1107	6/6	0.95	0.09	21,32,57,57	0
8	CL	A	1118	1/1	0.95	0.09	50,50,50,50	0
6	GOL	A	1108	6/6	0.97	0.06	28,36,49,49	0
5	MG	A	1104	1/1	0.97	0.06	29,29,29,29	0
2	ATP	A	1101	31/31	0.98	0.05	17,25,31,35	0
7	K	A	1117	1/1	1.00	0.04	20,20,20,20	1

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.

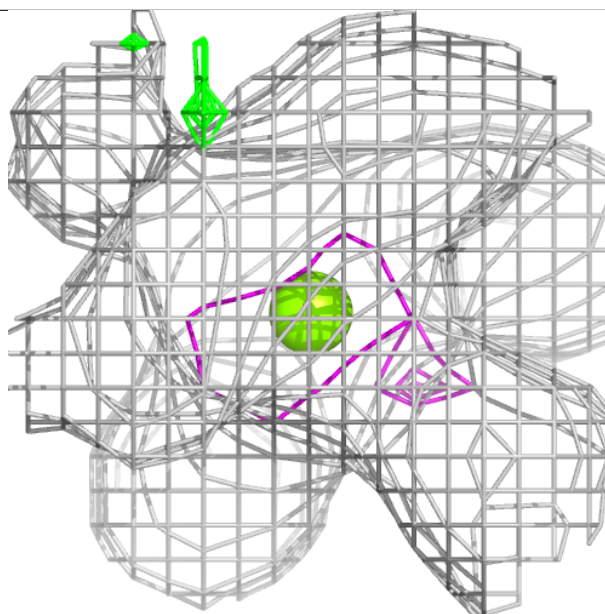
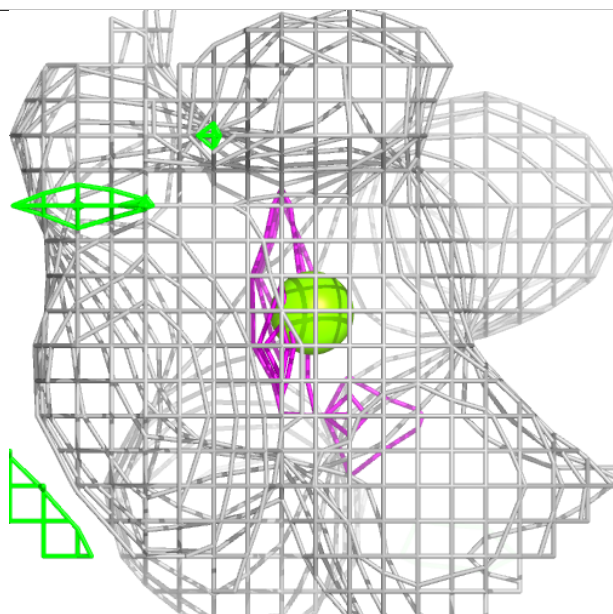
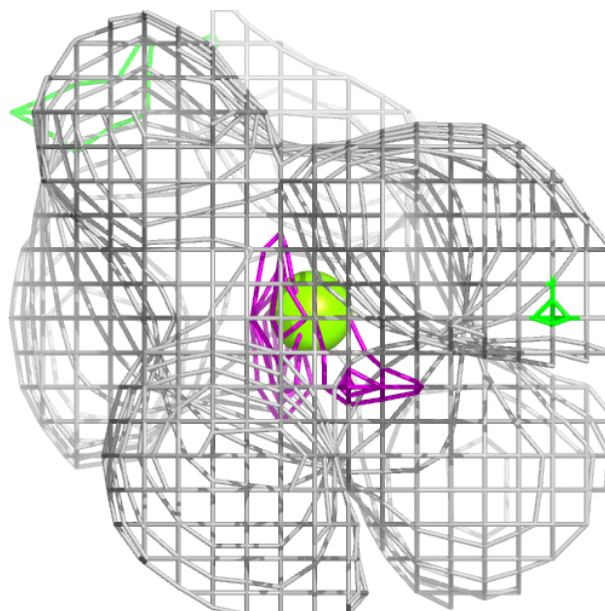
Electron density around MG A 1106:

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



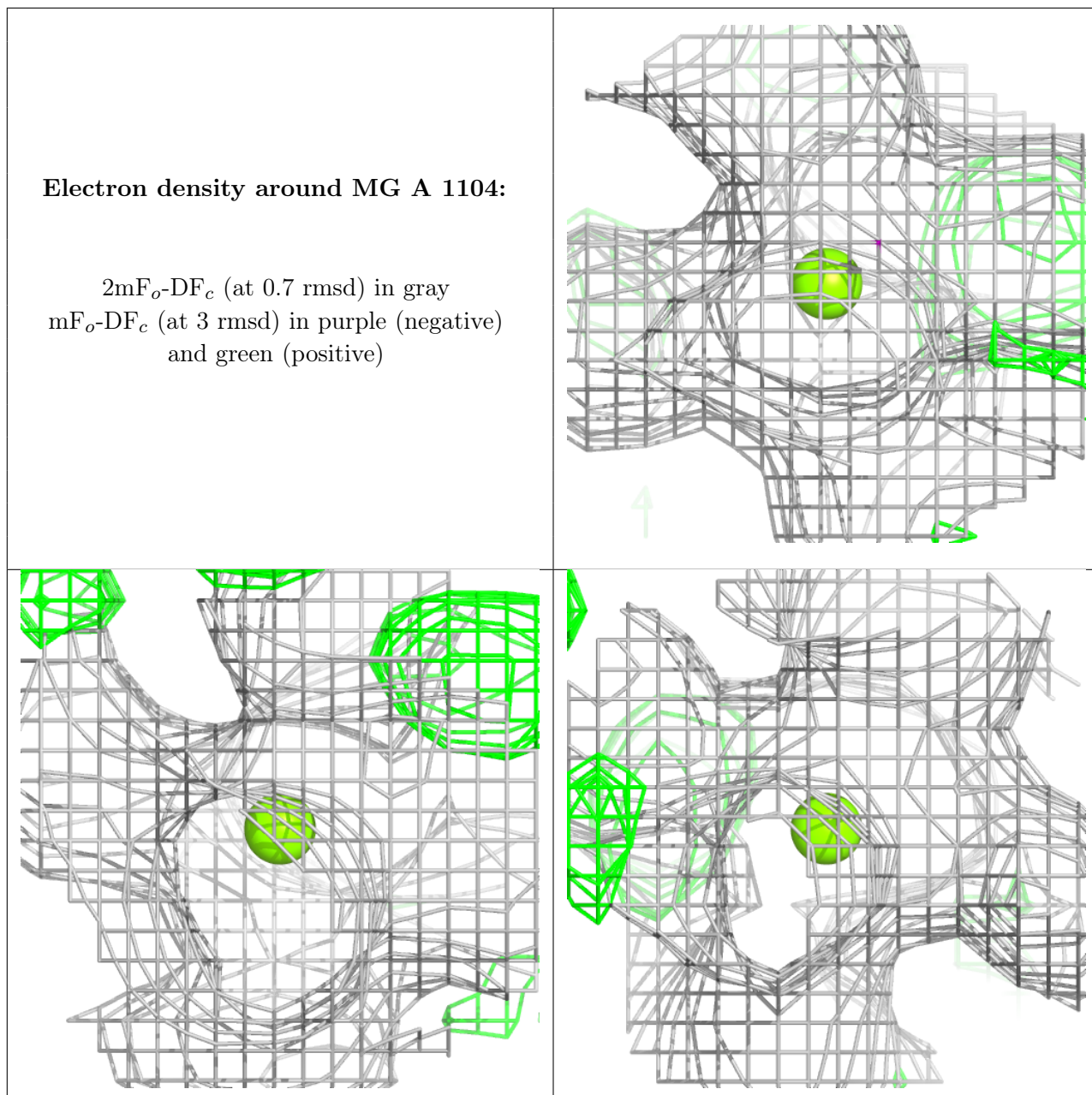
Electron density around MG A 1105:

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



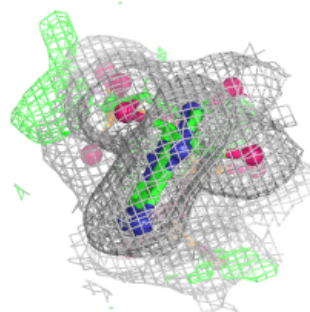
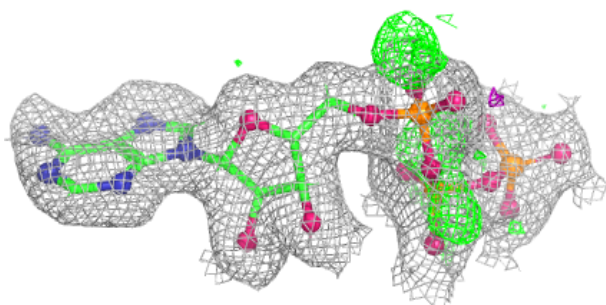
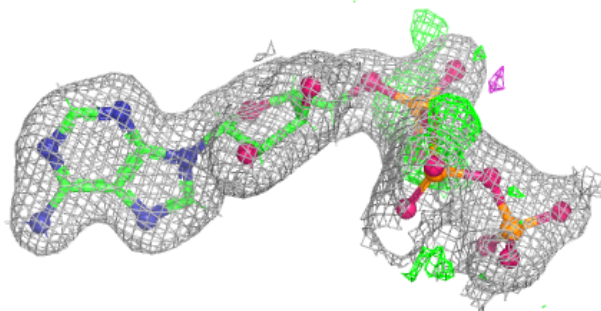
Electron density around MG A 1104:

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



Electron density around ATP A 1101:

$2mF_o - DF_c$ (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.