Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2022 – 04:35 pm BST

PDB ID	:	6ST5
Title	:	crystal structure of LicM2
Authors	:	Gonsior, M.; Mainz, A.; Hugelland, M.; Kuthning, A.; Tietzmann, M.; Dobbek, H.; Martins, B.M.; Sussmuth, R.
Deposited on	:	2019-09-10
Resolution	:	2.82 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:

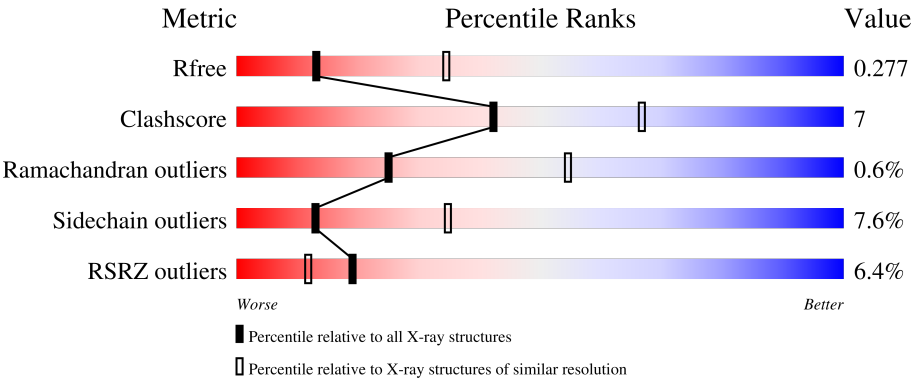
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 <=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	979	6% 75% 16% · 7%

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
4	GOL	A	1110	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14611 atoms, of which 7228 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.

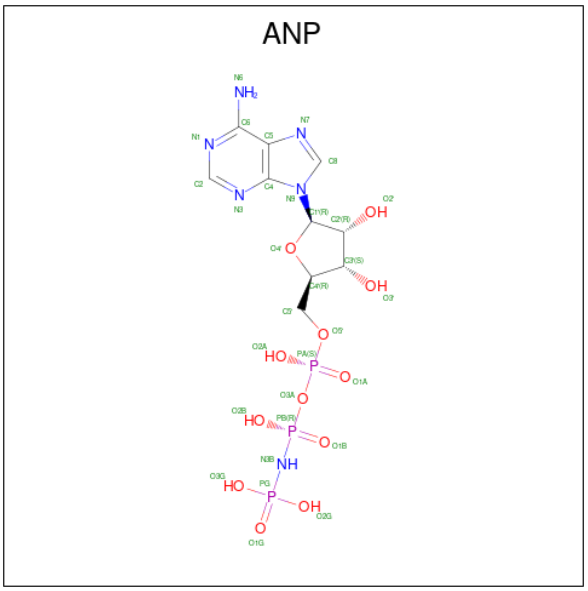
- Molecule 1 is a protein called LicM2.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
1	A	913	14408	4652	7138	1230	1361	8	19	0	2	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

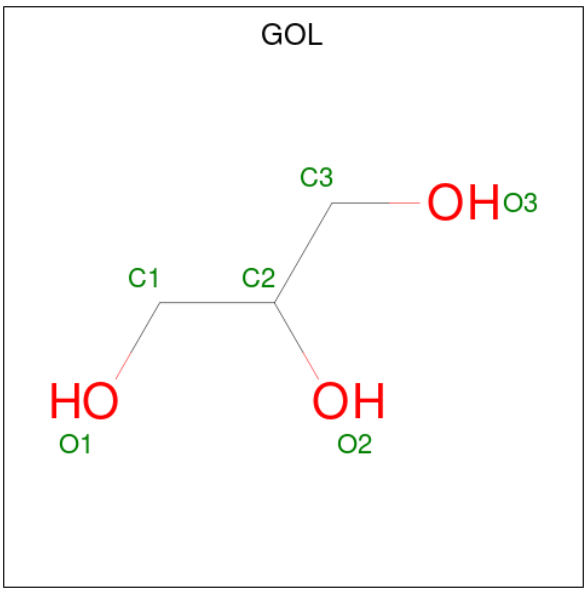
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
3	A	1	88	20	26	12	24	6	0	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 H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is water.

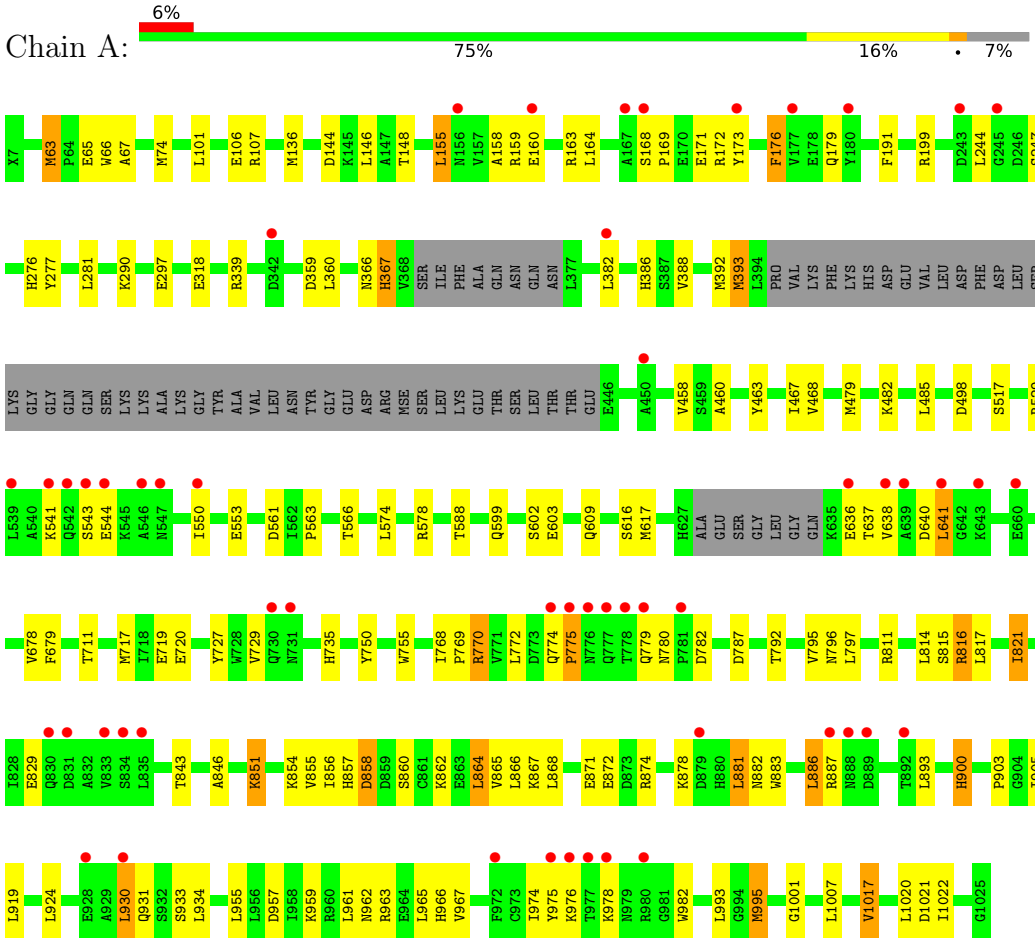
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0

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: LicM2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.36Å 128.41Å 141.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.50 – 2.82 48.56 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.50-2.82) 99.6 (48.56-2.82)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_1168	Depositor
R, R_{free}	0.224 , 0.272 0.235 , 0.277	Depositor DCC
R_{free} test set	1111 reflections (3.17%)	wwPDB-VP
Wilson B-factor (Å^2)	84.0	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14611	wwPDB-VP
Average B, all atoms (Å^2)	98.0	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, MG, ZN, ANP

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	0.28	0/7345	0.47	2/9897 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	995	MSE	CG-SE-CE	7.29	114.93	98.90
1	A	63	MSE	CG-SE-CE	5.37	110.71	98.90

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	7270	7138	7110	100	1
2	A	1	0	0	0	0
3	A	62	26	26	2	0
4	A	48	64	64	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
All	All	7383	7228	7200	101	1

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 7.

All (101) 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:881:LEU:O	1:A:933:SER:OG	2.00	0.79
1:A:267:LYS:NZ	1:A:359:ASP:OD1	2.16	0.77
1:A:787:ASP:OD2	1:A:816:ARG:NH1	2.18	0.76
1:A:482:LYS:NZ	1:A:599:GLN:O	2.17	0.74
1:A:636:GLU:HB2	1:A:978:LYS:HG2	1.67	0.74
1:A:318:GLU:OE2	1:A:463:TYR:OH	2.08	0.70
1:A:517:SER:OG	1:A:529:ARG:NH1	2.27	0.68
1:A:796:ASN:OD1	1:A:851:LYS:NZ	2.30	0.64
1:A:158:ALA:HB1	1:A:164:LEU:HD22	1.81	0.62
1:A:882:ASN:OD1	1:A:883:TRP:N	2.32	0.62
1:A:821:ILE:HD12	1:A:867:LYS:HZ1	1.63	0.62
1:A:858:ASP:OD2	1:A:858:ASP:N	2.32	0.62
1:A:164:LEU:CD1	1:A:172:ARG:HG2	2.32	0.60
1:A:386:HIS:O	1:A:386:HIS:ND1	2.36	0.58
1:A:872:GLU:OE2	1:A:909:ARG:NH1	2.38	0.56
1:A:995:MSE:O	1:A:1001:GLY:HA3	2.06	0.56
1:A:144:ASP:OD1	1:A:148:THR:OG1	2.24	0.55
1:A:158:ALA:CB	1:A:164:LEU:HD22	2.38	0.54
1:A:962:ASN:OD1	1:A:963:ARG:N	2.41	0.53
1:A:931:GLN:NE2	1:A:966:HIS:O	2.41	0.53
1:A:887:ARG:HG3	1:A:887:ARG:O	2.09	0.52
1:A:74:MSE:HE1	1:A:191:PHE:HB2	1.92	0.52
1:A:906:LEU:HA	1:A:930:LEU:HD13	1.92	0.52
1:A:168:SER:OG	1:A:171:GLU:HG3	2.11	0.51
1:A:637:THR:HG22	1:A:975:TYR:CE1	2.45	0.51
1:A:638:VAL:CG2	1:A:976:LYS:HE2	2.41	0.51
1:A:168:SER:HB2	1:A:169:PRO:HD2	1.92	0.51
1:A:636:GLU:N	1:A:976:LYS:O	2.44	0.50
1:A:155:LEU:HG	1:A:176:PHE:CD2	2.46	0.50
1:A:392:MSE:HE2	1:A:393:MSE:HB3	1.94	0.50
1:A:871:GLU:OE2	1:A:909:ARG:NH2	2.44	0.50
1:A:276:HIS:ND1	1:A:498:ASP:OD2	2.44	0.49
1:A:796:ASN:ND2	1:A:1020:LEU:O	2.45	0.49
1:A:846:ALA:HB1	1:A:864:LEU:HD23	1.95	0.49
1:A:868:LEU:CD2	1:A:924:LEU:HD23	2.43	0.49
1:A:670:ASN:HA	1:A:679:PHE:O	2.13	0.49
1:A:779:GLN:OE1	1:A:816:ARG:CZ	2.61	0.48
1:A:959:LYS:HB2	1:A:967:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:ILE:HG22	1:A:930:LEU:HD11	1.96	0.48
1:A:638:VAL:HG11	1:A:641:LEU:HD12	1.96	0.48
1:A:769:PRO:HA	1:A:772:LEU:HD23	1.96	0.48
1:A:967:VAL:HG23	1:A:967:VAL:O	2.14	0.48
1:A:63:MSE:HG2	1:A:67:ALA:HB3	1.97	0.47
1:A:367:HIS:NE2	1:A:588:THR:O	2.40	0.47
1:A:393:MSE:CE	1:A:616:SER:OG	2.62	0.47
1:A:393:MSE:HE2	1:A:616:SER:CB	2.44	0.47
1:A:959:LYS:HD3	1:A:967:VAL:CG2	2.45	0.47
1:A:962:ASN:HB3	1:A:965:LEU:HD12	1.95	0.47
1:A:729:VAL:HB	1:A:770:ARG:HD3	1.97	0.47
1:A:66:TRP:CD2	1:A:199:ARG:HG3	2.50	0.46
1:A:887:ARG:NH2	1:A:893:LEU:O	2.49	0.46
1:A:905:ILE:HB	1:A:930:LEU:HD21	1.97	0.46
1:A:768:ILE:HG22	1:A:772:LEU:HD21	1.96	0.46
1:A:934:LEU:CD1	1:A:955:LEU:HD21	2.46	0.46
1:A:768:ILE:CG2	1:A:772:LEU:HD21	2.46	0.46
1:A:164:LEU:HD23	1:A:164:LEU:H	1.80	0.46
1:A:906:LEU:HB2	1:A:930:LEU:HB3	1.98	0.45
1:A:995:MSE:HE3	1:A:1017:VAL:HG21	1.99	0.45
3:A:1102[B]:ANP:O2G	3:A:1102[B]:ANP:O1A	2.33	0.45
1:A:173:TYR:O	1:A:176:PHE:HB3	2.16	0.45
1:A:750:TYR:HA	1:A:1022:ILE:HD12	1.99	0.45
1:A:101:LEU:HB3	1:A:136:MSE:HE1	1.98	0.45
1:A:865:VAL:HG22	1:A:919:LEU:HD21	1.99	0.44
1:A:277:TYR:CE2	1:A:281:LEU:HD11	2.53	0.44
1:A:868:LEU:O	1:A:872:GLU:HG2	2.17	0.44
1:A:155:LEU:HG	1:A:176:PHE:HD2	1.82	0.43
1:A:905:ILE:HB	1:A:930:LEU:CD2	2.47	0.43
1:A:779:GLN:OE1	1:A:816:ARG:NH1	2.52	0.43
1:A:774:GLN:HB3	1:A:775:PRO:HD3	2.00	0.43
1:A:637:THR:HG22	1:A:975:TYR:CD1	2.54	0.43
1:A:903:PRO:HA	1:A:934:LEU:HD22	2.01	0.43
1:A:735:HIS:NE2	1:A:775:PRO:HD3	2.34	0.43
1:A:976:LYS:HD3	1:A:982:TRP:CE3	2.54	0.43
1:A:727:TYR:CD1	1:A:727:TYR:C	2.92	0.42
1:A:768:ILE:O	1:A:772:LEU:HD22	2.19	0.42
1:A:339:ARG:HB2	1:A:366:ASN:HD22	1.85	0.42
1:A:244:LEU:HD13	3:A:1102[B]:ANP:O3'	2.18	0.42
1:A:883:TRP:CZ3	1:A:930:LEU:CD2	3.03	0.42
1:A:159:ARG:HG2	1:A:172:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:LYS:O	1:A:854:LYS:HD3	2.19	0.42
1:A:553:GLU:HB2	1:A:563:PRO:CG	2.50	0.41
1:A:779:GLN:OE1	1:A:816:ARG:CD	2.68	0.41
1:A:467:ILE:HD12	1:A:617:MSE:HE2	2.03	0.41
1:A:672:ALA:HB2	1:A:678:VAL:HA	2.02	0.41
1:A:843:THR:HG21	1:A:905:ILE:HA	2.00	0.41
1:A:868:LEU:HD21	1:A:924:LEU:HD23	2.02	0.41
1:A:957:ASP:O	1:A:961:LEU:HB2	2.21	0.41
1:A:886:LEU:O	1:A:886:LEU:HD12	2.20	0.41
1:A:636:GLU:O	1:A:975:TYR:HA	2.21	0.41
1:A:792:THR:HA	1:A:795:VAL:HG12	2.02	0.41
1:A:817:LEU:O	1:A:821:ILE:HG12	2.21	0.41
1:A:479:MSE:HE1	1:A:602:SER:C	2.42	0.41
1:A:479:MSE:HE1	1:A:603:GLU:N	2.36	0.41
1:A:779:GLN:HE22	1:A:816:ARG:HD3	1.85	0.40
1:A:250:ASN:N	1:A:561:ASP:OD2	2.54	0.40
1:A:855:VAL:HG12	1:A:856:ILE:HG23	2.02	0.40
1:A:164:LEU:HG	1:A:172:ARG:CG	2.52	0.40
1:A:460:ALA:HB1	1:A:617:MSE:HE1	2.04	0.40
1:A:164:LEU:HD12	1:A:172:ARG:O	2.22	0.40
1:A:550:ILE:HA	1:A:553:GLU:HG2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLU:OE2	1:A:290:LYS:NZ[3_745]	2.12	0.08

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	892/979 (91%)	828 (93%)	59 (7%)	5 (1%)	25 54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	673	GLY
1	A	930	LEU
1	A	821	ILE
1	A	775	PRO
1	A	468	VAL

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	781/812 (96%)	721 (92%)	60 (8%)	13 34

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
1	A	107	ARG
1	A	146	LEU
1	A	155	LEU
1	A	160	GLU
1	A	163	ARG
1	A	176	PHE
1	A	179	GLN
1	A	247	SER
1	A	297	GLU
1	A	360	LEU
1	A	367	HIS
1	A	382	LEU
1	A	388	VAL
1	A	393	MSE
1	A	458	VAL

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Mol	Chain	Res	Type
1	A	485	LEU
1	A	534	ASP
1	A	538	MSE
1	A	541	LYS
1	A	543	SER
1	A	544	GLU
1	A	566	THR
1	A	574	LEU
1	A	578	ARG
1	A	609	GLN
1	A	640	ASP
1	A	641	LEU
1	A	711	THR
1	A	717	MSE
1	A	719	GLU
1	A	720	GLU
1	A	755	TRP
1	A	770	ARG
1	A	780	ASN
1	A	782	ASP
1	A	797	LEU
1	A	811	ARG
1	A	814	LEU
1	A	815	SER
1	A	816	ARG
1	A	829	GLU
1	A	851	LYS
1	A	857	HIS
1	A	858	ASP
1	A	860	SER
1	A	862	LYS
1	A	864	LEU
1	A	866	LEU
1	A	874	ARG
1	A	878	LYS
1	A	881	LEU
1	A	886	LEU
1	A	900[A]	HIS
1	A	900[B]	HIS
1	A	974	ILE
1	A	993	LEU
1	A	1007	LEU

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Mol	Chain	Res	Type
1	A	1017	VAL
1	A	1021	ASP

Sometimes 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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	1109	-	5,5,5	0.37	0	5,5,5	0.18	0
3	ANP	A	1102[B]	5	29,33,33	1.07	3 (10%)	31,52,52	1.06	2 (6%)
4	GOL	A	1106	-	5,5,5	0.38	0	5,5,5	0.18	0
4	GOL	A	1108	-	5,5,5	0.35	0	5,5,5	0.24	0
4	GOL	A	1103	-	5,5,5	0.37	0	5,5,5	0.19	0
4	GOL	A	1104	-	5,5,5	0.39	0	5,5,5	0.12	0
4	GOL	A	1105	-	5,5,5	0.38	0	5,5,5	0.21	0
3	ANP	A	1102[A]	5	29,33,33	1.09	4 (13%)	31,52,52	1.09	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	A	1110	-	5,5,5	0.37	0	5,5,5	0.21	0
4	GOL	A	1107	-	5,5,5	0.38	0	5,5,5	0.23	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
4	GOL	A	1109	-	-	0/4/4/4	-
3	ANP	A	1102[B]	5	-	6/14/38/38	0/3/3/3
4	GOL	A	1106	-	-	4/4/4/4	-
4	GOL	A	1108	-	-	0/4/4/4	-
4	GOL	A	1103	-	-	3/4/4/4	-
4	GOL	A	1104	-	-	2/4/4/4	-
4	GOL	A	1105	-	-	2/4/4/4	-
3	ANP	A	1102[A]	5	-	5/14/38/38	0/3/3/3
4	GOL	A	1110	-	-	1/4/4/4	-
4	GOL	A	1107	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102[A]	ANP	PG-N3B	2.51	1.69	1.63
3	A	1102[B]	ANP	PG-O1G	2.50	1.50	1.46
3	A	1102[A]	ANP	PG-O1G	2.50	1.50	1.46
3	A	1102[B]	ANP	PG-N3B	2.49	1.69	1.63
3	A	1102[A]	ANP	PB-O1B	2.34	1.49	1.46
3	A	1102[B]	ANP	PB-O1B	2.33	1.49	1.46
3	A	1102[A]	ANP	PB-O3A	-2.02	1.56	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1102[A]	ANP	PB-O3A-PA	-3.27	121.11	132.62
3	A	1102[B]	ANP	PB-O3A-PA	-3.05	121.88	132.62
3	A	1102[A]	ANP	C5-C6-N6	2.25	123.77	120.35
3	A	1102[B]	ANP	C5-C6-N6	2.23	123.74	120.35

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102[A]	ANP	PB-N3B-PG-O1G
3	A	1102[A]	ANP	C5'-O5'-PA-O3A
3	A	1102[B]	ANP	PB-N3B-PG-O1G
3	A	1102[B]	ANP	PA-O3A-PB-O1B
3	A	1102[B]	ANP	PA-O3A-PB-O2B
3	A	1102[B]	ANP	C5'-O5'-PA-O2A
3	A	1102[B]	ANP	C5'-O5'-PA-O3A
4	A	1106	GOL	C1-C2-C3-O3
4	A	1107	GOL	O1-C1-C2-C3
3	A	1102[A]	ANP	O4'-C4'-C5'-O5'
3	A	1102[A]	ANP	C3'-C4'-C5'-O5'
4	A	1106	GOL	O1-C1-C2-C3
4	A	1106	GOL	O2-C2-C3-O3
4	A	1107	GOL	O1-C1-C2-O2
4	A	1103	GOL	O1-C1-C2-O2
4	A	1106	GOL	O1-C1-C2-O2
4	A	1104	GOL	O1-C1-C2-O2
4	A	1105	GOL	O1-C1-C2-O2
3	A	1102[A]	ANP	C5'-O5'-PA-O1A
3	A	1102[B]	ANP	C5'-O5'-PA-O1A
4	A	1104	GOL	O1-C1-C2-C3
4	A	1105	GOL	O1-C1-C2-C3
4	A	1103	GOL	O1-C1-C2-C3
4	A	1103	GOL	O2-C2-C3-O3
4	A	1110	GOL	O1-C1-C2-O2

There are no ring outliers.

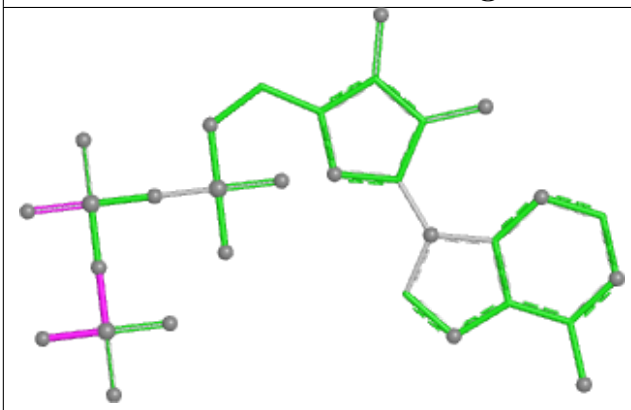
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102[B]	ANP	2	0

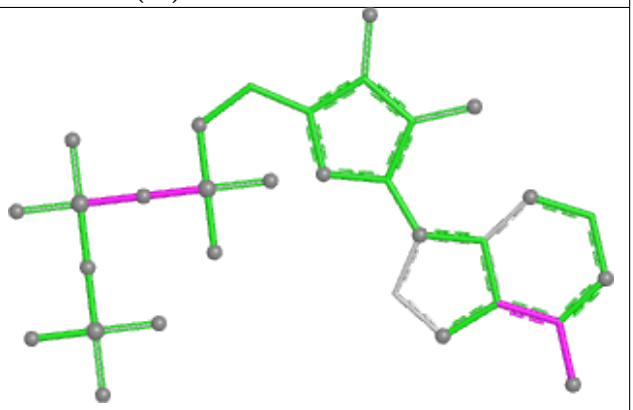
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

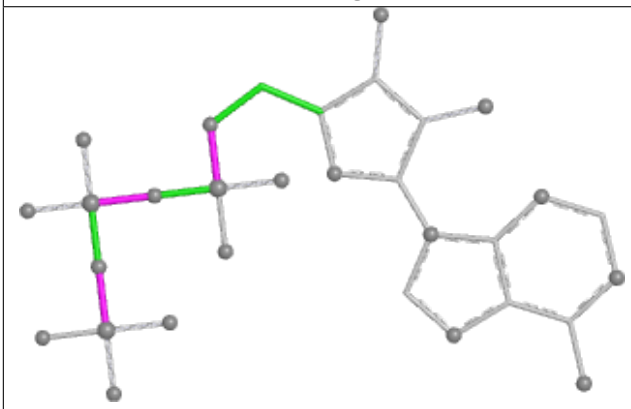
Ligand ANP A 1102 (B)



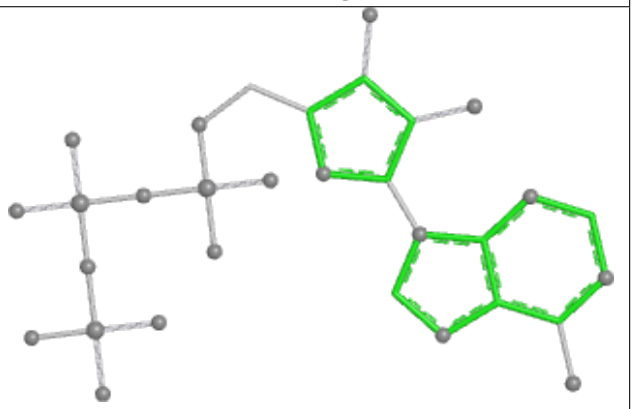
Bond lengths



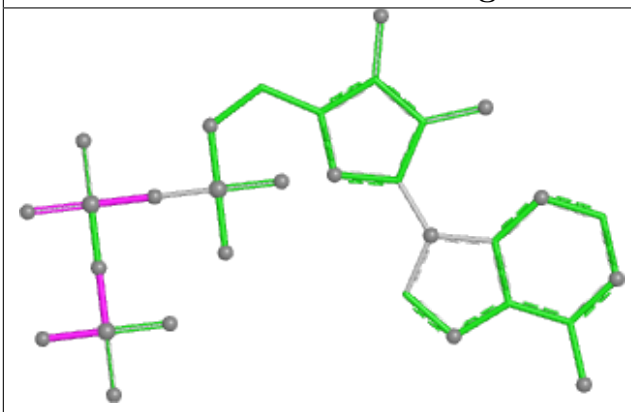
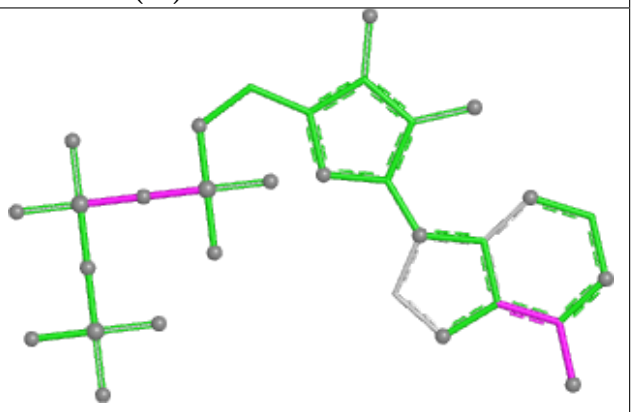
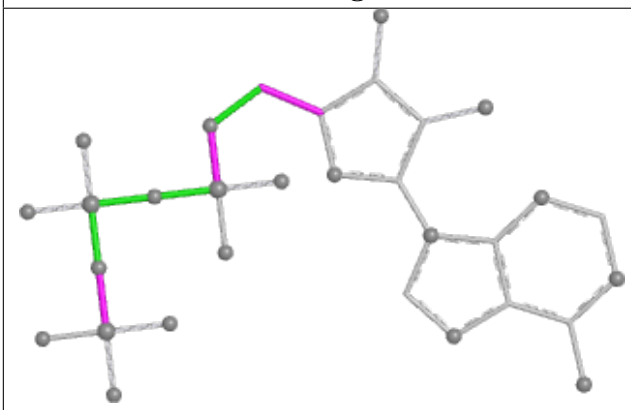
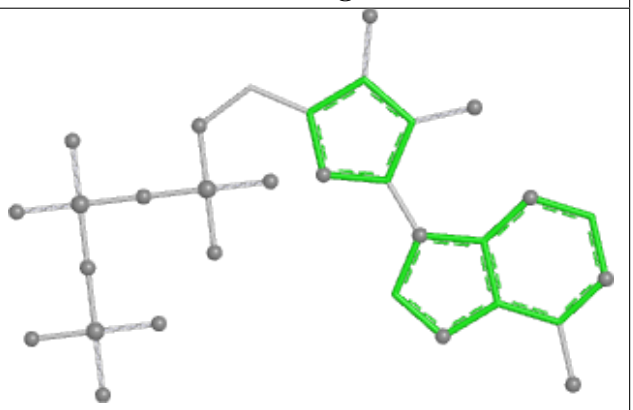
Bond angles



Torsions



Rings

Ligand ANP A 1102 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	21:UNK	C	62:LYS	N	11.36

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	879/979 (89%)	0.36	56 (6%) 19 12	47, 83, 137, 181	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	731	ASN	9.2
1	A	777	GLN	7.5
1	A	542	GLN	5.8
1	A	879	ASP	5.6
1	A	834	SER	5.3
1	A	831	ASP	5.2
1	A	660	GLU	5.0
1	A	976	LYS	4.6
1	A	827	SER	4.3
1	A	177	VAL	4.1
1	A	543	SER	4.0
1	A	888	ASN	3.9
1	A	776	ASN	3.8
1	A	541	LYS	3.7
1	A	180	TYR	3.7
1	A	243	ASP	3.6
1	A	774	GLN	3.4
1	A	975	TYR	3.3
1	A	930	LEU	3.2
1	A	978	LYS	3.2
1	A	824	LEU	3.2
1	A	544	GLU	3.2
1	A	779	GLN	3.1
1	A	382	LEU	3.1
1	A	781	PRO	3.1
1	A	889	ASP	3.0
1	A	156	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	833	VAL	2.9
1	A	928	GLU	2.9
1	A	887	ARG	2.7
1	A	641	LEU	2.7
1	A	546	ALA	2.7
1	A	730	GLN	2.6
1	A	245	GLY	2.6
1	A	835	LEU	2.6
1	A	639	ALA	2.5
1	A	636	GLU	2.5
1	A	638	VAL	2.5
1	A	830	GLN	2.4
1	A	778	THR	2.4
1	A	892	THR	2.4
1	A	342	ASP	2.4
1	A	160	GLU	2.3
1	A	826	ASP	2.3
1	A	775	PRO	2.3
1	A	539	LEU	2.3
1	A	450	ALA	2.3
1	A	547	ASN	2.3
1	A	643	LYS	2.2
1	A	167	ALA	2.2
1	A	173	TYR	2.2
1	A	550	ILE	2.1
1	A	972	PHE	2.1
1	A	977	THR	2.1
1	A	168	SER	2.0
1	A	980	ARG	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

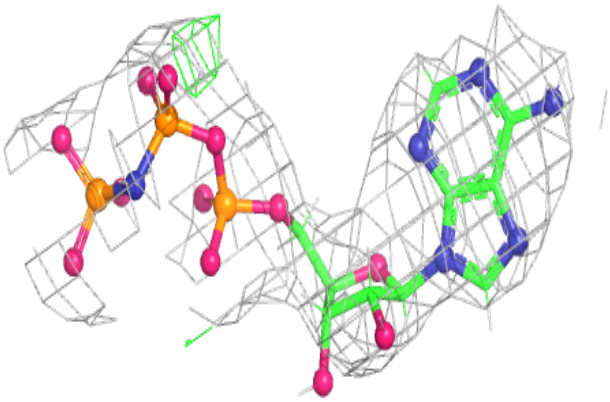
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

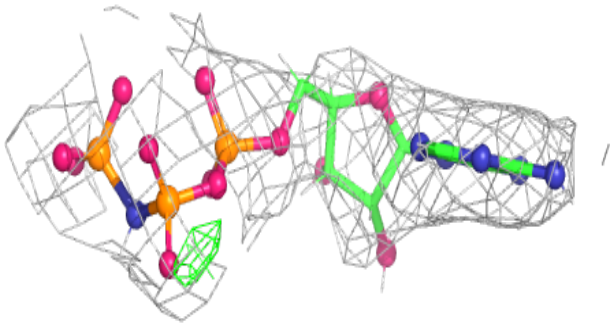
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	1106	6/6	0.72	0.16	85,108,140,140	0
4	GOL	A	1110	6/6	0.78	0.52	98,118,141,141	0
4	GOL	A	1103	6/6	0.79	0.30	97,117,136,140	0
4	GOL	A	1107	6/6	0.82	0.10	90,125,153,159	0
3	ANP	A	1102[A]	31/31	0.85	0.23	66,105,127,153	44
4	GOL	A	1108	6/6	0.85	0.08	104,125,145,147	0
3	ANP	A	1102[B]	31/31	0.85	0.23	63,108,134,149	44
4	GOL	A	1109	6/6	0.86	0.31	103,124,138,143	0
4	GOL	A	1104	6/6	0.88	0.43	74,91,118,119	0
5	MG	A	1111	1/1	0.91	0.16	74,74,74,74	0
4	GOL	A	1105	6/6	0.92	0.21	104,128,144,154	0
2	ZN	A	1101	1/1	0.99	0.18	79,79,79,79	0

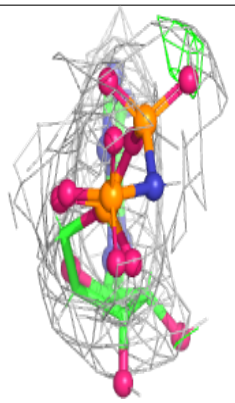
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 1102 (A):

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

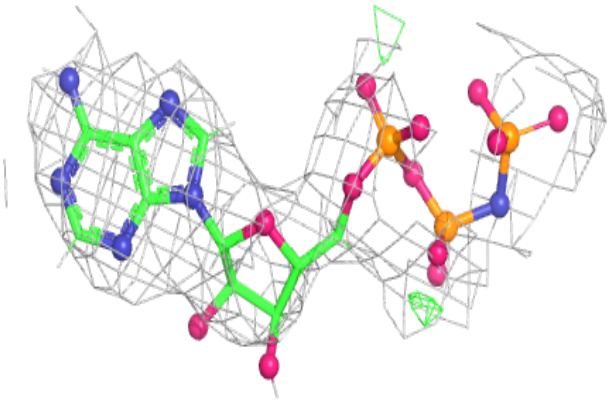


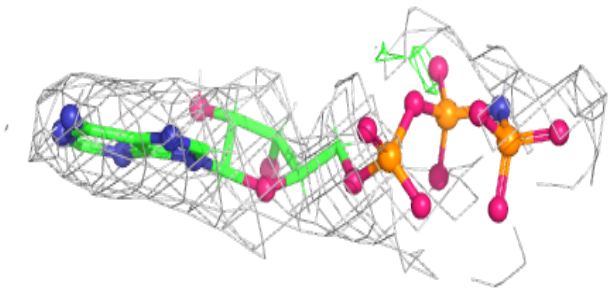


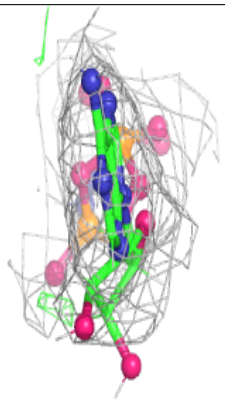


Electron density around ANP A 1102 (B):

$2mF_o$-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 1111:

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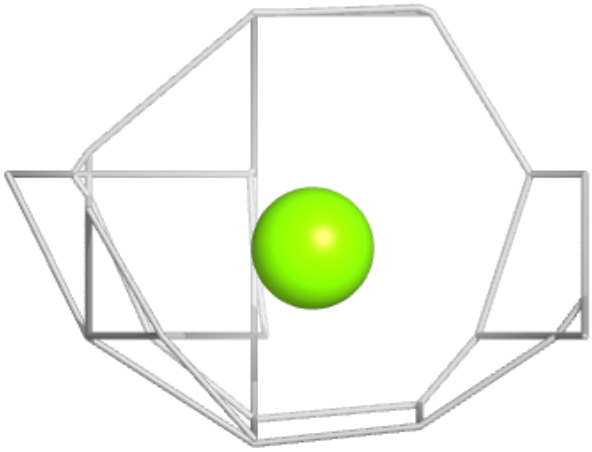
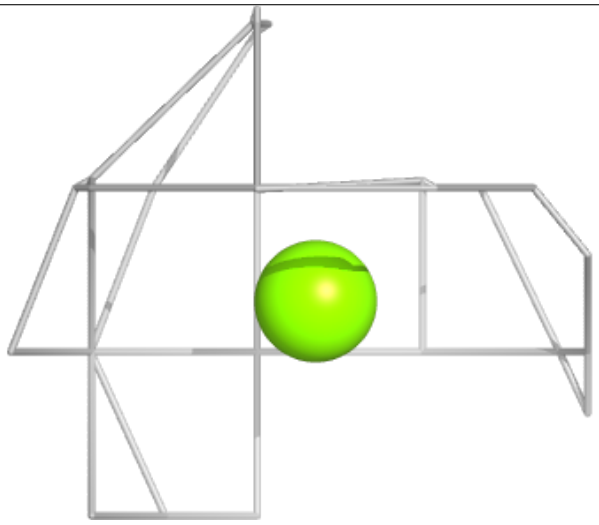
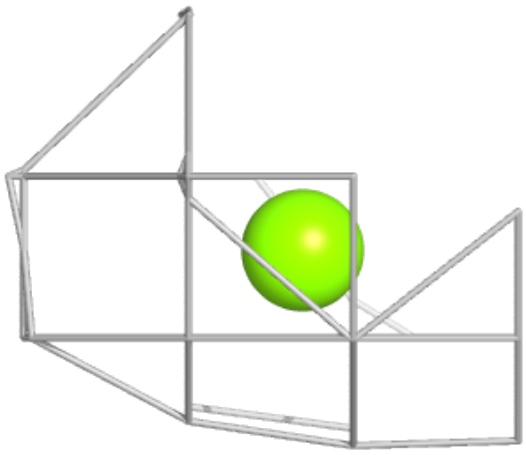
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around ZN A 1101:

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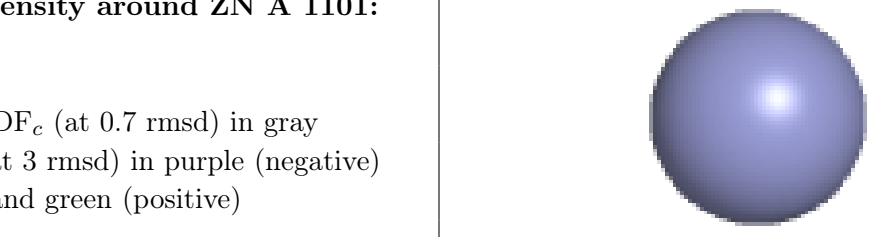
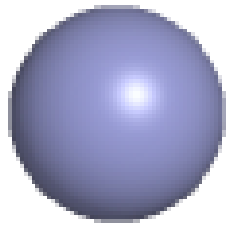
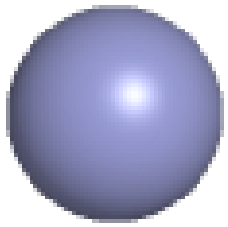
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers

There are no such residues in this entry.