



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:01 AM UTC

PDB ID : 6ST5 / pdb_00006st5
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	:	4-5-2 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

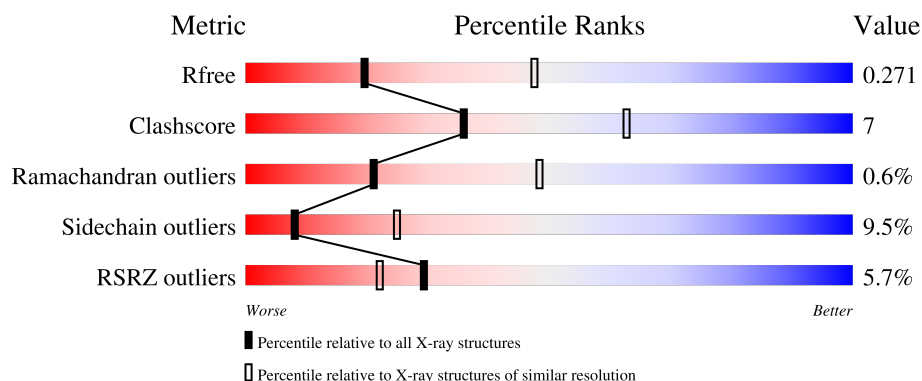
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (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 $\leq 5\%$. 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	979	

2 Entry composition [i](#)

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.

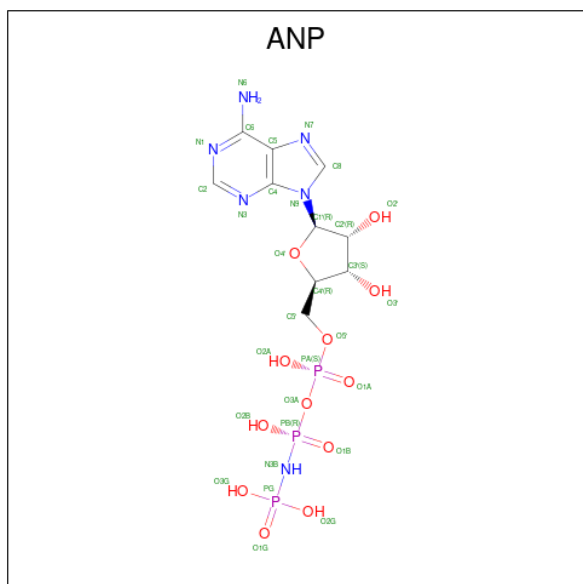
- Molecule 1 is a protein called LicM2.

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

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

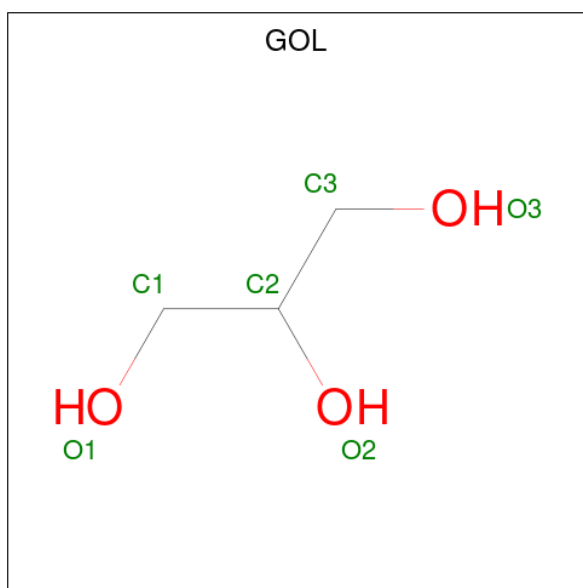
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		

- 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	1	Total	Mg	0	0
			1	1		

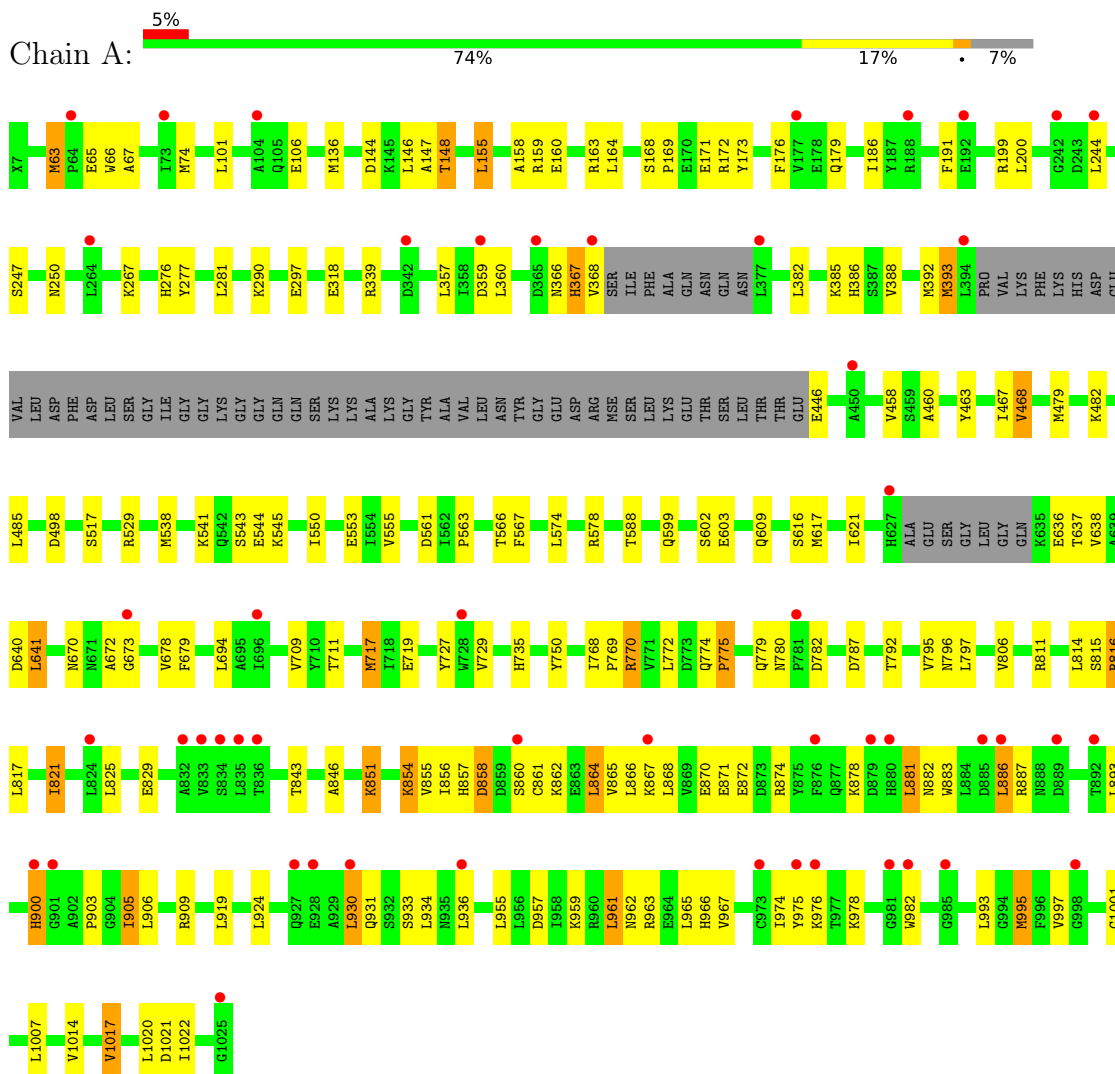
- Molecule 6 is water.

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

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: LicM2



4 Data and refinement statistics

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 47.50 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.50-2.82) 99.7 (47.50-2.82)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_1168	Depositor
R, R_{free}	0.224 , 0.272 0.238 , 0.271	Depositor DCC
R_{free} test set	1111 reflections (3.16%)	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)	0.36 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

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: GOL, ANP, ZN, 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	0.23	0/7345	0.41	4/9897 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	995	MSE	CG-SE-CE	7.28	114.93	98.92
1	A	997	VAL	CA-C-N	6.68	130.01	122.67
1	A	997	VAL	C-N-CA	6.68	130.01	122.67
1	A	63	MSE	CG-SE-CE	5.36	110.71	98.92

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	7270	7138	7110	105	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	106	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 (106) 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:821:ILE:HD12	1:A:867:LYS:HZ1	1.60	0.66
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:LYS:HB2	1:A:967:VAL:HG21	1.94	0.48
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:727:TYR:C	1:A:727:TYR:CD1	2.92	0.47
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:479:MSE:HE1	1:A:602:SER:C	2.42	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:C	1:A:729:VAL:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:467:ILE:O	1:A:468:VAL:C	2.63	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:567:PHE:CD1	1:A:567:PHE:C	2.98	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:603:GLU:N	2.36	0.41
1:A:779:GLN:HE22	1:A:816:ARG:HD3	1.85	0.40
1:A:147:ALA:O	1:A:148:THR:C	2.64	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:694:LEU:C	1:A:717:MSE:HE1	2.46	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 ⓘ

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	892/979 (91%)	828 (93%)	59 (7%)	5 (1%)	21 48

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%)	706 (90%)	75 (10%)	8 24

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
1	A	146	LEU
1	A	148	THR
1	A	155	LEU
1	A	160	GLU
1	A	163	ARG
1	A	179	GLN
1	A	186	ILE
1	A	200	LEU
1	A	247	SER
1	A	297	GLU
1	A	357	LEU

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Mol	Chain	Res	Type
1	A	360	LEU
1	A	367	HIS
1	A	368	VAL
1	A	382	LEU
1	A	385	LYS
1	A	388	VAL
1	A	393	MSE
1	A	446	GLU
1	A	458	VAL
1	A	485	LEU
1	A	538	MSE
1	A	541	LYS
1	A	543	SER
1	A	544	GLU
1	A	545	LYS
1	A	555	VAL
1	A	566	THR
1	A	574	LEU
1	A	578	ARG
1	A	609	GLN
1	A	621	ILE
1	A	640	ASP
1	A	641	LEU
1	A	709	VAL
1	A	711	THR
1	A	717	MSE
1	A	719	GLU
1	A	770	ARG
1	A	780	ASN
1	A	782	ASP
1	A	797	LEU
1	A	806	VAL
1	A	811	ARG
1	A	814	LEU
1	A	815	SER
1	A	816	ARG
1	A	825	LEU
1	A	829	GLU
1	A	851	LYS
1	A	854	LYS
1	A	857	HIS
1	A	858	ASP

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Mol	Chain	Res	Type
1	A	860	SER
1	A	861	CYS
1	A	862	LYS
1	A	864	LEU
1	A	866	LEU
1	A	870	GLU
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	905	ILE
1	A	936	LEU
1	A	961	LEU
1	A	974	ILE
1	A	993	LEU
1	A	1007	LEU
1	A	1014	VAL
1	A	1017	VAL
1	A	1021	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	497	HIS
1	A	502	HIS
1	A	627	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
3	ANP	A	1102[A]	5	33,33,33	0.93	4 (12%)	45,52,52	0.64	0
3	ANP	A	1102[B]	5	33,33,33	0.92	3 (9%)	45,52,52	0.64	0
4	GOL	A	1107	-	5,5,5	0.38	0	5,5,5	0.25	0
4	GOL	A	1103	-	5,5,5	0.37	0	5,5,5	0.21	0
4	GOL	A	1110	-	5,5,5	0.38	0	5,5,5	0.24	0
4	GOL	A	1104	-	5,5,5	0.40	0	5,5,5	0.13	0
4	GOL	A	1108	-	5,5,5	0.36	0	5,5,5	0.27	0
4	GOL	A	1109	-	5,5,5	0.38	0	5,5,5	0.21	0
4	GOL	A	1106	-	5,5,5	0.39	0	5,5,5	0.20	0
4	GOL	A	1105	-	5,5,5	0.38	0	5,5,5	0.24	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
3	ANP	A	1102[A]	5	-	5/18/38/38	0/3/3/3
3	ANP	A	1102[B]	5	-	6/18/38/38	0/3/3/3
4	GOL	A	1107	-	-	2/4/4/4	-
4	GOL	A	1103	-	-	2/4/4/4	-
4	GOL	A	1110	-	-	1/4/4/4	-
4	GOL	A	1104	-	-	1/4/4/4	-
4	GOL	A	1108	-	-	0/4/4/4	-
4	GOL	A	1109	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	1106	-	-	4/4/4/4	-
4	GOL	A	1105	-	-	1/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102[B]	ANP	PG-O1G	2.60	1.50	1.46
3	A	1102[A]	ANP	PG-O1G	2.60	1.50	1.46
3	A	1102[A]	ANP	PG-N3B	2.51	1.69	1.63
3	A	1102[B]	ANP	PG-N3B	2.49	1.69	1.63
3	A	1102[A]	ANP	PB-O1B	2.42	1.49	1.46
3	A	1102[B]	ANP	PB-O1B	2.42	1.49	1.46
3	A	1102[A]	ANP	PB-O3A	-2.05	1.56	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

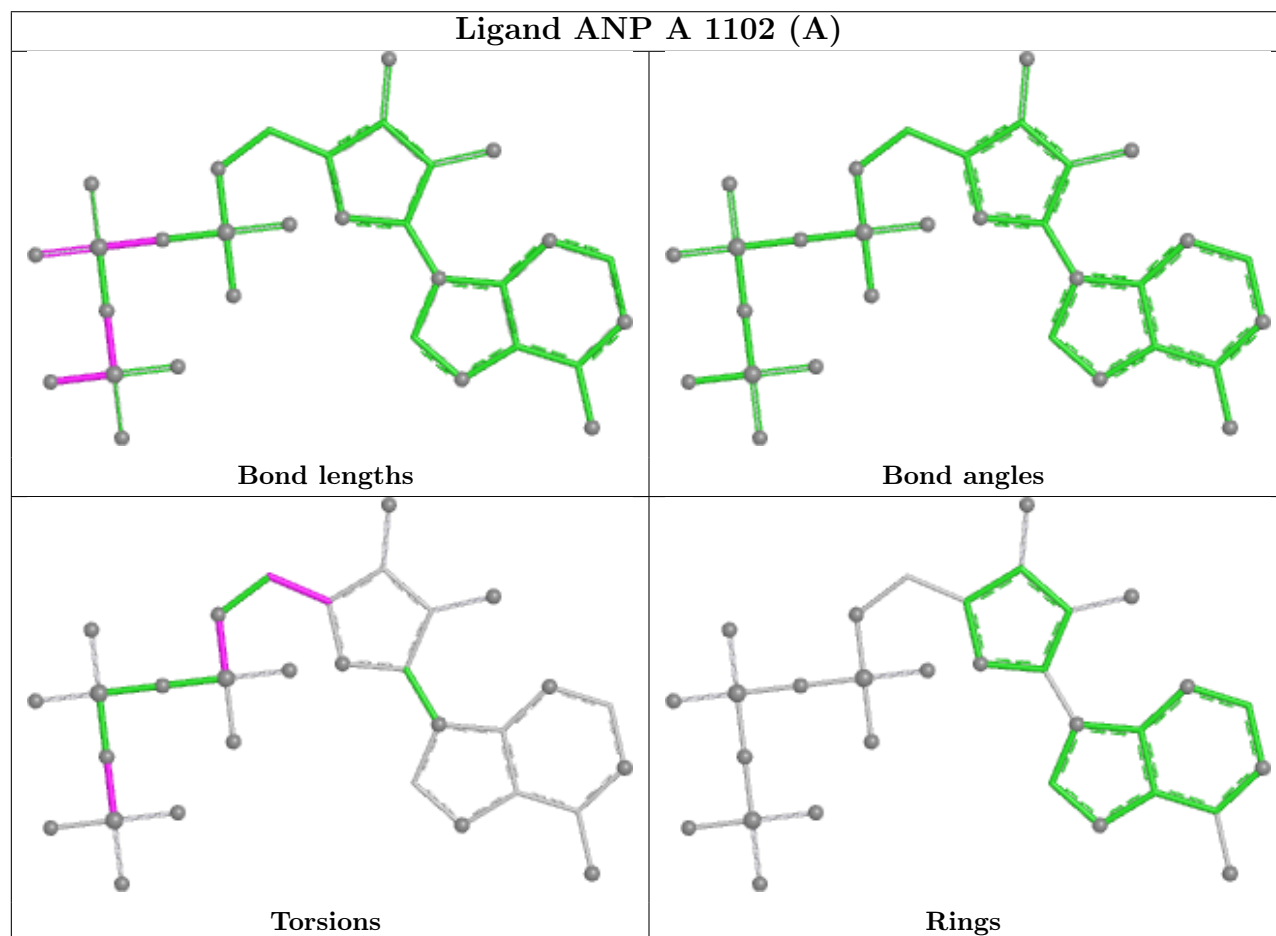
Mol	Chain	Res	Type	Atoms
3	A	1102[A]	ANP	PB-N3B-PG-O1G
3	A	1102[A]	ANP	C5'-O5'-PA-O3A
3	A	1102[B]	ANP	PB-N3B-PG-O1G
3	A	1102[B]	ANP	PA-O3A-PB-O2B
3	A	1102[B]	ANP	C5'-O5'-PA-O2A
4	A	1106	GOL	C1-C2-C3-O3
4	A	1107	GOL	O1-C1-C2-C3
3	A	1102[A]	ANP	O4'-C4'-C5'-O5'
3	A	1102[A]	ANP	C3'-C4'-C5'-O5'
4	A	1106	GOL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

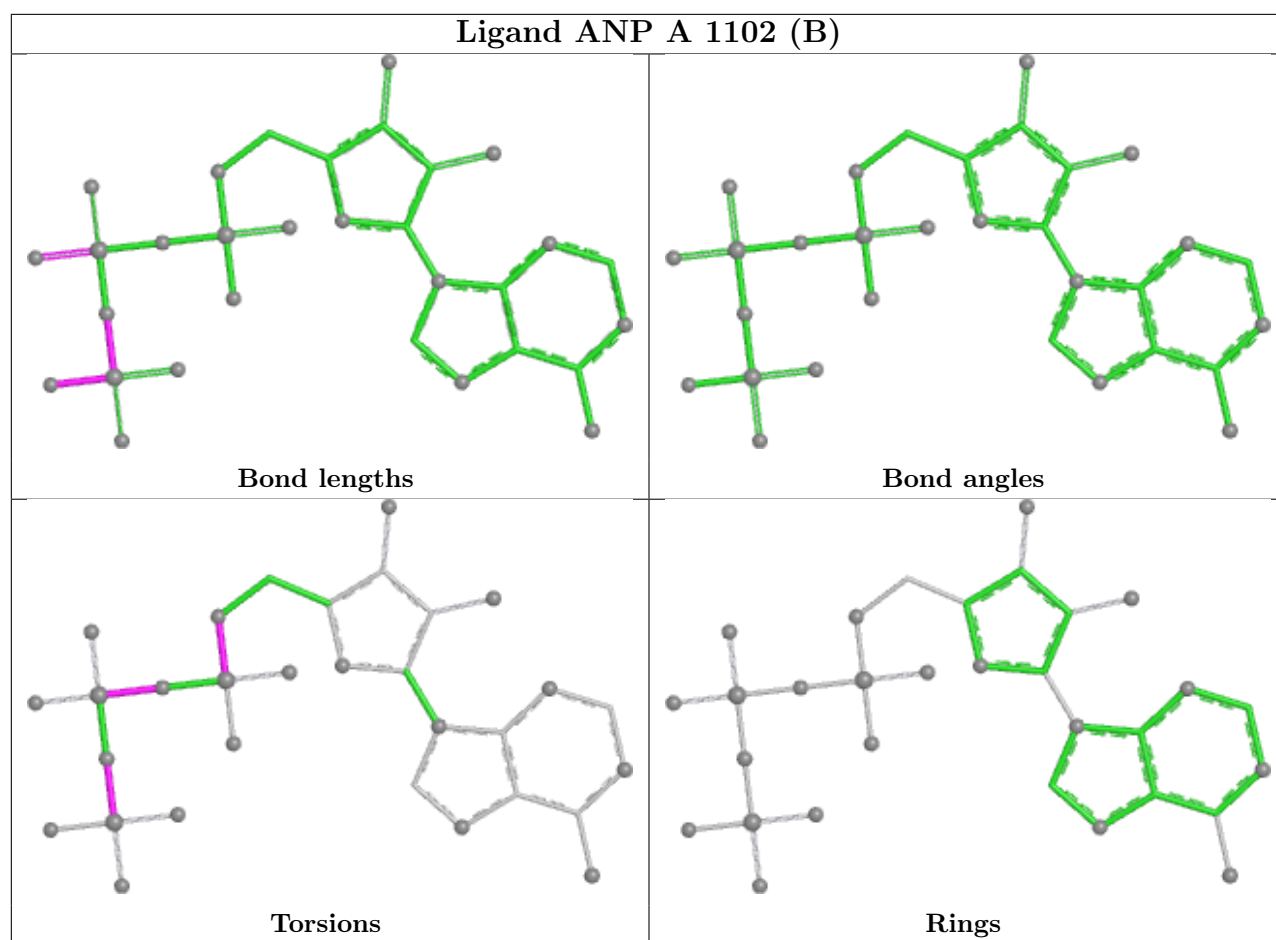
There are no ring outliers.

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 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](#)

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, 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	879/979 (89%)	0.36	50 (5%)	29 22	51, 91, 150, 196	2 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	930	LEU	6.4
1	A	900[A]	HIS	6.4
1	A	835	LEU	4.4
1	A	368	VAL	4.3
1	A	901	GLY	3.8
1	A	781	PRO	3.6
1	A	1025	GLY	3.6
1	A	886	LEU	3.5
1	A	928	GLU	3.4
1	A	976	LYS	3.4
1	A	673	GLY	3.3
1	A	927	GLN	3.1
1	A	860	SER	3.0
1	A	377	LEU	3.0
1	A	104	ALA	3.0
1	A	394	LEU	2.9
1	A	985	GLY	2.9
1	A	627	HIS	2.9
1	A	833	VAL	2.8
1	A	885	ASP	2.8
1	A	867	LYS	2.7
1	A	177	VAL	2.6
1	A	936	LEU	2.6
1	A	836	THR	2.6
1	A	832	ALA	2.6
1	A	889	ASP	2.5
1	A	973	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	696	ILE	2.4
1	A	188	ARG	2.4
1	A	242	GLY	2.4
1	A	365	ASP	2.4
1	A	342	ASP	2.3
1	A	982	TRP	2.3
1	A	824	LEU	2.3
1	A	876	PHE	2.2
1	A	880	HIS	2.2
1	A	359	ASP	2.2
1	A	879	ASP	2.2
1	A	892	THR	2.2
1	A	73	ILE	2.2
1	A	728	TRP	2.2
1	A	264	LEU	2.2
1	A	244	LEU	2.2
1	A	834	SER	2.1
1	A	64	PRO	2.1
1	A	450	ALA	2.1
1	A	998	GLY	2.1
1	A	975	TYR	2.1
1	A	981	GLY	2.0
1	A	192	GLU	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.

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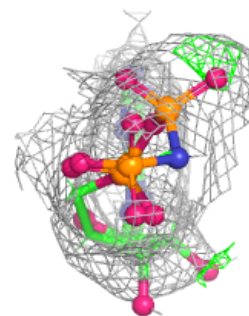
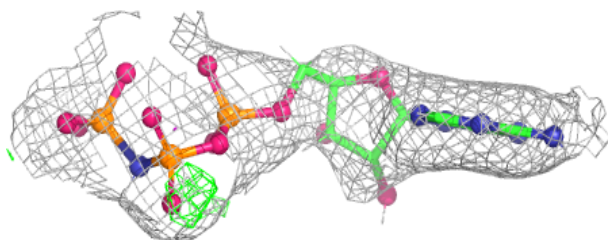
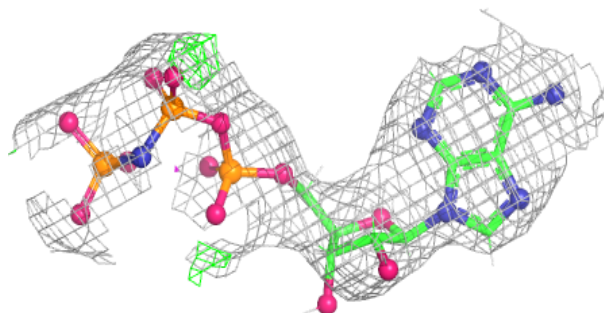
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	1109	6/6	0.49	0.13	103,124,138,143	0
4	GOL	A	1110	6/6	0.56	0.17	98,118,141,141	0
4	GOL	A	1105	6/6	0.63	0.14	104,128,144,154	0
4	GOL	A	1108	6/6	0.66	0.15	104,125,145,147	0
4	GOL	A	1103	6/6	0.68	0.16	97,117,136,140	0
4	GOL	A	1106	6/6	0.78	0.17	85,108,140,140	0
4	GOL	A	1107	6/6	0.82	0.12	90,125,153,159	0
4	GOL	A	1104	6/6	0.86	0.33	74,91,118,119	0
3	ANP	A	1102[A]	31/31	0.87	0.13	66,105,127,153	44
3	ANP	A	1102[B]	31/31	0.87	0.13	63,108,134,149	44
5	MG	A	1111	1/1	0.94	0.12	74,74,74,74	0
2	ZN	A	1101	1/1	1.00	0.04	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.

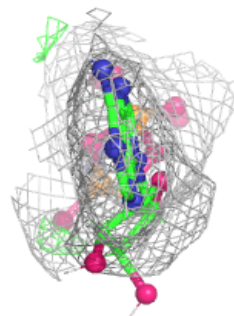
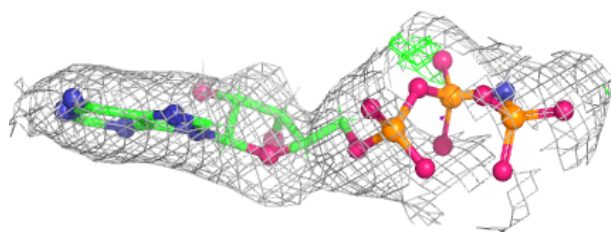
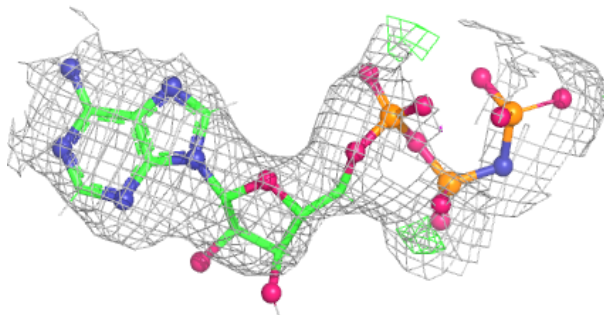
Electron density around ANP A 1102 (A):

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



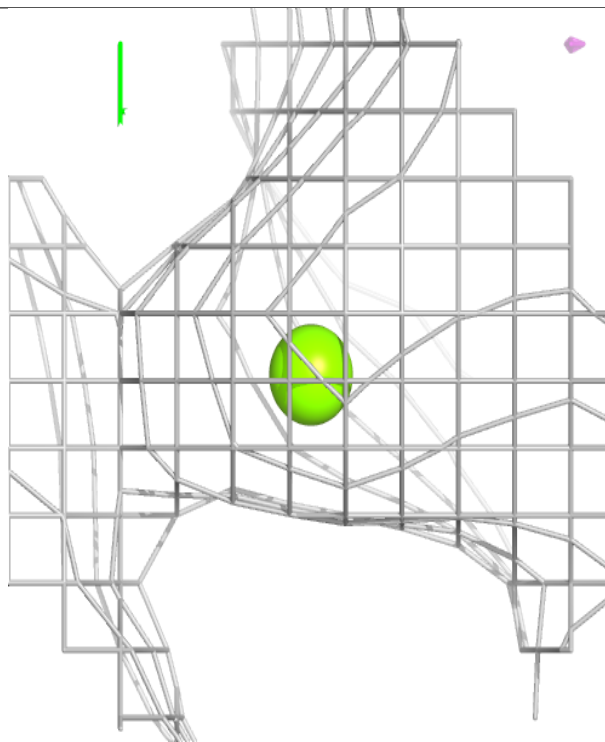
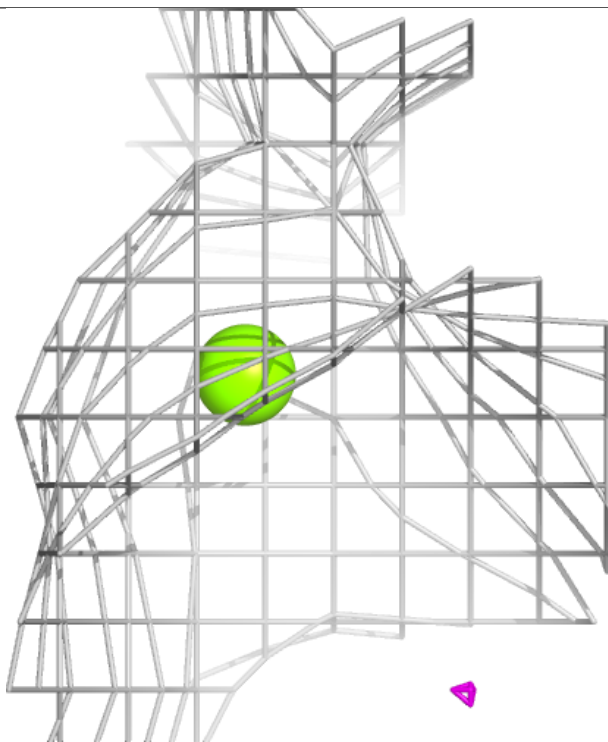
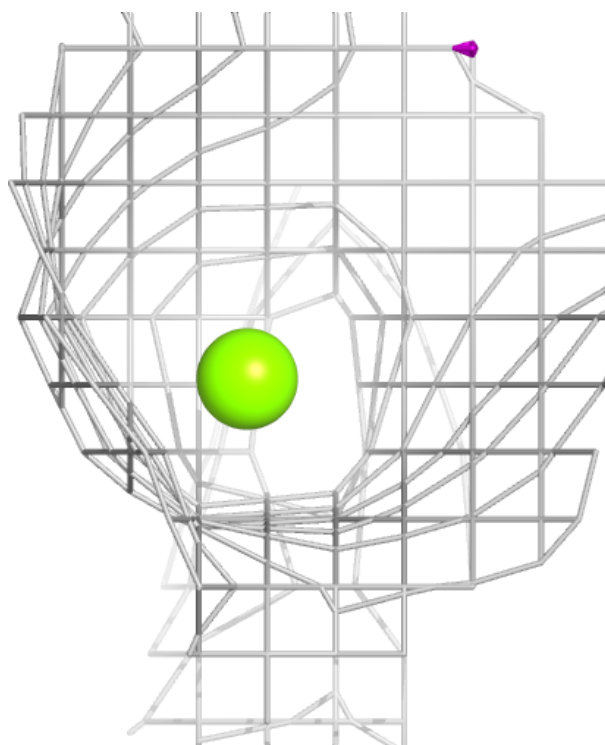
Electron density around ANP A 1102 (B):

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



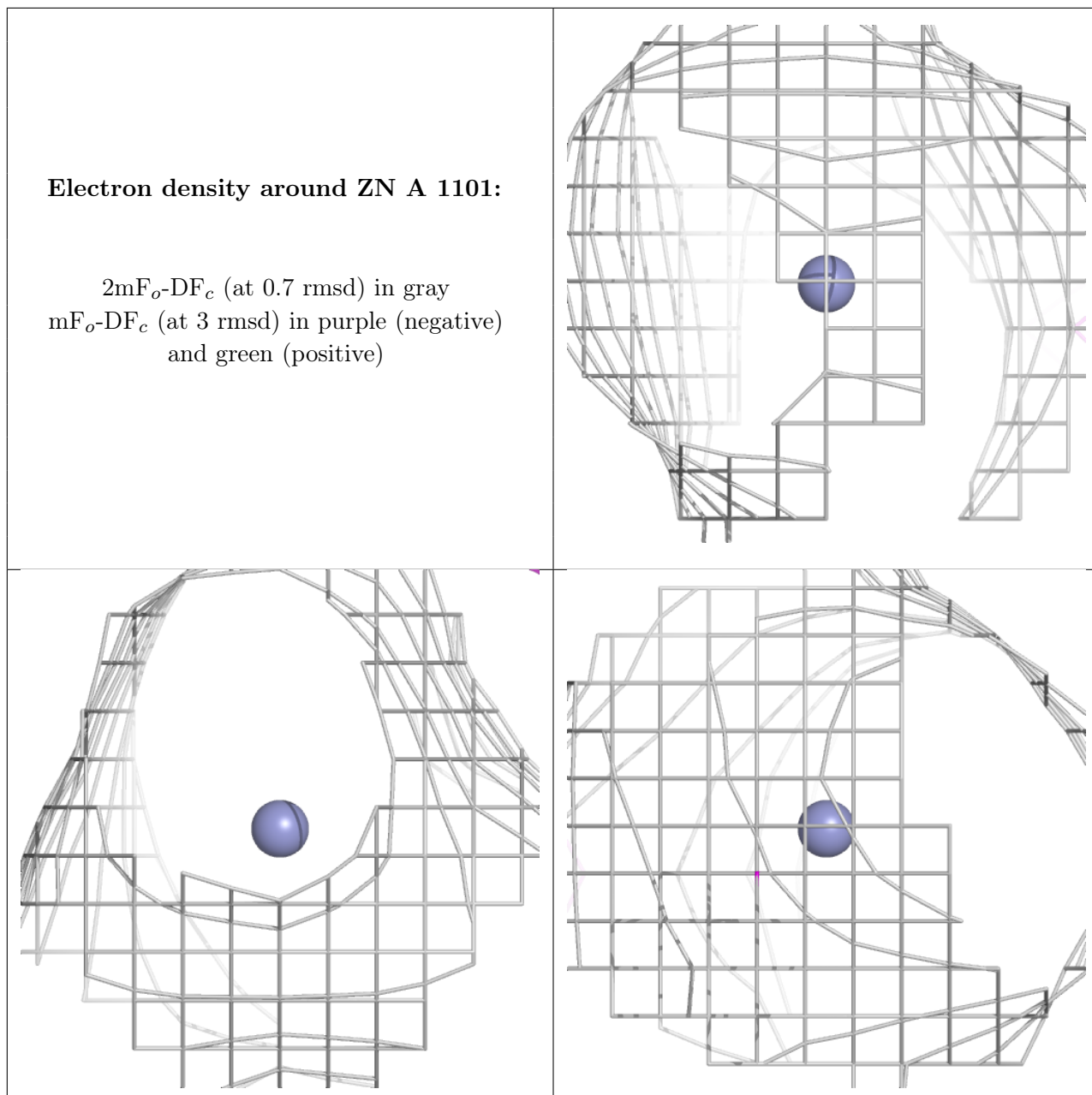
Electron density around MG A 1111:

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



Electron density around ZN 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 ⓘ

There are no such residues in this entry.