



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:59 PM UTC

PDB ID : 8PME / pdb_00008pme
Title : Structure of Nall indica cultivar IR64, construct 88-458
Authors : Huang, L.Y.; Rety, S.; Xi, X.G.
Deposited on : 2023-06-28
Resolution : 2.15 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

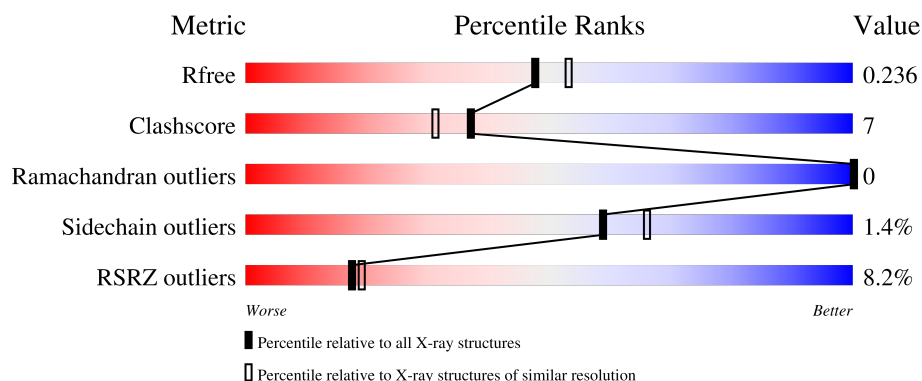
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	371	9% 80% 15% • •
1	B	371	8% 76% 13% • 10%
1	C	371	5% 78% 15% 8%

2 Entry composition [i](#)

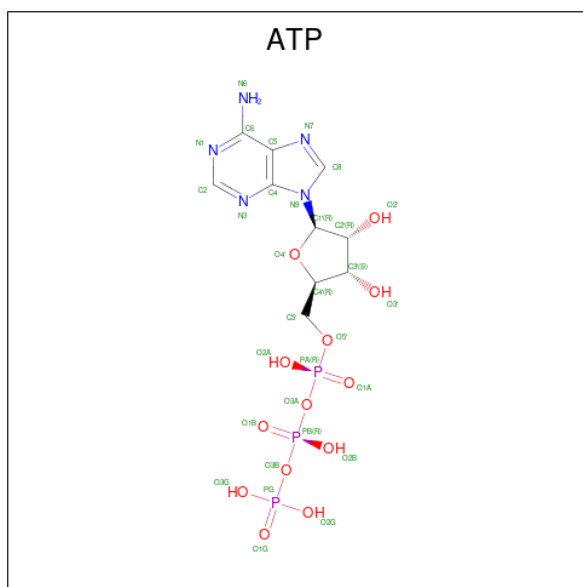
There are 5 unique types of molecules in this entry. The entry contains 8165 atoms, of which 2 are hydrogens and 0 are deuteriums.

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 Narrow leaf 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	Se	0	0	0
			2747	1739	477	520	7	4			
1	B	333	Total	C	N	O	S	Se	0	0	0
			2557	1614	453	479	7	4			
1	C	343	Total	C	N	O	S	Se	0	0	0
			2632	1665	462	494	7	4			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

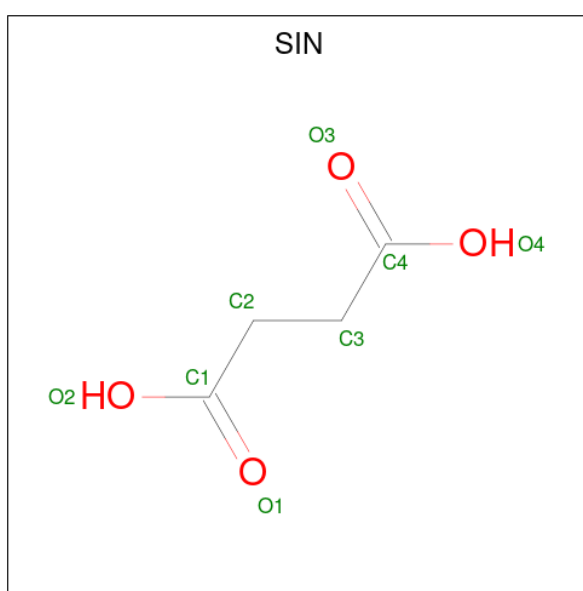


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is SUCCINIC ACID (CCD ID: SIN) (formula: C₄H₆O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 4 4	0	0
4	A	1	Total C O 8 4 4	0	0
4	B	1	Total C H O 10 4 2 4	0	0
4	C	1	Total C O 8 4 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	30	Total O 30 30	0	0

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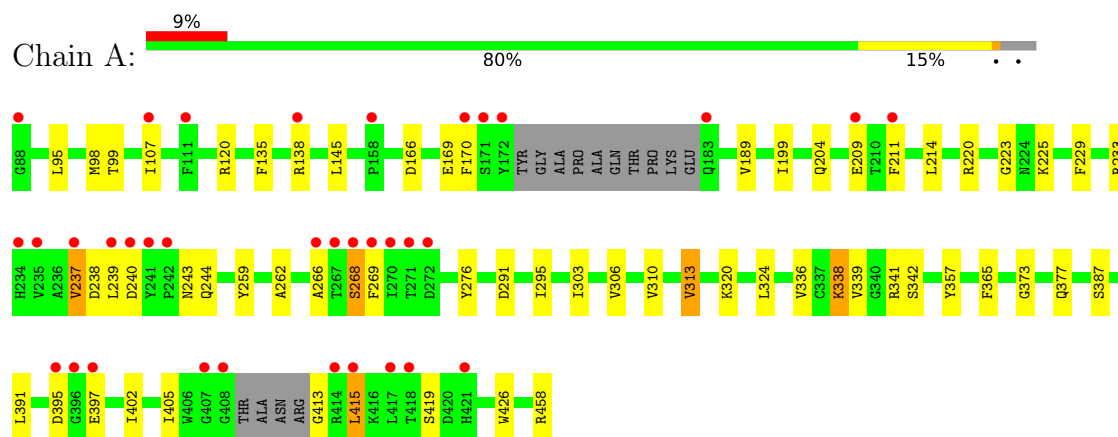
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	28	Total	O	0	0
			28	28		
5	C	41	Total	O	0	0
			41	41		

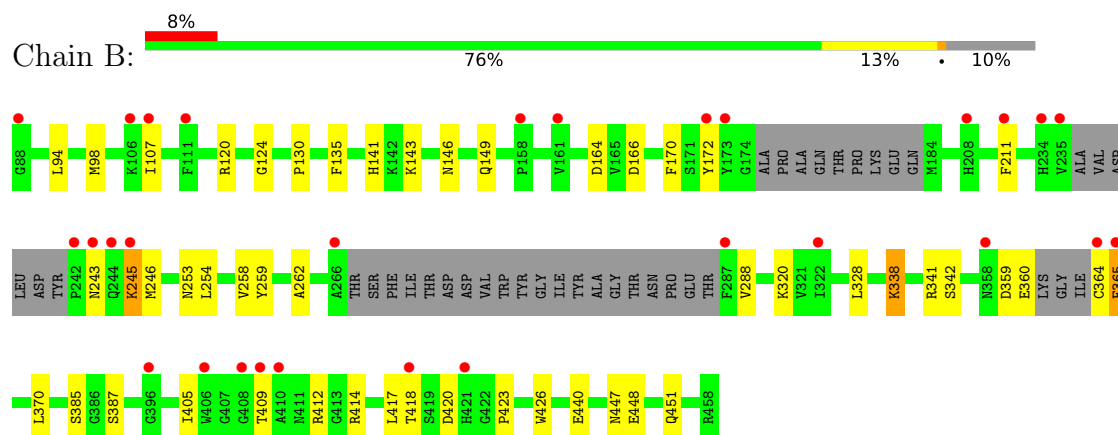
3 Residue-property plots [i](#)

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.

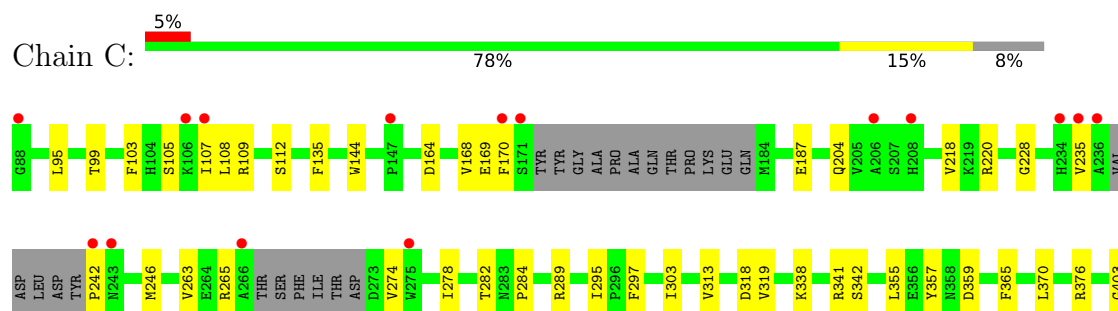
• Molecule 1: Narrow leaf 1

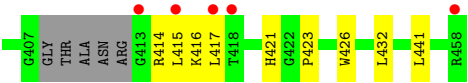


• Molecule 1: Narrow leaf 1



• Molecule 1: Narrow leaf 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.28Å 103.73Å 143.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.64 – 2.15 39.64 – 2.15	Depositor EDS
% Data completeness (in resolution range)	72.8 (39.64-2.15) 73.0 (39.64-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874+SVN, PHENIX 1.18.2_3874+SVN	Depositor
R, R_{free}	0.194 , 0.235 0.195 , 0.236	Depositor DCC
R_{free} test set	2321 reflections (3.56%)	wwPDB-VI
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8165	wwPDB-VI
Average B, all atoms (Å ²)	61.0	wwPDB-VI

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: MG, SIN, ATP

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	0.16	0/2796	0.46	0/3784
1	B	0.15	0/2599	0.43	0/3509
1	C	0.13	0/2677	0.40	0/3618
All	All	0.15	0/8072	0.43	0/10911

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	268	SER	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	2747	0	2724	41	2
1	B	2557	0	2551	39	0
1	C	2632	0	2624	36	0
2	A	31	0	12	1	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	16	0	8	1	0
4	B	8	2	4	3	0
4	C	8	0	4	0	1
5	A	30	0	0	0	0
5	B	28	0	0	2	0
5	C	41	0	0	1	0
All	All	8163	2	7951	114	2

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 (114) 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:413:GLY:HA3	1:A:426:TRP:HE1	1.41	0.86
1:A:209:GLU:OE2	1:A:238:ASP:HB3	1.83	0.79
1:B:245:LYS:HB3	1:B:259:TYR:HE1	1.47	0.78
1:B:258:VAL:HG13	1:C:144:TRP:HA	1.67	0.76
1:B:320:LYS:NZ	5:B:1101:HOH:O	2.17	0.73
1:A:413:GLY:HA3	1:A:426:TRP:NE1	2.05	0.70
1:B:418:THR:HG22	1:B:420:ASP:H	1.57	0.70
1:A:138:ARG:NH1	1:A:169:GLU:OE2	2.24	0.70
1:B:107:ILE:HD12	1:B:107:ILE:H	1.57	0.70
1:B:211:PHE:HB3	4:B:1003:SIN:H21	1.73	0.70
1:B:245:LYS:HG3	1:B:262:ALA:HB2	1.74	0.69
1:B:448:GLU:OE1	1:B:448:GLU:N	2.27	0.68
1:A:95:LEU:O	1:A:99:THR:HG23	1.96	0.65
1:A:395:ASP:HB2	1:A:397:GLU:OE1	1.97	0.63
1:C:282:THR:O	1:C:284:PRO:HD3	2.00	0.62
1:B:245:LYS:HB3	1:B:259:TYR:CE1	2.33	0.62
1:B:172:TYR:CE1	1:B:409:THR:HG22	2.36	0.61
1:A:237:VAL:HG12	1:A:239:LEU:HG	1.82	0.61
1:B:211:PHE:HB3	4:B:1003:SIN:C2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LYS:HG3	1:B:262:ALA:CB	2.34	0.57
1:C:169:GLU:HB3	1:C:416:LYS:HB3	1.87	0.57
1:A:107:ILE:HD12	1:A:107:ILE:H	1.70	0.56
1:C:355:LEU:HD22	1:C:370:LEU:HD13	1.87	0.56
1:B:172:TYR:HE1	1:B:409:THR:HG22	1.70	0.56
1:B:447:ASN:O	1:B:451:GLN:HG3	2.05	0.55
1:B:243:ASN:HB3	1:B:245:LYS:HD2	1.87	0.55
1:B:146:ASN:O	1:B:149:GLN:HG2	2.06	0.55
1:B:135:PHE:HB3	1:B:170:PHE:HB3	1.89	0.55
1:C:246:MSE:HG3	1:C:295:ILE:HG12	1.88	0.55
1:C:242:PRO:HB2	1:C:265:ARG:CZ	2.37	0.55
1:A:211:PHE:HB3	4:A:1003:SIN:H21	1.89	0.54
1:A:419:SER:OG	1:C:187:GLU:OE2	2.25	0.53
1:A:240:ASP:O	1:A:243:ASN:N	2.41	0.53
1:C:103:PHE:O	5:C:1101:HOH:O	2.18	0.53
1:C:357:TYR:HB3	1:C:365:PHE:HB3	1.90	0.53
1:C:218:VAL:HG21	1:C:441:LEU:HD13	1.90	0.53
1:A:233:ARG:CZ	1:A:266:ALA:HB2	2.39	0.52
1:B:288:VAL:O	1:B:365:PHE:HA	2.10	0.52
1:C:289:ARG:HH11	1:C:289:ARG:HG2	1.73	0.52
1:A:204:GLN:OE1	1:A:341:ARG:NE	2.42	0.51
1:A:214:LEU:HG	1:A:229:PHE:CD1	2.46	0.51
1:C:274:VAL:O	1:C:278:ILE:HG13	2.11	0.51
1:A:320:LYS:HB3	1:A:402:ILE:HG22	1.93	0.51
1:B:414:ARG:HB2	1:B:423:PRO:HB2	1.94	0.50
1:C:220:ARG:HA	1:C:441:LEU:HD23	1.94	0.49
1:A:98:MSE:HE1	1:A:324:LEU:HD13	1.93	0.49
1:C:95:LEU:O	1:C:99:THR:HG23	2.13	0.49
1:B:341:ARG:HG3	1:B:342:SER:N	2.26	0.49
1:A:209:GLU:CD	1:A:243:ASN:HB3	2.39	0.48
1:A:220:ARG:HB2	1:A:225:LYS:HA	1.96	0.48
1:A:170:PHE:CE1	1:A:415:LEU:HD12	2.48	0.48
1:B:94:LEU:O	1:B:98:MSE:HG3	2.13	0.48
1:B:135:PHE:HB3	1:B:170:PHE:CB	2.44	0.48
1:C:235:VAL:HG22	1:C:235:VAL:O	2.13	0.48
1:C:415:LEU:HD22	1:C:417:LEU:HG	1.95	0.48
1:B:338:LYS:HD2	1:B:338:LYS:C	2.39	0.47
1:B:245:LYS:HA	1:B:262:ALA:HA	1.96	0.47
1:C:341:ARG:HG3	1:C:342:SER:N	2.29	0.47
1:C:204:GLN:OE1	1:C:341:ARG:NE	2.44	0.47
1:A:341:ARG:HG3	1:A:342:SER:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ARG:HB3	1:C:423:PRO:HB2	1.97	0.47
1:C:105:SER:O	1:C:109:ARG:HG3	2.15	0.47
1:A:310:VAL:HG12	1:A:313:VAL:HG13	1.96	0.47
1:C:263:VAL:HA	1:C:295:ILE:HG13	1.97	0.46
1:C:318:ASP:OD1	1:C:319:VAL:HG12	2.15	0.46
1:A:415:LEU:HD23	1:A:415:LEU:O	2.15	0.46
1:C:303:ILE:HG22	1:C:303:ILE:O	2.16	0.46
1:B:387:SER:HB2	1:B:405:ILE:HD12	1.96	0.46
1:A:240:ASP:H	1:A:243:ASN:HD22	1.61	0.46
1:C:415:LEU:CD2	1:C:417:LEU:HG	2.47	0.45
1:C:108:LEU:O	1:C:112:SER:OG	2.29	0.45
1:C:318:ASP:OD1	1:C:319:VAL:N	2.50	0.44
1:A:170:PHE:HE1	1:A:415:LEU:HD12	1.83	0.44
1:A:269:PHE:HZ	1:A:291:ASP:CG	2.25	0.44
1:C:359:ASP:OD1	1:C:359:ASP:C	2.61	0.44
1:B:364:CYS:SG	5:B:1108:HOH:O	2.60	0.44
1:A:244:GLN:O	1:A:262:ALA:HA	2.17	0.44
1:B:253:ASN:ND2	1:B:254:LEU:HG	2.32	0.44
1:A:233:ARG:NE	1:A:266:ALA:HB2	2.33	0.44
1:C:135:PHE:HA	1:C:168:VAL:O	2.18	0.44
1:A:295:ILE:HD12	1:A:295:ILE:N	2.33	0.43
1:B:120:ARG:HG3	1:B:166:ASP:OD1	2.18	0.43
1:A:387:SER:HB2	1:A:405:ILE:HD12	2.00	0.43
1:C:107:ILE:HD12	1:C:107:ILE:N	2.34	0.43
1:C:228:GLY:HA2	1:C:297:PHE:CD2	2.54	0.43
1:C:319:VAL:HG23	1:C:432:LEU:HD23	2.01	0.43
1:B:120:ARG:NH1	1:B:166:ASP:OD1	2.51	0.43
1:A:373:GLY:HA3	1:A:377:GLN:O	2.18	0.43
1:C:403:GLY:HA2	1:C:432:LEU:HB2	2.00	0.42
1:B:124:GLY:HA2	1:B:417:LEU:O	2.19	0.42
1:A:120:ARG:HG3	1:A:166:ASP:OD1	2.19	0.42
1:A:199:ILE:O	1:A:306:VAL:HA	2.19	0.42
1:A:223:GLY:O	1:A:458:ARG:HD2	2.19	0.42
1:A:338:LYS:HG2	1:A:339:VAL:N	2.29	0.42
1:A:135:PHE:HB3	1:A:170:PHE:CB	2.50	0.42
1:A:303:ILE:O	1:A:303:ILE:HG22	2.20	0.42
1:C:107:ILE:HD12	1:C:107:ILE:H	1.84	0.41
1:A:145:LEU:HD11	2:A:1001:ATP:C4	2.56	0.41
1:B:172:TYR:O	1:B:412:ARG:HB3	2.20	0.41
1:C:170:PHE:HE2	1:C:426:TRP:NE1	2.18	0.41
1:B:130:PRO:HB3	1:B:328:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:MSE:HE3	1:B:246:MSE:HB3	1.93	0.41
1:B:107:ILE:HD12	1:B:107:ILE:N	2.31	0.41
1:B:141:HIS:CE1	1:B:143:LYS:HG3	2.55	0.41
1:A:189:VAL:HG13	1:A:341:ARG:O	2.21	0.41
1:A:268:SER:O	1:A:269:PHE:CD2	2.74	0.41
1:A:336:VAL:HG12	1:A:391:LEU:HD23	2.02	0.40
1:C:376:ARG:HH11	1:C:421:HIS:CG	2.38	0.40
1:B:254:LEU:CD1	4:B:1003:SIN:H32	2.52	0.40
1:B:359:ASP:HB3	1:B:360:GLU:CD	2.47	0.40
1:B:370:LEU:HD11	1:B:426:TRP:HB2	2.04	0.40
1:C:289:ARG:HG2	1:C:289:ARG:NH1	2.36	0.40
1:A:357:TYR:HB3	1:A:365:PHE:HB3	2.03	0.40
1:B:385:SER:HA	1:B:405:ILE:HG22	2.03	0.40

All (2) 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:259:TYR:OH	1:A:397:GLU:OE2[4_557]	2.05	0.15
1:A:276:TYR:OH	4:C:1003:SIN:O4[2_455]	2.13	0.07

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	351/371 (95%)	351 (100%)	0	0	100	100
1	B	323/371 (87%)	323 (100%)	0	0	100	100
1	C	333/371 (90%)	333 (100%)	0	0	100	100
All	All	1007/1113 (90%)	1007 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/305 (98%)	295 (99%)	4 (1%)	61	68
1	B	278/305 (91%)	273 (98%)	5 (2%)	51	58
1	C	286/305 (94%)	283 (99%)	3 (1%)	68	75
All	All	863/915 (94%)	851 (99%)	12 (1%)	59	66

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	VAL
1	A	313	VAL
1	A	338	LYS
1	A	415	LEU
1	B	164	ASP
1	B	245	LYS
1	B	338	LYS
1	B	365	PHE
1	B	440	GLU
1	C	164	ASP
1	C	313	VAL
1	C	338	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	A	243	ASN
1	A	335	GLN
1	A	377	GLN
1	A	421	HIS
1	B	335	GLN
1	B	394	GLN
1	C	283	ASN
1	C	335	GLN

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Mol	Chain	Res	Type
1	C	394	GLN

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 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	SIN	A	1004	-	7,7,7	1.07	0	8,8,8	1.45	1 (12%)
2	ATP	C	1001	3	32,33,33	1.36	5 (15%)	48,52,52	1.76	9 (18%)
4	SIN	C	1003	-	7,7,7	1.10	0	8,8,8	1.54	2 (25%)
4	SIN	A	1003	-	7,7,7	1.05	0	8,8,8	1.60	2 (25%)
2	ATP	A	1001	3	32,33,33	1.39	4 (12%)	48,52,52	1.75	10 (20%)
2	ATP	B	1001	3	32,33,33	1.43	5 (15%)	48,52,52	1.75	8 (16%)
4	SIN	B	1003	-	7,7,7	1.14	0	8,8,8	1.66	1 (12%)

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	SIN	A	1004	-	-	4/5/5/5	-
2	ATP	C	1001	3	-	2/22/38/38	0/3/3/3
4	SIN	C	1003	-	-	2/5/5/5	-
4	SIN	A	1003	-	-	3/5/5/5	-
2	ATP	A	1001	3	-	3/22/38/38	0/3/3/3
2	ATP	B	1001	3	-	2/22/38/38	0/3/3/3
4	SIN	B	1003	-	-	3/5/5/5	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	ATP	C5-C4	4.76	1.47	1.39
2	B	1001	ATP	C5-C4	4.72	1.47	1.39
2	A	1001	ATP	C5-C4	4.71	1.47	1.39
2	B	1001	ATP	C5-C6	2.73	1.48	1.41
2	A	1001	ATP	C5-C6	2.67	1.48	1.41
2	C	1001	ATP	C5-C6	2.62	1.48	1.41
2	B	1001	ATP	PB-O3B	2.43	1.62	1.59
2	A	1001	ATP	C8-N7	2.37	1.36	1.31
2	A	1001	ATP	C5-N7	-2.31	1.34	1.39
2	B	1001	ATP	C8-N7	2.31	1.36	1.31
2	C	1001	ATP	C5-N7	-2.31	1.34	1.39
2	C	1001	ATP	C8-N7	2.28	1.36	1.31
2	B	1001	ATP	C5-N7	-2.25	1.35	1.39
2	C	1001	ATP	PB-O3B	2.07	1.61	1.59

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	ATP	C5-C4-N3	-5.84	118.67	126.72
2	A	1001	ATP	C5-C4-N3	-5.79	118.75	126.72
2	C	1001	ATP	C5-C4-N3	-5.68	118.89	126.72
2	B	1001	ATP	N3-C4-N9	4.67	135.10	127.17
2	C	1001	ATP	N3-C4-N9	4.62	135.03	127.17
2	A	1001	ATP	N3-C4-N9	4.55	134.91	127.17
2	B	1001	ATP	C2-N3-C4	3.74	120.97	111.83
2	A	1001	ATP	C2-N3-C4	3.63	120.70	111.83
2	C	1001	ATP	C2-N3-C4	3.61	120.64	111.83
2	A	1001	ATP	C4-C5-N7	-3.50	106.58	110.58
2	B	1001	ATP	C4-C5-N7	-3.42	106.67	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	ATP	C4-C5-N7	-3.33	106.78	110.58
2	B	1001	ATP	N3-C2-N1	-3.29	123.61	128.58
2	C	1001	ATP	N3-C2-N1	-3.21	123.72	128.58
2	A	1001	ATP	N3-C2-N1	-3.14	123.83	128.58
2	C	1001	ATP	C4-N9-C8	2.75	108.63	105.74
2	C	1001	ATP	C2'-C1'-N9	-2.75	106.47	113.30
2	B	1001	ATP	C4-N9-C8	2.68	108.55	105.74
2	A	1001	ATP	C4-N9-C8	2.64	108.51	105.74
2	A	1001	ATP	C5-N7-C8	2.61	107.55	103.45
2	B	1001	ATP	C5-N7-C8	2.51	107.40	103.45
2	C	1001	ATP	C5-N7-C8	2.49	107.36	103.45
4	B	1003	SIN	O4-C4-C3	2.34	121.41	114.00
2	A	1001	ATP	C3'-C2'-C1'	2.25	105.71	101.46
4	C	1003	SIN	O2-C1-C2	2.17	120.86	114.00
2	A	1001	ATP	C6-C5-N7	2.07	136.09	132.09
2	B	1001	ATP	C6-C5-N7	2.06	136.06	132.09
2	C	1001	ATP	O3G-PG-O2G	2.06	115.51	107.80
2	A	1001	ATP	N9-C8-N7	-2.05	111.03	113.94
4	A	1003	SIN	O2-C1-C2	2.04	120.43	114.00
4	A	1004	SIN	O2-C1-C2	2.03	120.42	114.00
4	A	1003	SIN	O4-C4-C3	2.02	120.38	114.00
4	C	1003	SIN	O4-C4-C3	2.00	120.33	114.00

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	SIN	C1-C2-C3-C4
4	B	1003	SIN	C1-C2-C3-C4
2	A	1001	ATP	PA-O3A-PB-O2B
2	B	1001	ATP	PA-O3A-PB-O2B
2	C	1001	ATP	PA-O3A-PB-O2B
2	A	1001	ATP	C3'-C4'-C5'-O5'
4	A	1004	SIN	C2-C3-C4-O4
4	A	1004	SIN	O1-C1-C2-C3
4	A	1004	SIN	C2-C3-C4-O3
4	A	1004	SIN	O2-C1-C2-C3
2	C	1001	ATP	PA-O3A-PB-O1B
4	A	1003	SIN	O2-C1-C2-C3
4	C	1003	SIN	O2-C1-C2-C3
4	C	1003	SIN	O1-C1-C2-C3
4	A	1003	SIN	O1-C1-C2-C3

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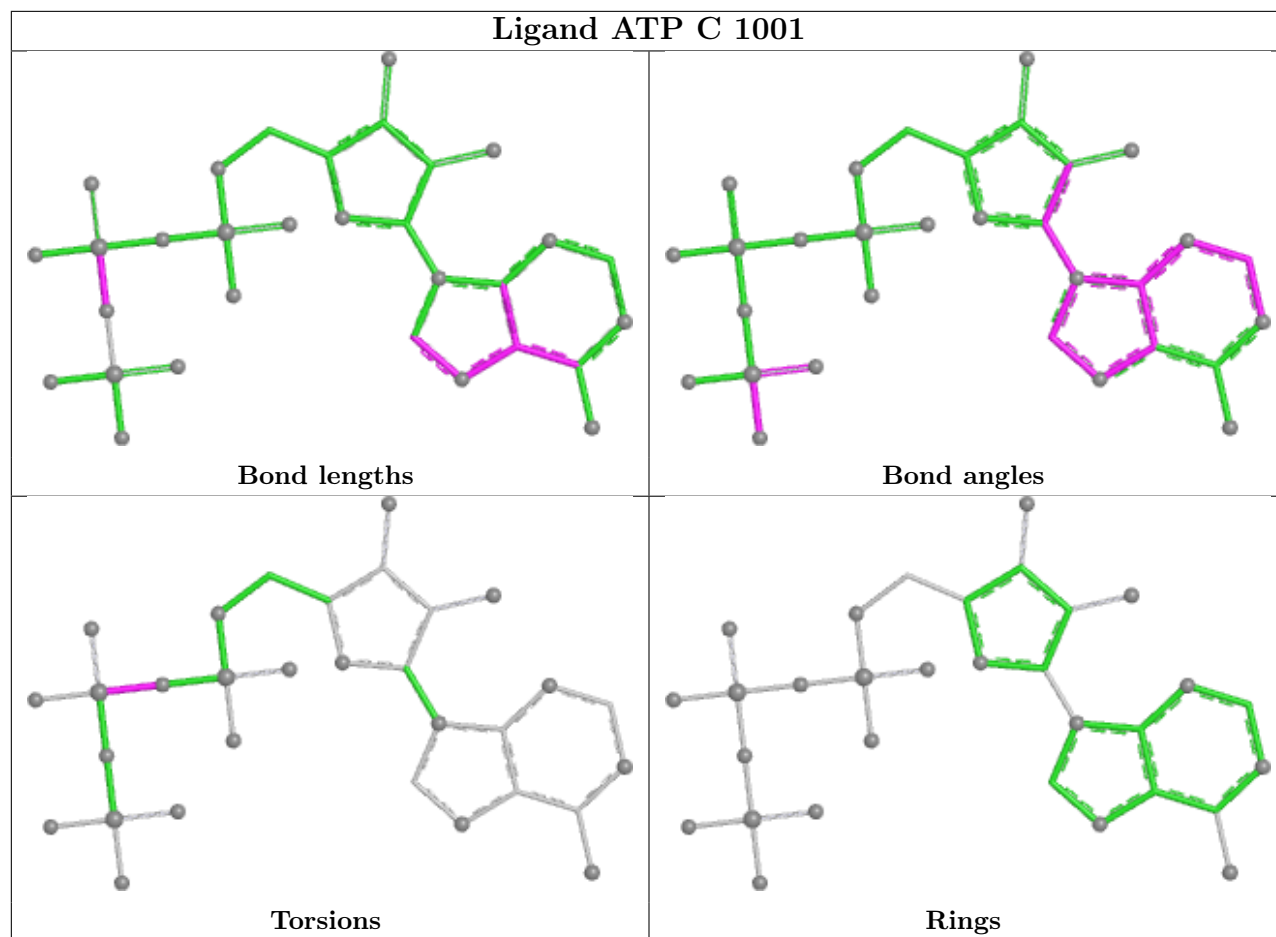
Mol	Chain	Res	Type	Atoms
2	A	1001	ATP	PA-O3A-PB-O1B
2	B	1001	ATP	PA-O3A-PB-O1B
4	B	1003	SIN	O1-C1-C2-C3
4	B	1003	SIN	O2-C1-C2-C3

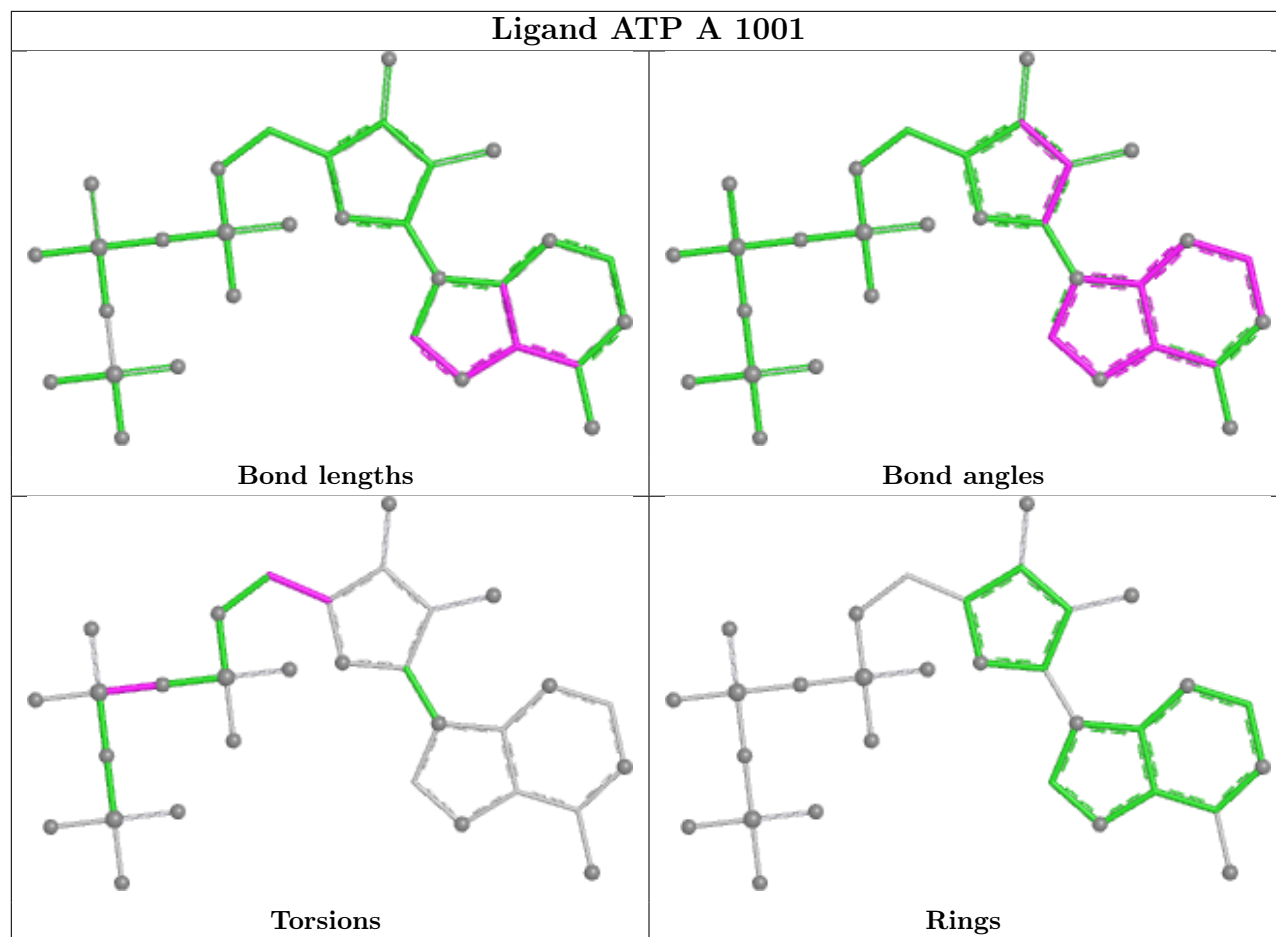
There are no ring outliers.

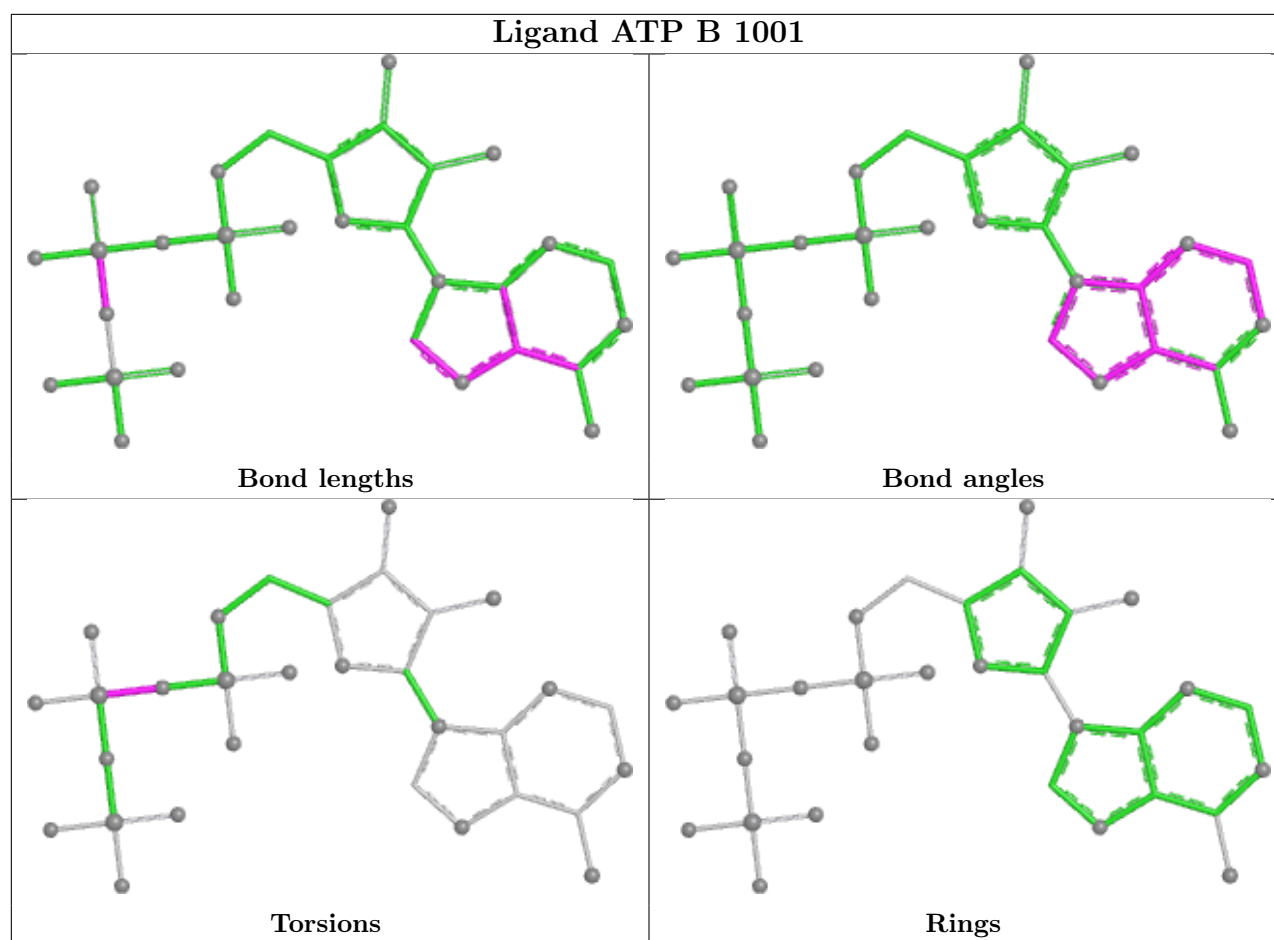
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1003	SIN	0	1
4	A	1003	SIN	1	0
2	A	1001	ATP	1	0
4	B	1003	SIN	3	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	353/371 (95%)	0.40	35 (9%) 13 14	35, 53, 102, 140	0
1	B	329/371 (88%)	0.52	29 (8%) 15 17	40, 60, 103, 127	0
1	C	339/371 (91%)	0.28	20 (5%) 28 32	40, 54, 87, 132	0
All	All	1021/1113 (91%)	0.40	84 (8%) 17 19	35, 56, 98, 140	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	410	ALA	5.5
1	A	408	GLY	5.4
1	A	270	ILE	5.4
1	B	235	VAL	5.1
1	C	242	PRO	5.1
1	A	241	TYR	5.0
1	A	397	GLU	4.9
1	A	271	THR	4.4
1	C	236	ALA	4.4
1	A	239	LEU	4.3
1	B	409	THR	4.3
1	C	266	ALA	4.2
1	B	408	GLY	4.0
1	A	395	ASP	3.9
1	A	268	SER	3.9
1	A	170	PHE	3.8
1	B	111	PHE	3.8
1	A	269	PHE	3.8
1	B	244	GLN	3.6
1	A	396	GLY	3.4
1	A	407	GLY	3.4
1	A	172	TYR	3.4
1	B	172	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	173	TYR	3.2
1	C	170	PHE	3.1
1	B	322	ILE	3.1
1	B	287	PHE	3.1
1	C	235	VAL	3.1
1	B	421	HIS	3.1
1	C	206	ALA	3.1
1	A	111	PHE	3.0
1	B	107	ILE	3.0
1	A	418	THR	3.0
1	B	266	ALA	3.0
1	B	243	ASN	3.0
1	A	242	PRO	3.0
1	C	208	HIS	2.9
1	B	242	PRO	2.9
1	A	171	SER	2.9
1	B	245	LYS	2.9
1	A	266	ALA	2.8
1	B	106	LYS	2.8
1	A	183	GLN	2.8
1	B	365	PHE	2.8
1	C	417	LEU	2.7
1	A	267	THR	2.7
1	B	406	TRP	2.7
1	A	88	GLY	2.7
1	A	209	GLU	2.6
1	A	158	PRO	2.6
1	B	364	CYS	2.6
1	A	417	LEU	2.6
1	B	88	GLY	2.5
1	B	396	GLY	2.5
1	C	107	ILE	2.5
1	A	235	VAL	2.4
1	C	413	GLY	2.4
1	C	418	THR	2.4
1	C	243	ASN	2.4
1	A	211	PHE	2.3
1	B	211	PHE	2.3
1	A	234	HIS	2.3
1	A	414	ARG	2.3
1	B	208	HIS	2.3
1	C	234	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	158	PRO	2.3
1	C	106	LYS	2.3
1	A	138	ARG	2.2
1	C	458	ARG	2.2
1	A	415	LEU	2.2
1	C	275	TRP	2.2
1	C	147	PRO	2.2
1	B	234	HIS	2.1
1	C	415	LEU	2.1
1	A	272	ASP	2.1
1	B	418	THR	2.1
1	A	107	ILE	2.1
1	A	421	HIS	2.1
1	B	161	VAL	2.1
1	C	171	SER	2.1
1	B	358	ASN	2.1
1	C	88	GLY	2.1
1	A	237	VAL	2.1
1	A	240	ASP	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.

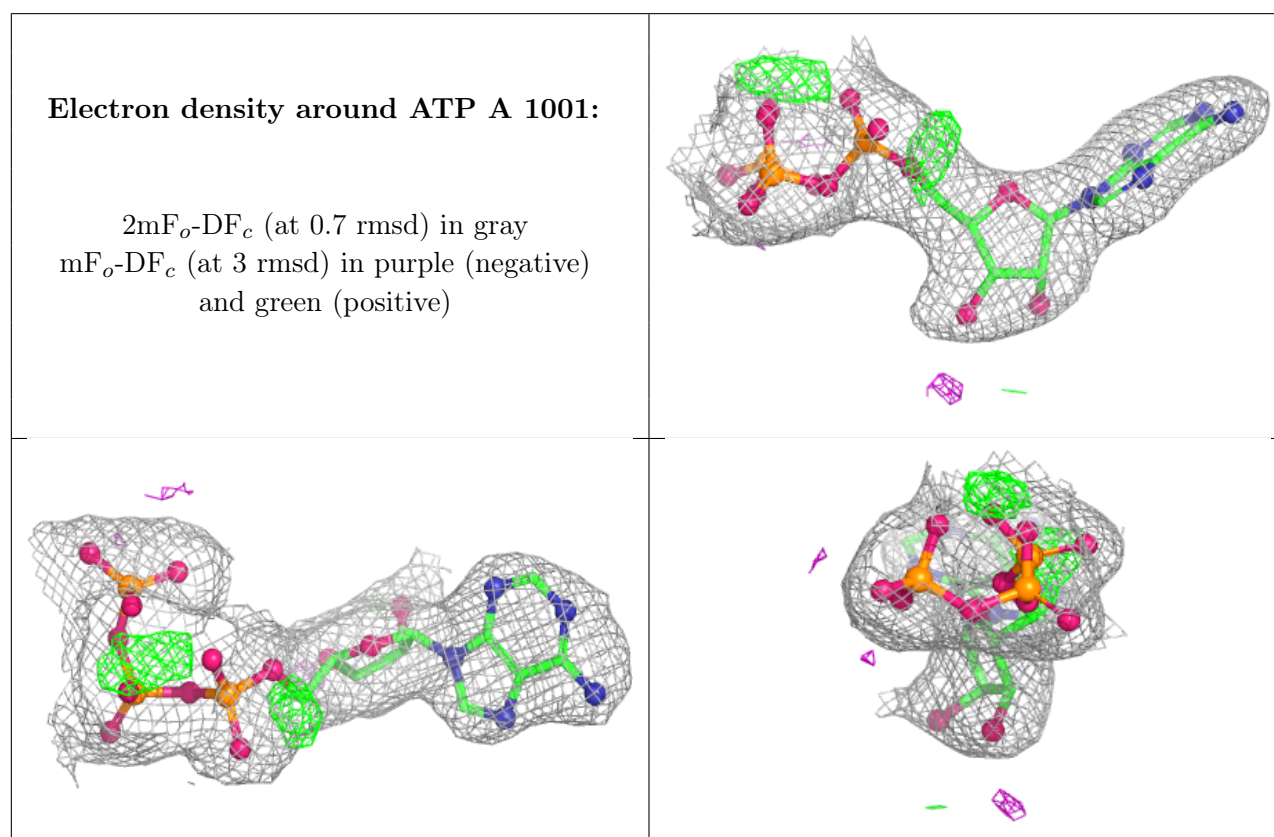
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SIN	A	1004	8/8	0.63	0.18	75,78,83,87	0
4	SIN	A	1003	8/8	0.77	0.15	60,69,73,74	0
4	SIN	B	1003	8/8	0.79	0.20	103,125,131,133	0
4	SIN	C	1003	8/8	0.81	0.17	56,65,72,77	0

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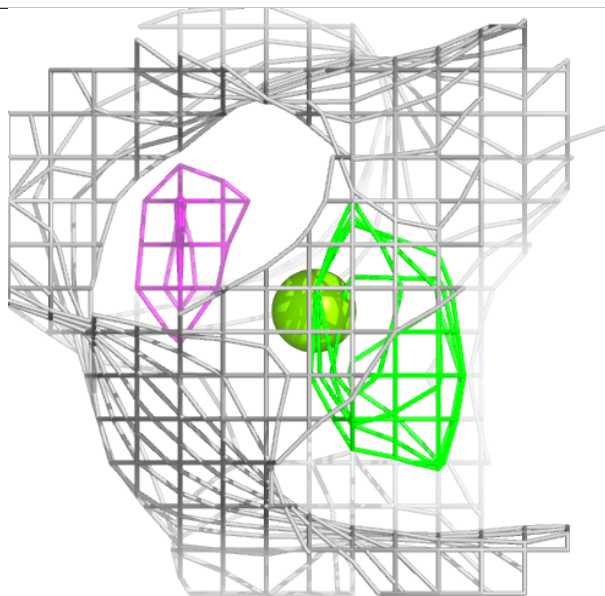
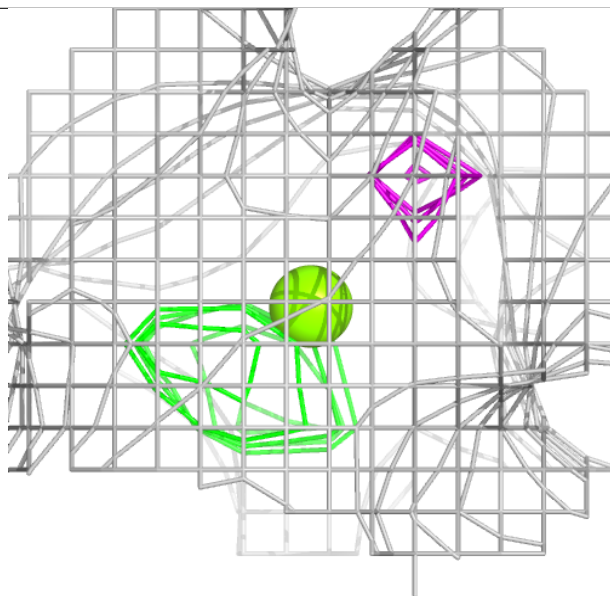
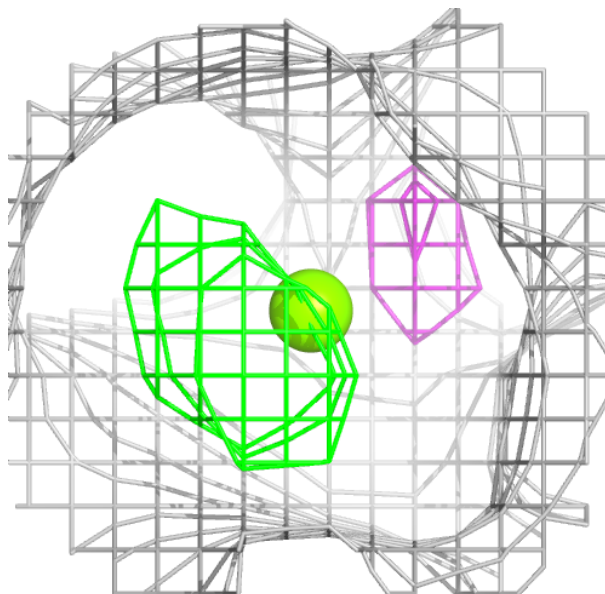
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	A	1001	31/31	0.95	0.08	45,53,58,65	0
3	MG	B	1002	1/1	0.95	0.08	43,43,43,43	0
3	MG	A	1002	1/1	0.96	0.08	48,48,48,48	0
3	MG	C	1002	1/1	0.96	0.06	43,43,43,43	0
2	ATP	C	1001	31/31	0.97	0.07	43,51,56,59	0
2	ATP	B	1001	31/31	0.97	0.06	44,51,54,60	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.



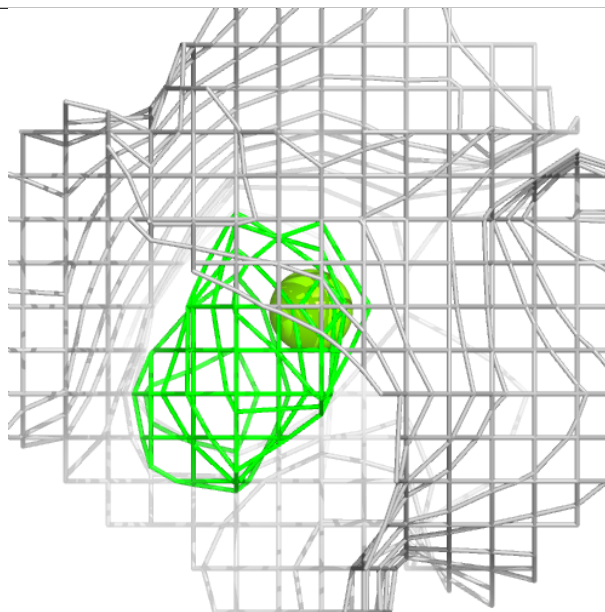
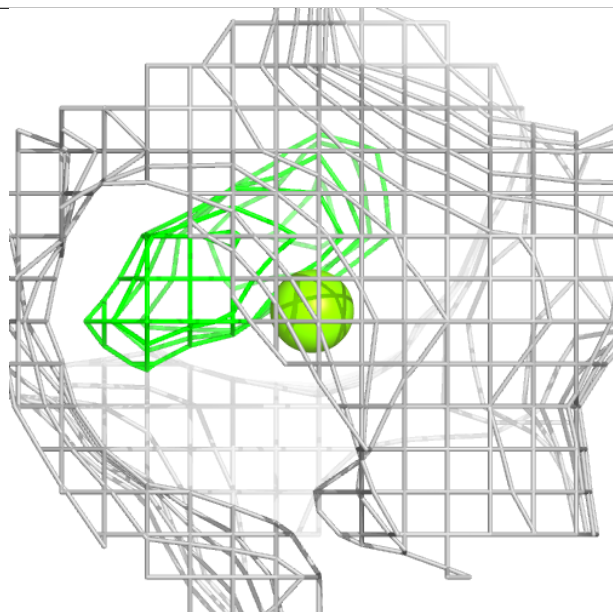
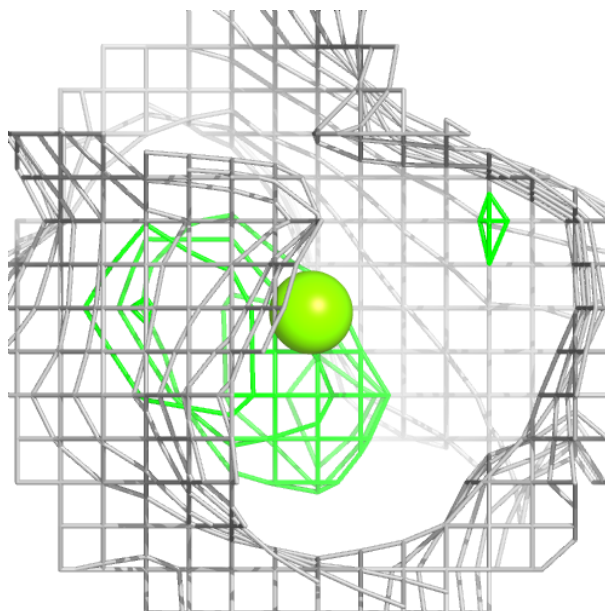
Electron density around MG B 1002:

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



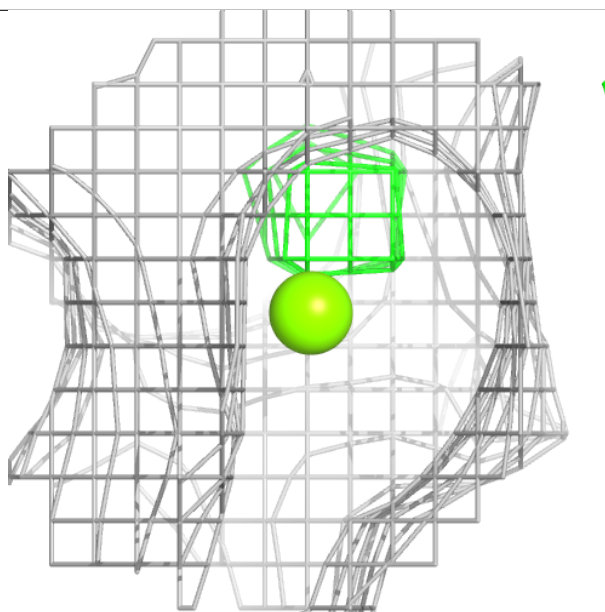
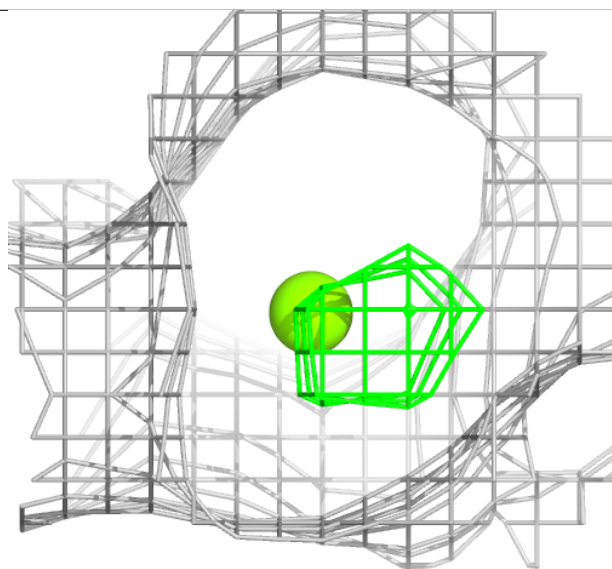
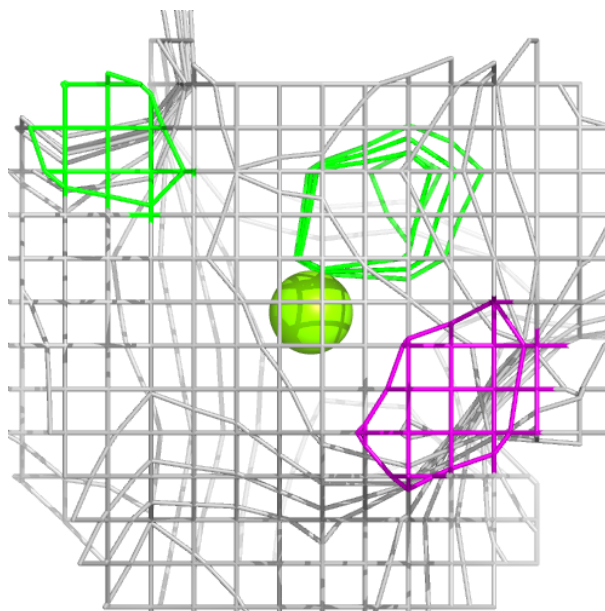
Electron density around MG A 1002:

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



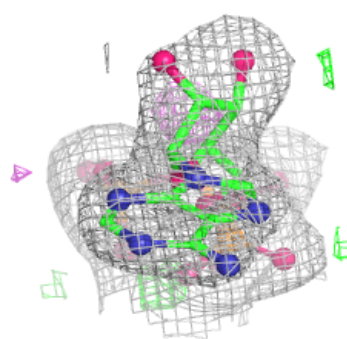
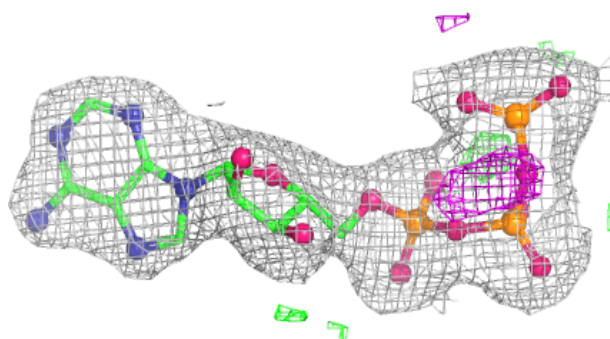
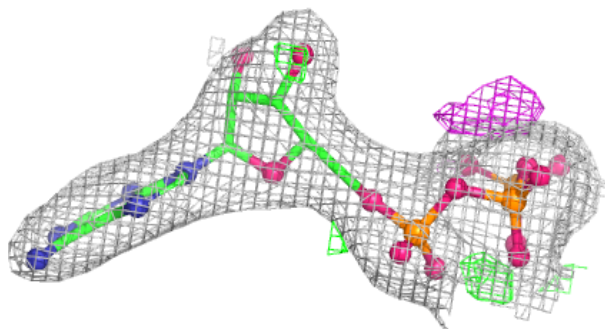
Electron density around MG C 1002:

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

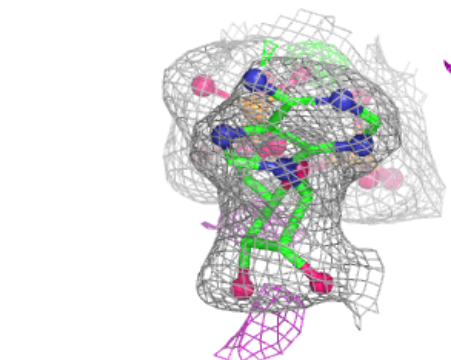
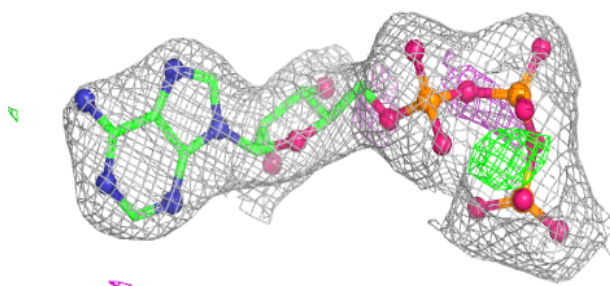
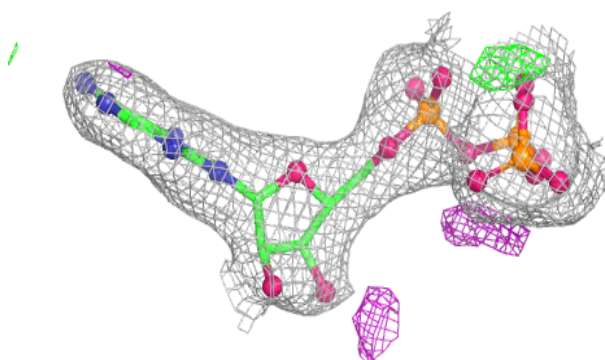


Electron density around ATP C 1001:

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

**Electron density around ATP B 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.