



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:30 PM UTC

PDB ID : 6KC0 / pdb_00006kc0
Title : fused To-MtbCsm1 with 2ATP
Authors : Li, T.; Huo, Y.; Jiang, T.
Deposited on : 2019-06-26
Resolution : 2.29 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

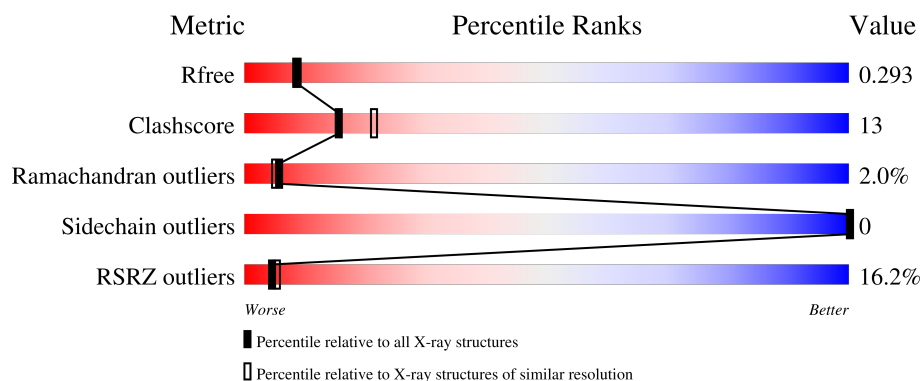
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	776	14% 63% 23% • 13%

2 Entry composition [i](#)

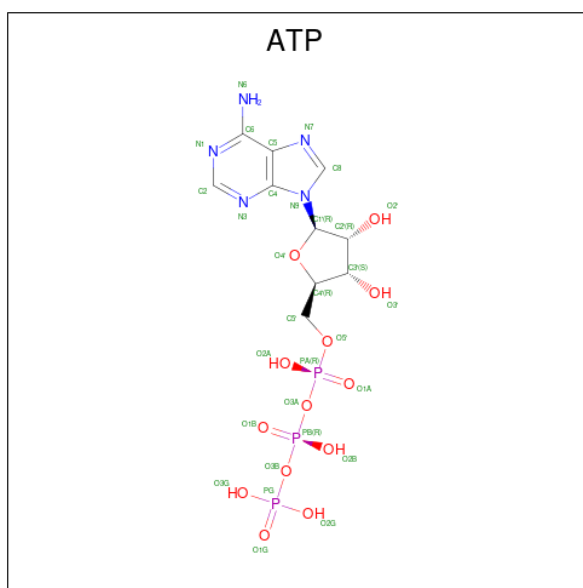
There are 4 unique types of molecules in this entry. The entry contains 5668 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A), CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	674	Total	C	N	O	S	0	0	0
			5423	3485	944	977	17			

- 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	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

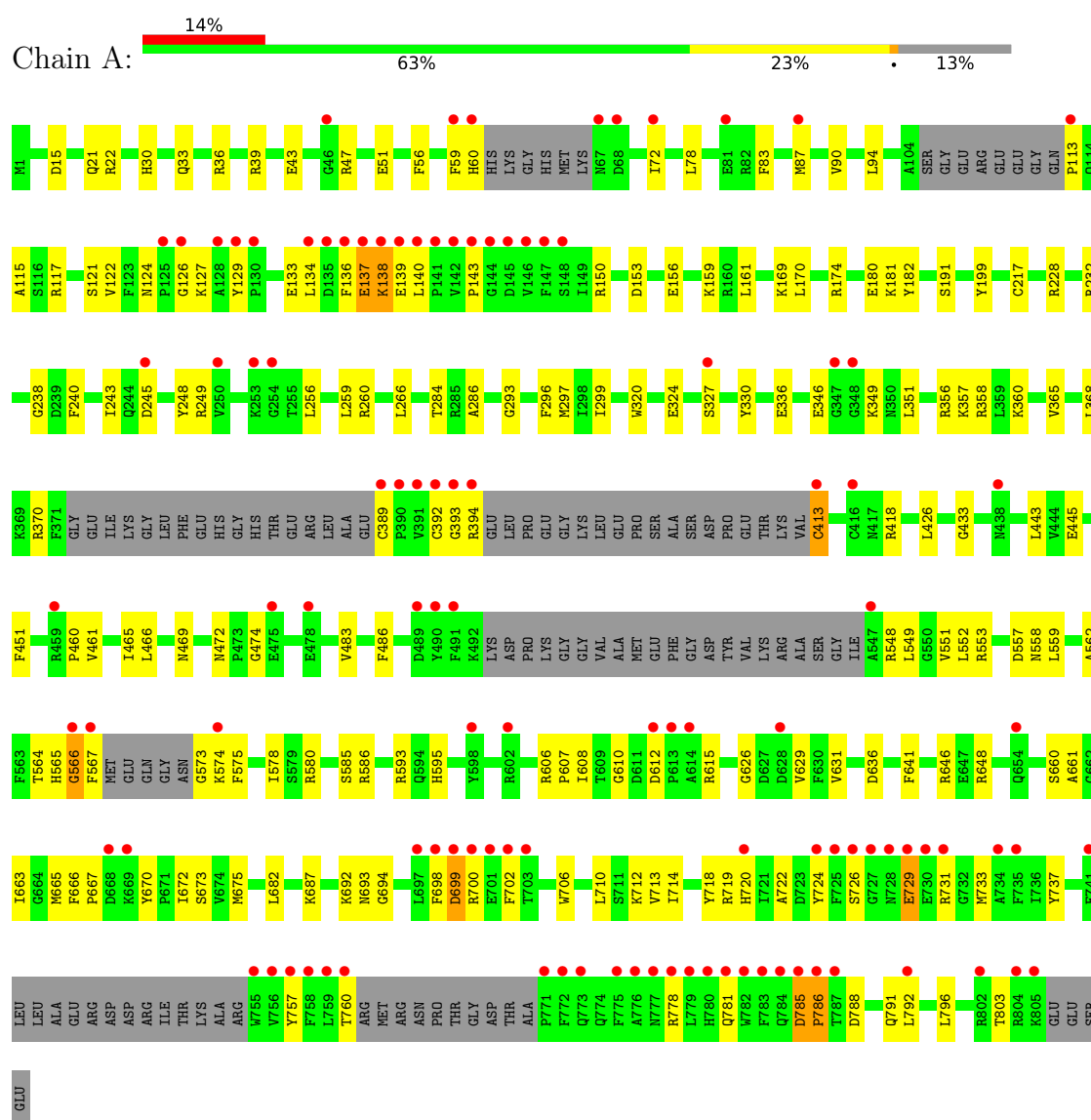
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	180	Total 180	O 180	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: CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A), CRISPR system single-strand-specific deoxyribonuclease Cas10/Csm1 (subtype III-A)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.63Å 53.62Å 130.31Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	64.36 – 2.29 64.36 – 2.29	Depositor EDS
% Data completeness (in resolution range)	96.6 (64.36-2.29) 96.2 (64.36-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.14_3247: ???)	Depositor
R, R_{free}	0.213 , 0.286 (Not available) , 0.293	Depositor DCC
R_{free} test set	1980 reflections (5.57%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5668	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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: 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	0.37	0/5543	0.62	3/7471 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	413	CYS	CA-CB-SG	8.71	134.42	114.40
1	A	558	ASN	CA-C-N	-6.95	109.75	120.31
1	A	558	ASN	C-N-CA	-6.95	109.75	120.31

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	5423	0	5401	145	0
2	A	62	0	24	3	0
3	A	3	0	0	0	0
4	A	180	0	0	9	0
All	All	5668	0	5425	145	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 13.

All (145) 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:284:THR:HG22	1:A:286:ALA:H	1.33	0.92
1:A:327:SER:O	1:A:370:ARG:NH2	2.08	0.86
1:A:78:LEU:O	1:A:78:LEU:HD13	1.78	0.83
1:A:562:ALA:HA	1:A:566:GLY:HA3	1.60	0.81
1:A:573:GLY:N	4:A:1001:HOH:O	2.14	0.81
1:A:610:GLY:O	1:A:615:ARG:NH2	2.16	0.78
1:A:593:ARG:HH22	1:A:626:GLY:H	1.35	0.74
1:A:137:GLU:O	1:A:139:GLU:N	2.21	0.73
1:A:698:PHE:O	1:A:700:ARG:N	2.23	0.71
1:A:228:ARG:NH1	4:A:1003:HOH:O	2.23	0.69
1:A:15:ASP:OD1	1:A:60:HIS:NE2	2.26	0.69
1:A:786:PRO:HG2	1:A:788:ASP:HB2	1.75	0.69
1:A:336:GLU:OE2	1:A:358:ARG:NH1	2.27	0.68
1:A:445:GLU:OE2	4:A:1002:HOH:O	2.14	0.65
1:A:243:ILE:HD12	1:A:266:LEU:HD21	1.78	0.65
1:A:559:LEU:HB3	2:A:902:ATP:H5'2	1.80	0.64
1:A:30:HIS:HE2	1:A:60:HIS:CD2	2.15	0.64
1:A:713:VAL:HG22	1:A:791:GLN:HB3	1.80	0.63
1:A:719:ARG:HH11	1:A:719:ARG:HB2	1.63	0.63
1:A:121:SER:HB2	1:A:143:PRO:HB3	1.80	0.62
1:A:59:PHE:HD1	1:A:60:HIS:N	1.98	0.61
1:A:733:MET:HE1	1:A:803:THR:HB	1.83	0.61
1:A:169:LYS:HE2	1:A:174:ARG:HG3	1.83	0.60
1:A:169:LYS:CE	1:A:169:LYS:H	2.14	0.60
1:A:127:LYS:HB2	1:A:143:PRO:HB2	1.83	0.60
1:A:719:ARG:HA	1:A:722:ALA:HB3	1.84	0.59
1:A:169:LYS:HE2	1:A:169:LYS:H	1.68	0.59
1:A:593:ARG:NH2	1:A:626:GLY:H	2.01	0.58
1:A:284:THR:HG21	4:A:1031:HOH:O	2.03	0.58
1:A:389:CYS:SG	1:A:413:CYS:HB3	2.44	0.58
1:A:136:PHE:H	1:A:138:LYS:HD2	1.68	0.57
1:A:460:PRO:HB2	1:A:465:ILE:HD13	1.85	0.57
1:A:785:ASP:N	1:A:786:PRO:HD3	2.21	0.56
1:A:731:ARG:HE	1:A:731:ARG:HA	1.70	0.56
1:A:433:GLY:HA3	1:A:461:VAL:O	2.05	0.56
1:A:552:LEU:HD12	1:A:663:ILE:HG12	1.88	0.56
1:A:169:LYS:HE3	1:A:174:ARG:NH1	2.21	0.55
1:A:121:SER:HA	1:A:129:TYR:HE1	1.71	0.55
1:A:217:CYS:SG	1:A:232:ARG:NH1	2.80	0.55
1:A:181:LYS:NZ	1:A:472:ASN:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:VAL:HG21	1:A:675:MET:HE2	1.91	0.53
1:A:731:ARG:HG3	1:A:733:MET:H	1.74	0.53
1:A:127:LYS:CB	1:A:143:PRO:HB2	2.39	0.53
1:A:418:ARG:HD3	1:A:443:LEU:O	2.08	0.53
1:A:580:ARG:NH2	4:A:1014:HOH:O	2.42	0.53
1:A:21:GLN:HG2	1:A:33:GLN:NE2	2.24	0.53
1:A:349:LYS:HE2	1:A:351:LEU:HD21	1.90	0.52
1:A:150:ARG:NH1	1:A:153:ASP:OD1	2.42	0.52
1:A:59:PHE:CD1	1:A:60:HIS:N	2.76	0.52
1:A:389:CYS:SG	1:A:392:CYS:N	2.72	0.51
1:A:256:LEU:O	1:A:260:ARG:HG3	2.10	0.51
1:A:169:LYS:CE	1:A:174:ARG:HG3	2.41	0.51
1:A:733:MET:HG3	1:A:737:TYR:CE2	2.46	0.51
1:A:548:ARG:HG3	1:A:665:MET:HE3	1.92	0.51
1:A:39:ARG:O	1:A:43:GLU:HG2	2.11	0.50
1:A:757:TYR:O	1:A:760:THR:OG1	2.26	0.50
1:A:710:LEU:O	1:A:714:ILE:HB	2.12	0.49
1:A:389:CYS:SG	1:A:413:CYS:SG	3.08	0.49
1:A:629:VAL:HG12	1:A:631:VAL:HG23	1.93	0.49
1:A:729:GLU:H	1:A:729:GLU:CD	2.19	0.49
1:A:47:ARG:N	4:A:1018:HOH:O	2.46	0.48
1:A:248:TYR:O	1:A:673:SER:HA	2.14	0.48
1:A:297:MET:HE1	1:A:356:ARG:NE	2.29	0.48
1:A:293:GLY:N	4:A:1020:HOH:O	2.47	0.48
1:A:140:LEU:HG	1:A:595:HIS:CD2	2.48	0.48
1:A:136:PHE:N	1:A:138:LYS:HD2	2.30	0.47
1:A:720:HIS:CE1	1:A:724:TYR:HE2	2.31	0.47
1:A:30:HIS:NE2	1:A:60:HIS:CD2	2.83	0.47
1:A:365:VAL:HA	1:A:368:LEU:HD12	1.95	0.47
1:A:36:ARG:HH11	1:A:36:ARG:HG3	1.77	0.47
1:A:692:LYS:O	1:A:694:GLY:N	2.47	0.47
1:A:792:LEU:O	1:A:796:LEU:HG	2.15	0.47
1:A:121:SER:CB	1:A:143:PRO:HB3	2.46	0.46
1:A:238:GLY:HA3	1:A:296:PHE:CZ	2.51	0.46
1:A:564:THR:HG1	1:A:565:HIS:CE1	2.32	0.46
1:A:682:LEU:HD21	1:A:699:ASP:HA	1.98	0.46
1:A:140:LEU:HA	1:A:595:HIS:CE1	2.50	0.46
1:A:562:ALA:HA	1:A:566:GLY:CA	2.37	0.46
1:A:180:GLU:HB2	1:A:199:TYR:CZ	2.50	0.46
1:A:698:PHE:C	1:A:700:ARG:H	2.25	0.45
1:A:702:PHE:HD1	1:A:702:PHE:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LYS:HA	1:A:357:LYS:HD3	1.44	0.45
1:A:714:ILE:O	1:A:718:TYR:HB3	2.17	0.45
1:A:56:PHE:HA	1:A:59:PHE:CE2	2.52	0.45
1:A:648:ARG:HD3	1:A:648:ARG:HA	1.79	0.44
1:A:330:TYR:CG	1:A:370:ARG:HB2	2.52	0.44
1:A:22:ARG:HG2	1:A:115:ALA:HB1	2.00	0.44
1:A:299:ILE:HD11	1:A:578:ILE:HG12	2.00	0.44
1:A:240:PHE:HB3	1:A:243:ILE:HD11	2.00	0.44
1:A:156:GLU:OE2	1:A:159:LYS:NZ	2.30	0.44
1:A:78:LEU:HD11	1:A:83:PHE:HE2	1.83	0.44
1:A:259:LEU:HD11	1:A:672:ILE:HD13	2.00	0.44
1:A:636:ASP:OD1	1:A:636:ASP:N	2.43	0.44
1:A:133:GLU:HG2	1:A:134:LEU:O	2.18	0.43
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.70	0.43
1:A:137:GLU:O	1:A:137:GLU:HG3	2.18	0.43
1:A:778:ARG:NH1	1:A:781:GLN:OE1	2.52	0.43
1:A:113:PRO:HD2	1:A:191:SER:N	2.32	0.43
1:A:113:PRO:HB2	1:A:117:ARG:NH2	2.34	0.43
1:A:389:CYS:HB3	1:A:392:CYS:HB2	2.00	0.43
1:A:660:SER:HA	1:A:694:GLY:O	2.17	0.43
1:A:389:CYS:SG	1:A:392:CYS:CB	3.07	0.43
1:A:426:LEU:HD23	1:A:426:LEU:HA	1.88	0.43
1:A:666:PHE:HB2	1:A:675:MET:HE3	2.00	0.43
1:A:51:GLU:HB3	1:A:78:LEU:HD21	2.01	0.43
1:A:567:PHE:N	1:A:567:PHE:CD1	2.87	0.43
1:A:719:ARG:HB2	1:A:719:ARG:NH1	2.31	0.43
1:A:180:GLU:OE2	1:A:586:ARG:NH1	2.52	0.42
1:A:553:ARG:O	1:A:661:ALA:HA	2.19	0.42
1:A:180:GLU:HB2	1:A:199:TYR:CE1	2.54	0.42
1:A:549:LEU:HD11	1:A:675:MET:HE1	2.01	0.42
1:A:606:ARG:NH2	1:A:615:ARG:HG3	2.35	0.42
1:A:245:ASP:O	1:A:249:ARG:HB2	2.19	0.42
1:A:133:GLU:HG3	1:A:182:TYR:CE1	2.55	0.42
1:A:169:LYS:H	1:A:169:LYS:CD	2.32	0.42
1:A:346:GLU:OE1	4:A:1003:HOH:O	2.22	0.42
1:A:320:TRP:CZ2	1:A:324:GLU:HG3	2.55	0.42
1:A:357:LYS:NZ	1:A:360:LYS:HD2	2.35	0.42
1:A:433:GLY:O	1:A:451:PHE:HA	2.19	0.42
1:A:667:PRO:HG2	1:A:670:TYR:CD1	2.54	0.42
1:A:574:LYS:O	1:A:580:ARG:HD3	2.19	0.42
1:A:124:ASN:C	1:A:126:GLY:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ASP:HA	1:A:687:LYS:NZ	2.34	0.42
1:A:712:LYS:HD3	1:A:791:GLN:HE22	1.85	0.42
1:A:698:PHE:C	1:A:700:ARG:N	2.77	0.42
1:A:122:VAL:HG13	1:A:575:PHE:CE1	2.55	0.41
1:A:393:GLY:O	1:A:394:ARG:HG3	2.20	0.41
1:A:259:LEU:HD11	1:A:672:ILE:HG21	2.01	0.41
1:A:346:GLU:HB2	1:A:349:LYS:HB2	2.02	0.41
1:A:585:SER:OG	2:A:902:ATP:N1	2.49	0.41
1:A:559:LEU:HD23	2:A:902:ATP:C8	2.55	0.41
1:A:136:PHE:O	1:A:137:GLU:C	2.63	0.41
1:A:180:GLU:HG3	1:A:586:ARG:NH2	2.36	0.41
1:A:646:ARG:HD3	1:A:646:ARG:C	2.46	0.41
1:A:39:ARG:HD3	4:A:1061:HOH:O	2.20	0.41
1:A:161:LEU:HA	1:A:161:LEU:HD23	1.86	0.41
1:A:284:THR:HG22	1:A:286:ALA:N	2.16	0.40
1:A:646:ARG:HG3	1:A:706:TRP:CD2	2.57	0.40
1:A:357:LYS:HZ3	1:A:360:LYS:HD2	1.87	0.40
1:A:469:ASN:HA	1:A:486:PHE:CD2	2.57	0.40
1:A:72:ILE:HG23	1:A:87:MET:CE	2.51	0.40
1:A:90:VAL:O	1:A:94:LEU:HG	2.20	0.40
1:A:631:VAL:HG21	1:A:641:PHE:HE2	1.87	0.40
1:A:169:LYS:HE3	1:A:174:ARG:HH11	1.86	0.40
1:A:466:LEU:HA	1:A:483:VAL:O	2.21	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	656/776 (84%)	605 (92%)	38 (6%)	13 (2%)	6 5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	GLU
1	A	138	LYS
1	A	612	ASP
1	A	693	ASN
1	A	699	ASP
1	A	726	SER
1	A	474	GLY
1	A	729	GLU
1	A	566	GLY
1	A	608	ILE
1	A	785	ASP
1	A	786	PRO
1	A	607	PRO

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	569/651 (87%)	569 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	194	ASN
1	A	438	ASN
1	A	595	HIS
1	A	784	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
2	ATP	A	901	-	32,33,33	1.41	5 (15%)	48,52,52	1.80	10 (20%)
2	ATP	A	902	3	32,33,33	1.73	7 (21%)	48,52,52	2.25	15 (31%)

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
2	ATP	A	901	-	-	4/22/38/38	0/3/3/3
2	ATP	A	902	3	-	2/22/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	ATP	PA-O3A	4.74	1.64	1.59
2	A	901	ATP	C5-C4	4.22	1.46	1.39
2	A	902	ATP	C5-C4	4.16	1.46	1.39
2	A	902	ATP	PB-O3A	3.66	1.63	1.59
2	A	902	ATP	PB-O1B	3.21	1.61	1.50
2	A	901	ATP	C5-C6	2.89	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ATP	PB-O3A	2.83	1.62	1.59
2	A	902	ATP	C5-C6	2.56	1.48	1.41
2	A	901	ATP	PA-O3A	2.51	1.62	1.59
2	A	902	ATP	PB-O3B	2.51	1.62	1.59
2	A	901	ATP	C8-N7	2.35	1.36	1.31
2	A	902	ATP	C8-N7	2.01	1.35	1.31

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	ATP	O2B-PB-O3A	6.86	125.83	107.27
2	A	901	ATP	C5-C4-N3	-5.53	119.11	126.72
2	A	902	ATP	C5-C4-N3	-5.48	119.18	126.72
2	A	902	ATP	N3-C4-N9	4.56	134.92	127.17
2	A	901	ATP	N3-C4-N9	4.29	134.47	127.17
2	A	901	ATP	C2-N3-C4	3.99	121.58	111.83
2	A	902	ATP	N3-C2-N1	-3.87	122.73	128.58
2	A	902	ATP	C2-N3-C4	3.84	121.20	111.83
2	A	901	ATP	N3-C2-N1	-3.75	122.91	128.58
2	A	902	ATP	O3B-PB-O1B	3.62	121.60	110.70
2	A	901	ATP	C4-C5-N7	-3.39	106.71	110.58
2	A	902	ATP	O3A-PB-O1B	3.24	120.44	110.70
2	A	902	ATP	C4-C5-N7	-3.10	107.04	110.58
2	A	902	ATP	C4-N9-C8	3.06	108.95	105.74
2	A	901	ATP	O4'-C1'-N9	2.98	113.82	108.09
2	A	901	ATP	C4-N9-C8	2.86	108.74	105.74
2	A	902	ATP	O2B-PB-O3B	-2.75	99.84	107.27
2	A	902	ATP	O3'-C3'-C4'	-2.59	103.64	111.08
2	A	902	ATP	O2G-PG-O1G	2.57	120.85	110.83
2	A	901	ATP	C5-N7-C8	2.51	107.39	103.45
2	A	901	ATP	C6-C5-N7	2.45	136.82	132.09
2	A	902	ATP	C5-N7-C8	2.45	107.29	103.45
2	A	901	ATP	N9-C8-N7	-2.26	110.73	113.94
2	A	902	ATP	C6-C5-N7	2.24	136.41	132.09
2	A	902	ATP	N9-C8-N7	-2.22	110.79	113.94

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	902	ATP	PB-O3B-PG-O1G
2	A	901	ATP	C2'-C1'-N9-C8

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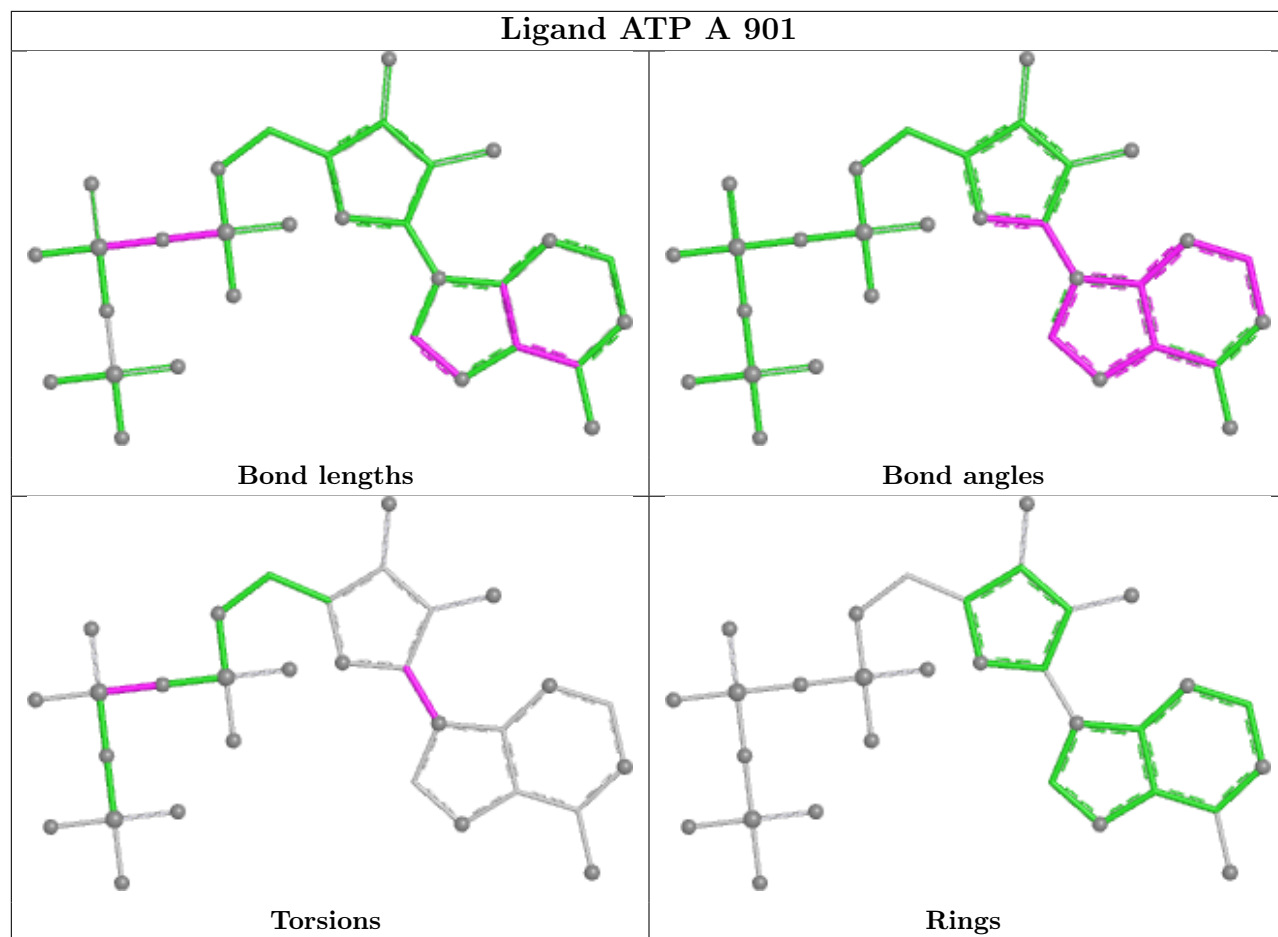
Mol	Chain	Res	Type	Atoms
2	A	901	ATP	PA-O3A-PB-O2B
2	A	902	ATP	C5'-O5'-PA-O2A
2	A	901	ATP	O4'-C1'-N9-C8
2	A	901	ATP	PA-O3A-PB-O1B

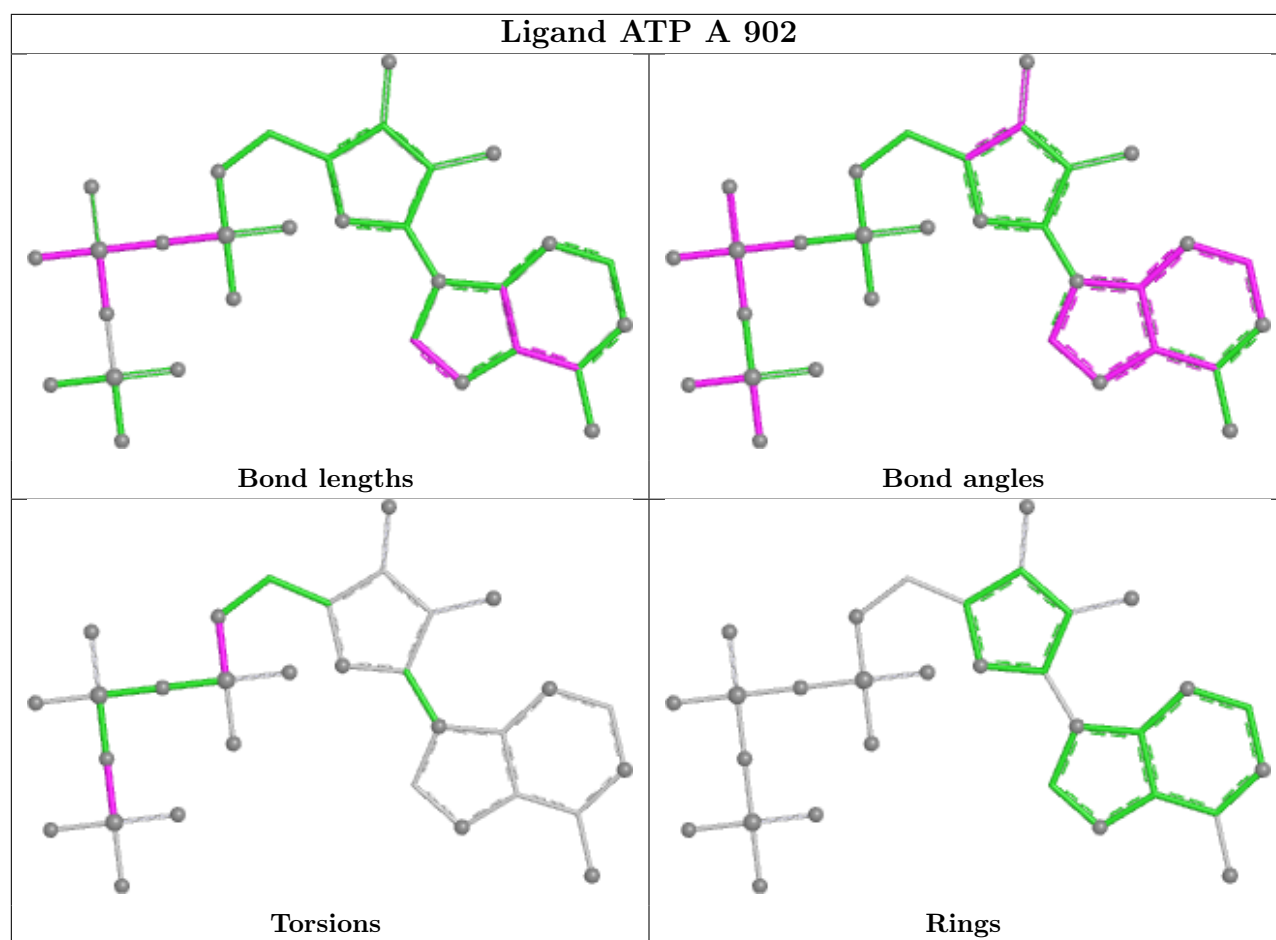
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	ATP	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	674/776 (86%)	0.74	109 (16%) 4 5	9, 34, 89, 141	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	755	TRP	7.0
1	A	140	LEU	6.9
1	A	135	ASP	6.6
1	A	59	PHE	5.6
1	A	136	PHE	5.5
1	A	756	VAL	5.5
1	A	758	PHE	5.5
1	A	67	ASN	5.4
1	A	147	PHE	5.4
1	A	142	VAL	5.3
1	A	491	PHE	5.3
1	A	757	TYR	5.3
1	A	146	VAL	5.2
1	A	699	ASP	5.2
1	A	783	PHE	5.1
1	A	759	LEU	5.1
1	A	760	THR	4.9
1	A	143	PRO	4.8
1	A	60	HIS	4.6
1	A	113	PRO	4.6
1	A	786	PRO	4.6
1	A	702	PHE	4.4
1	A	547	ALA	4.2
1	A	612	ASP	4.1
1	A	701	GLU	4.0
1	A	724	TYR	4.0
1	A	772	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	775	PHE	3.8
1	A	348	GLY	3.8
1	A	490	TYR	3.7
1	A	139	GLU	3.7
1	A	129	TYR	3.6
1	A	148	SER	3.6
1	A	141	PRO	3.6
1	A	776	ALA	3.5
1	A	138	LYS	3.4
1	A	771	PRO	3.4
1	A	416	CYS	3.4
1	A	144	GLY	3.4
1	A	697	LEU	3.4
1	A	478	GLU	3.3
1	A	734	ALA	3.3
1	A	698	PHE	3.3
1	A	598	TYR	3.3
1	A	413	CYS	3.2
1	A	475	GLU	3.2
1	A	125	PRO	3.2
1	A	785	ASP	3.1
1	A	130	PRO	3.1
1	A	805	LYS	3.1
1	A	727	GLY	3.0
1	A	87	MET	3.0
1	A	703	THR	2.9
1	A	784	GLN	2.9
1	A	726	SER	2.8
1	A	778	ARG	2.8
1	A	145	ASP	2.8
1	A	391	VAL	2.8
1	A	613	PRO	2.7
1	A	741	GLU	2.7
1	A	729	GLU	2.6
1	A	68	ASP	2.6
1	A	567	PHE	2.6
1	A	773	GLN	2.6
1	A	134	LEU	2.6
1	A	730	GLU	2.6
1	A	392	CYS	2.5
1	A	566	GLY	2.5
1	A	787	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	725	PHE	2.5
1	A	459	ARG	2.5
1	A	72	ILE	2.5
1	A	250	VAL	2.5
1	A	731	ARG	2.5
1	A	628	ASP	2.5
1	A	668	ASP	2.4
1	A	728	ASN	2.4
1	A	390	PRO	2.4
1	A	394	ARG	2.4
1	A	700	ARG	2.4
1	A	327	SER	2.4
1	A	489	ASP	2.4
1	A	81	GLU	2.4
1	A	669	LYS	2.4
1	A	137	GLU	2.4
1	A	438	ASN	2.3
1	A	347	GLY	2.3
1	A	128	ALA	2.3
1	A	393	GLY	2.3
1	A	602	ARG	2.2
1	A	654	GLN	2.2
1	A	779	LEU	2.2
1	A	781	GLN	2.2
1	A	782	TRP	2.2
1	A	777	ASN	2.2
1	A	245	ASP	2.2
1	A	126	GLY	2.2
1	A	254	GLY	2.2
1	A	735	PHE	2.1
1	A	389	CYS	2.1
1	A	720	HIS	2.1
1	A	780	HIS	2.1
1	A	614	ALA	2.1
1	A	253	LYS	2.1
1	A	46	GLY	2.1
1	A	802	ARG	2.1
1	A	574	LYS	2.0
1	A	792	LEU	2.0
1	A	804	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

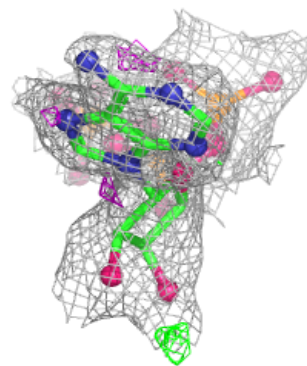
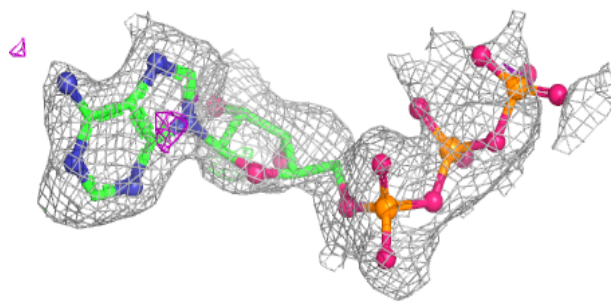
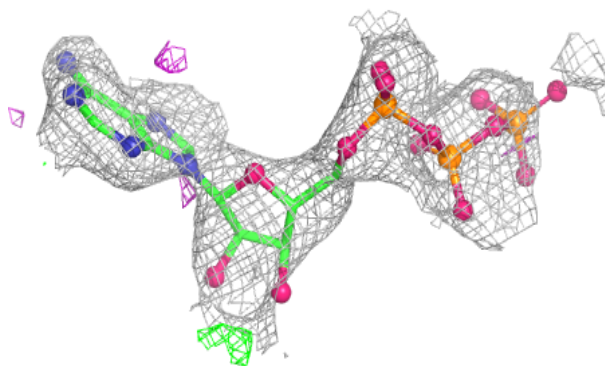
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	ATP	A	901	31/31	0.77	0.16	32,69,120,123	0
3	MG	A	905	1/1	0.91	0.10	64,64,64,64	0
2	ATP	A	902	31/31	0.93	0.09	9,19,46,54	0
3	MG	A	904	1/1	0.97	0.06	41,41,41,41	0
3	MG	A	903	1/1	0.98	0.11	15,15,15,15	0

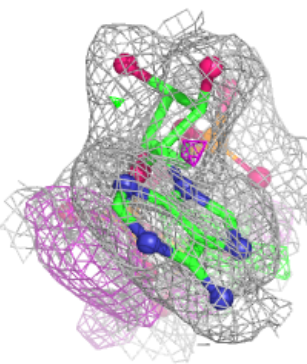
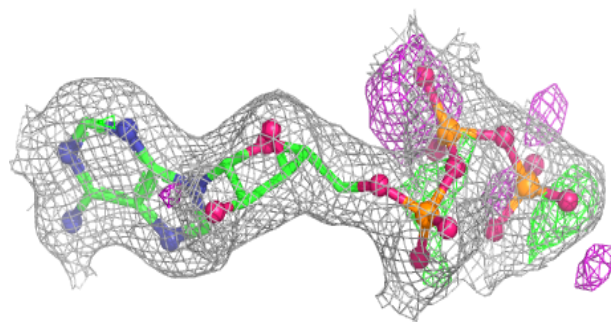
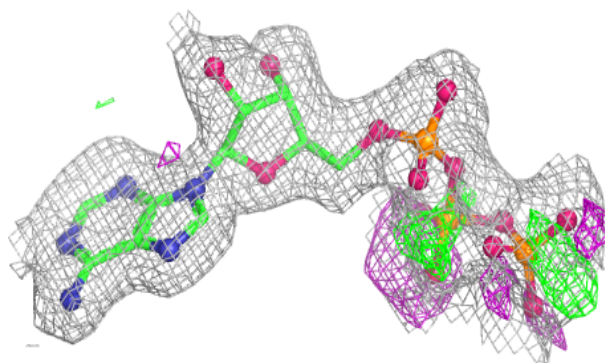
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 901:

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

**Electron density around ATP A 902:**

$2mF_o-DF_c$ (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.