



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:24 AM UTC

PDB ID : 5K8F / pdb_00005k8f
Title : Crystal structure of Acetyl-CoA Synthetase in complex with ATP and Acetyl-AMP from *Cryptococcus neoformans* H99
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID); Fox III, D.; Delker, S.L.; Potts, K.T.; Lorimer, D.D.; Edwards, T.E.; Mutz, M.W.
Deposited on : 2016-05-30
Resolution : 2.45 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

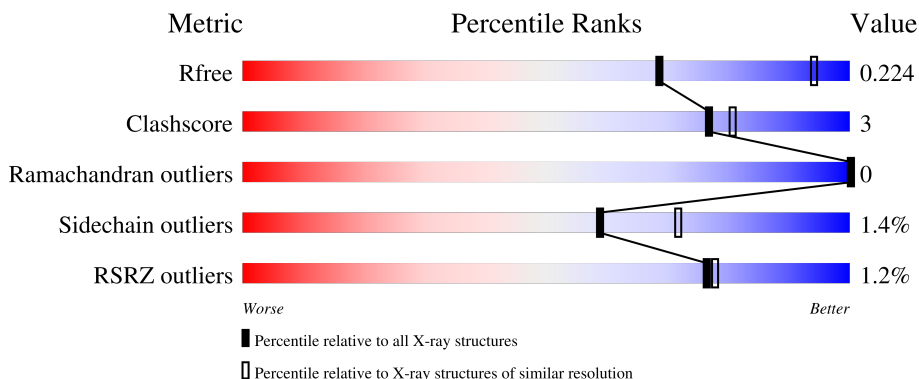
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	694	85% 9% 5%
1	B	694	86% 8% 6%
1	C	694	86% 7% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15624 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 Acetyl-coenzyme A synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	0	5	0
			5054	3216	864	947	27			
1	B	655	Total	C	N	O	S	0	5	0
			4985	3180	854	925	26			
1	C	651	Total	C	N	O	S	0	7	0
			4992	3193	851	921	27			

There are 45 discrepancies between the modelled and reference sequences:

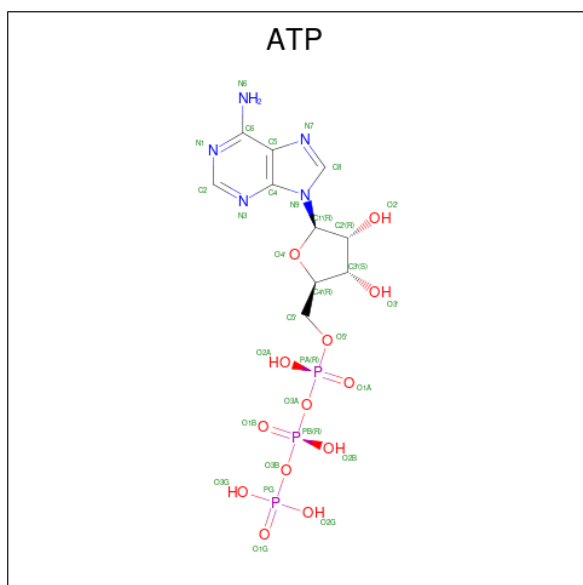
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP J9VFT1
A	-12	HIS	-	expression tag	UNP J9VFT1
A	-11	HIS	-	expression tag	UNP J9VFT1
A	-10	HIS	-	expression tag	UNP J9VFT1
A	-9	HIS	-	expression tag	UNP J9VFT1
A	-8	HIS	-	expression tag	UNP J9VFT1
A	-7	HIS	-	expression tag	UNP J9VFT1
A	-6	HIS	-	expression tag	UNP J9VFT1
A	-5	HIS	-	expression tag	UNP J9VFT1
A	-4	GLU	-	expression tag	UNP J9VFT1
A	-3	ASN	-	expression tag	UNP J9VFT1
A	-2	LEU	-	expression tag	UNP J9VFT1
A	-1	TYR	-	expression tag	UNP J9VFT1
A	0	PHE	-	expression tag	UNP J9VFT1
A	1	GLN	-	expression tag	UNP J9VFT1
B	-13	MET	-	expression tag	UNP J9VFT1
B	-12	HIS	-	expression tag	UNP J9VFT1
B	-11	HIS	-	expression tag	UNP J9VFT1
B	-10	HIS	-	expression tag	UNP J9VFT1
B	-9	HIS	-	expression tag	UNP J9VFT1
B	-8	HIS	-	expression tag	UNP J9VFT1
B	-7	HIS	-	expression tag	UNP J9VFT1
B	-6	HIS	-	expression tag	UNP J9VFT1

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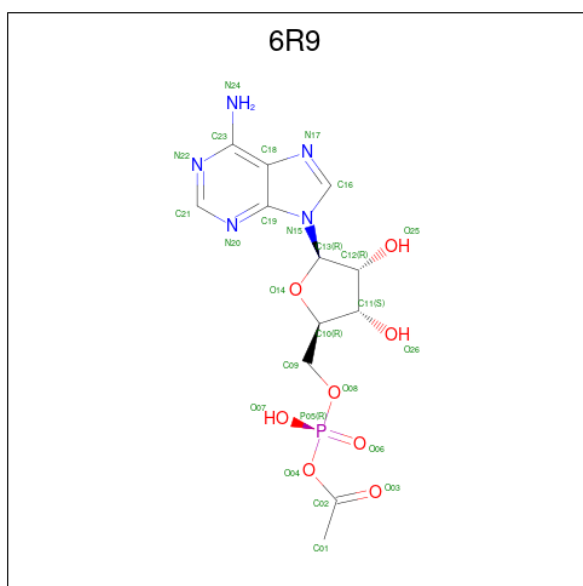
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression tag	UNP J9VFT1
B	1	GLN	-	expression tag	UNP J9VFT1
C	-13	MET	-	expression tag	UNP J9VFT1
C	-12	HIS	-	expression tag	UNP J9VFT1
C	-11	HIS	-	expression tag	UNP J9VFT1
C	-10	HIS	-	expression tag	UNP J9VFT1
C	-9	HIS	-	expression tag	UNP J9VFT1
C	-8	HIS	-	expression tag	UNP J9VFT1
C	-7	HIS	-	expression tag	UNP J9VFT1
C	-6	HIS	-	expression tag	UNP J9VFT1
C	-5	HIS	-	expression tag	UNP J9VFT1
C	-4	GLU	-	expression tag	UNP J9VFT1
C	-3	ASN	-	expression tag	UNP J9VFT1
C	-2	LEU	-	expression tag	UNP J9VFT1
C	-1	TYR	-	expression tag	UNP J9VFT1
C	0	PHE	-	expression tag	UNP J9VFT1
C	1	GLN	-	expression tag	UNP J9VFT1

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

- Molecule 3 is [[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] ethanoate (CCD ID: 6R9) (formula: C₁₂H₁₆N₅O₈P) (labeled as "Ligand of Interest" by depositor).

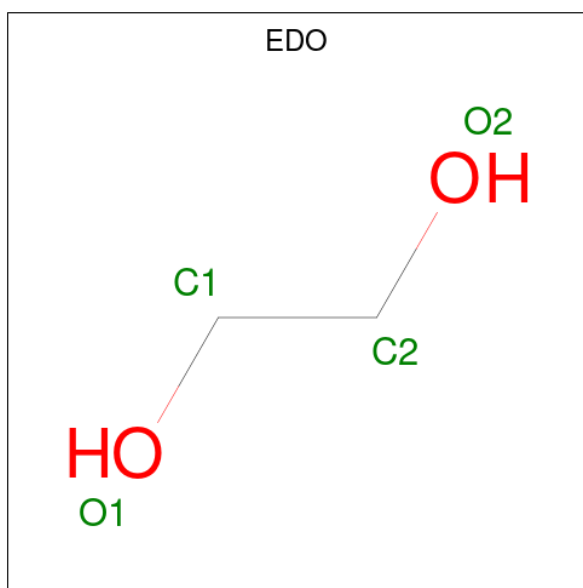


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			26	12	5	8	1		
3	B	1	Total	C	N	O	P	0	1
			26	12	5	8	1		
3	C	1	Total	C	N	O	P	0	1
			26	12	5	8	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

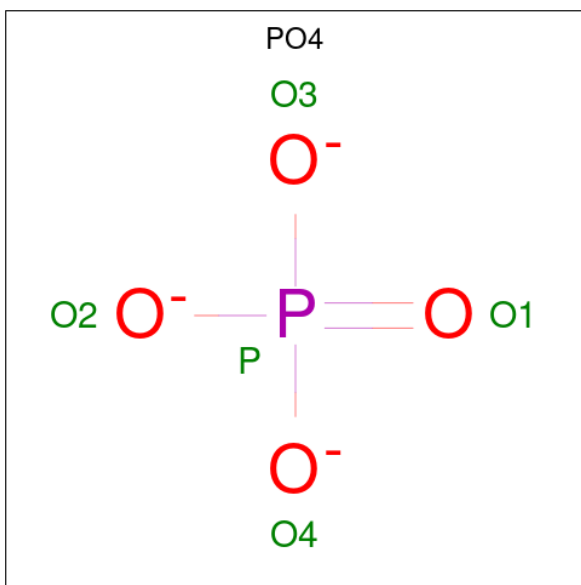
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	1
			1	1		
4	B	1	Total	Mg	0	1
			1	1		
4	C	2	Total	Mg	0	1
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



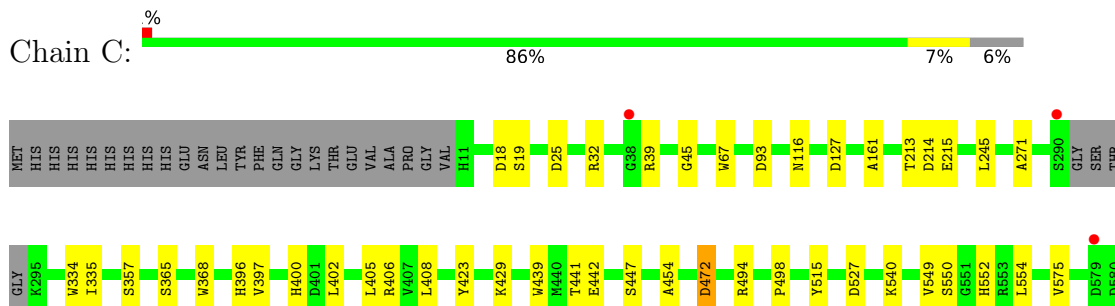
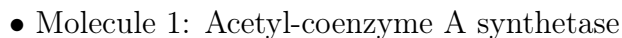
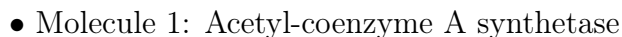
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			5	4	1		

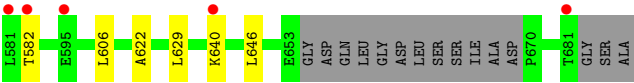
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	188	Total	O	0	3
			190	190		
7	B	85	Total	O	0	2
			87	87		
7	C	98	Total	O	0	2
			100	100		

i

- Molecule 1: Acetyl-coenzyme A synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.37Å 83.92Å 101.57Å 110.06° 105.24° 87.65°	Depositor
Resolution (Å)	26.62 – 2.45 26.62 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.6 (26.62-2.45) 98.5 (26.62-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.19rc4_4035	Depositor
R, R_{free}	0.188 , 0.224 0.188 , 0.224	Depositor DCC
R_{free} test set	2000 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.7	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	0.95	EDS
Total number of atoms	15624	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, PO4, ATP, 6R9, EDO

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	0.10	0/5202	0.28	0/7101
1	B	0.09	0/5135	0.26	0/7018
1	C	0.10	0/5148	0.27	1/7033 (0.0%)
All	All	0.10	0/15485	0.27	1/21152 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	406	ARG	N-CA-C	-5.12	108.78	114.62

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	5054	0	4776	31	0
1	B	4985	0	4657	29	0
1	C	4992	0	4699	27	0
2	A	31	0	12	0	0
2	B	31	0	12	1	0
2	C	31	0	12	1	0
3	A	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	0	0	0
3	C	26	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	16	0	24	0	0
5	B	12	0	18	0	0
5	C	8	0	12	2	0
6	C	5	0	0	0	0
7	A	190	0	0	0	0
7	B	87	0	0	0	0
7	C	100	0	0	0	0
All	All	15624	0	14222	84	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (84) 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:C:549:VAL:HG23	1:C:552:HIS:HB2	1.85	0.59
1:C:554:LEU:HD11	1:C:622:ALA:HA	1.84	0.59
1:C:540:LYS:HG2	5:C:705:EDO:H21	1.84	0.59
1:B:472:ASP:OD2	1:B:494:ARG:NH2	2.37	0.57
1:B:93:ASP:HB3	1:C:271:ALA:HB3	1.86	0.56
1:A:271:ALA:HB3	1:C:93:ASP:HB3	1.86	0.56
1:C:606:LEU:HD23	1:C:629:LEU:HD21	1.87	0.56
1:C:527:ASP:OD1	3:C:702[A]:6R9:O25	2.25	0.54
1:B:572:THR:HG22	1:B:590:VAL:HG13	1.91	0.53
1:A:213:THR:HG22	1:A:245:LEU:HB3	1.91	0.52
1:C:335:ILE:HG12	1:C:441:THR:HA	1.92	0.52
1:A:405:LEU:HD13	1:A:408:LEU:HD21	1.91	0.51
1:B:190[B]:PHE:HZ	1:B:334[B]:TRP:HB2	1.74	0.51
1:A:615:ARG:HG2	1:A:620:PRO:HA	1.92	0.51
1:C:472:ASP:OD2	1:C:494:ARG:NH1	2.44	0.51
1:A:93:ASP:HB3	1:B:271:ALA:HB3	1.94	0.50
1:A:295:LYS:O	1:A:510:ARG:NH2	2.37	0.50
1:C:127:ASP:HA	1:C:357:SER:HB2	1.94	0.50
1:A:314:LEU:HD22	1:A:345:PRO:HA	1.94	0.50
1:B:405:LEU:HD13	1:B:408:LEU:HD21	1.94	0.50
1:A:439:TRP:HB3	1:A:447:SER:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:THR:HG22	1:B:245:LEU:HB3	1.95	0.49
1:C:439:TRP:HB3	1:C:447:SER:H	1.76	0.49
1:B:190[B]:PHE:CZ	1:B:334[B]:TRP:HB2	2.47	0.49
1:B:440:MET:HG3	1:B:443:THR:HG23	1.94	0.48
1:A:110:ASP:N	1:A:110:ASP:OD1	2.47	0.48
1:C:214:ASP:OD1	1:C:215:GLU:N	2.43	0.48
1:B:127:ASP:HA	1:B:357:SER:HB2	1.95	0.48
1:B:493:ALA:HB3	1:B:523:PHE:HB3	1.96	0.47
1:A:649:ILE:HG21	1:A:676:VAL:HG12	1.95	0.47
1:A:368:TRP:HB3	1:A:402:LEU:HD21	1.96	0.47
1:B:214:ASP:OD1	1:B:215:GLU:N	2.47	0.47
1:B:513:GLU:HA	1:B:517:LYS:HG3	1.96	0.47
1:B:440:MET:HB3	2:B:701[A]:ATP:H5'1	1.96	0.46
1:A:328:CYS:HA	1:A:380:TYR:HB3	1.96	0.46
1:A:373:LYS:HD2	1:A:374:TRP:CE2	2.51	0.46
1:C:213:THR:HG22	1:C:245:LEU:HB3	1.97	0.46
1:A:638:SER:HB2	1:A:640:LYS:HD2	1.97	0.46
1:A:58:THR:HG22	1:A:66:TRP:CD2	2.51	0.45
1:B:58:THR:HG21	1:B:467:PHE:HB3	1.98	0.45
1:B:448:ILE:HA	1:B:465:PRO:HA	1.98	0.45
1:A:313:THR:HG21	1:A:445:SER:HB2	1.98	0.45
1:B:575:VAL:HG12	1:B:643:ARG:HB3	1.99	0.45
1:A:442:GLU:HG2	1:A:515:TYR:CZ	2.52	0.45
1:B:614:VAL:HG13	1:B:618:ILE:HD12	1.99	0.45
1:C:400:HIS:O	1:C:429:LYS:NZ	2.40	0.45
1:A:472:ASP:OD2	1:A:494:ARG:NH1	2.48	0.44
1:C:640[B]:LYS:NZ	2:C:701[B]:ATP:O5'	2.50	0.44
1:C:575:VAL:HG11	1:C:646:LEU:HB2	1.99	0.44
1:C:32:ARG:HD3	1:C:39:ARG:HE	1.82	0.44
1:A:360:VAL:HA	1:A:364:PRO:HA	2.00	0.44
1:C:67:TRP:CZ3	1:C:498:PRO:HG2	2.52	0.43
1:C:442:GLU:HG2	1:C:515:TYR:CZ	2.53	0.43
1:B:58:THR:HG22	1:B:66:TRP:CD2	2.53	0.43
1:C:368:TRP:HB3	1:C:402:LEU:HD21	2.00	0.43
1:C:45:GLY:HA2	1:C:454:ALA:HB2	2.01	0.43
1:B:471:VAL:HB	1:B:491:LEU:HD11	2.01	0.43
1:B:442:GLU:HG2	1:B:515:TYR:CZ	2.54	0.42
1:B:17:PRO:HD2	1:B:561:SER:HB2	2.00	0.42
1:A:325[B]:ARG:HG3	1:A:376:ALA:HA	2.01	0.42
1:A:440:MET:HB2	1:A:443:THR:HG23	2.02	0.42
1:B:11:HIS:O	1:B:14:HIS:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:SER:N	1:C:582:THR:O	2.39	0.42
1:A:334:TRP:CD1	1:A:335:ILE:H	2.38	0.42
1:C:334[B]:TRP:CD1	1:C:335:ILE:H	2.38	0.42
1:A:67:TRP:CZ3	1:A:498:PRO:HG2	2.55	0.41
1:A:214:ASP:OD1	1:A:215:GLU:N	2.51	0.41
1:A:332:ILE:HA	1:A:337:GLY:HA3	2.02	0.41
1:B:67:TRP:CZ3	1:B:498:PRO:HG2	2.55	0.41
1:B:327:ALA:HA	1:B:353:ALA:HB3	2.02	0.41
1:C:161:ALA:H	5:C:704:EDO:H11	1.85	0.41
1:A:554:LEU:HD21	1:A:621:PHE:HE2	1.85	0.41
1:B:390:ARG:NH2	1:B:418:GLU:OE2	2.54	0.41
1:C:405:LEU:HD13	1:C:408:LEU:HD21	2.02	0.41
1:A:644:ARG:HA	1:A:647:ARG:NH1	2.36	0.41
1:A:18:ASP:OD1	1:A:19:SER:N	2.54	0.41
1:A:463:THR:OG1	1:A:464:PHE:N	2.53	0.41
1:C:18:ASP:OD1	1:C:19:SER:N	2.53	0.41
1:B:190[A]:PHE:HB3	1:B:193:PHE:CD1	2.56	0.40
1:A:391:ARG:HH21	1:A:392:MET:HE1	1.86	0.40
1:C:365:SER:HB3	1:C:396:HIS:HB3	2.02	0.40
1:A:588:ALA:HB3	1:A:627:ILE:HG12	2.04	0.40
1:B:363:THR:HG1	1:B:365:SER:HG	1.68	0.40
1:B:400:HIS:O	1:B:429:LYS:NZ	2.38	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	657/694 (95%)	638 (97%)	19 (3%)	0	100	100
1	B	655/694 (94%)	636 (97%)	19 (3%)	0	100	100
1	C	652/694 (94%)	636 (98%)	16 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1964/2082 (94%)	1910 (97%)	54 (3%)	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	512/576 (89%)	502 (98%)	10 (2%)	48	63
1	B	492/576 (85%)	485 (99%)	7 (1%)	59	72
1	C	498/576 (86%)	493 (99%)	5 (1%)	68	77
All	All	1502/1728 (87%)	1480 (98%)	22 (2%)	59	70

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	116	ASN
1	A	297	LYS
1	A	325[A]	ARG
1	A	325[B]	ARG
1	A	397	VAL
1	A	472	ASP
1	A	481	VAL
1	A	640	LYS
1	A	642	MET
1	B	25	ASP
1	B	116	ASN
1	B	234	GLN
1	B	297	LYS
1	B	440	MET
1	B	472	ASP
1	B	640	LYS
1	C	25	ASP

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Mol	Chain	Res	Type
1	C	116	ASN
1	C	397	VAL
1	C	423	TYR
1	C	472	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
1	A	485	ASN
1	B	91	HIS
1	C	91	HIS
1	C	95	GLN
1	C	241	ASN
1	C	548	ASN

5.3.3 RNA [i](#)

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 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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
5	EDO	A	705	-	3,3,3	0.43	0	2,2,2	0.37	0
2	ATP	C	701[B]	4	32,33,33	0.25	0	48,52,52	0.28	0
5	EDO	B	704	-	3,3,3	0.43	0	2,2,2	0.40	0
6	PO4	C	707	-	4,4,4	0.96	0	6,6,6	0.45	0
3	6R9	A	702[A]	-	27,28,28	2.79	7 (25%)	39,42,42	1.97	10 (25%)
5	EDO	A	707	-	3,3,3	0.44	0	2,2,2	0.30	0
3	6R9	B	702[B]	-	27,28,28	2.78	7 (25%)	39,42,42	1.99	10 (25%)
5	EDO	B	706	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	C	704	-	3,3,3	0.43	0	2,2,2	0.34	0
2	ATP	B	701[A]	-	32,33,33	0.27	0	48,52,52	0.30	0
5	EDO	A	704	-	3,3,3	0.42	0	2,2,2	0.37	0
5	EDO	A	706	-	3,3,3	0.43	0	2,2,2	0.36	0
2	ATP	A	701[B]	4	32,33,33	0.26	0	48,52,52	0.28	0
5	EDO	B	705	-	3,3,3	0.42	0	2,2,2	0.38	0
3	6R9	C	702[A]	-	27,28,28	2.78	7 (25%)	39,42,42	1.97	10 (25%)
5	EDO	C	705	-	3,3,3	0.42	0	2,2,2	0.42	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
5	EDO	A	705	-	-	0/1/1/1	-
2	ATP	C	701[B]	4	-	8/22/38/38	0/3/3/3
5	EDO	B	704	-	-	0/1/1/1	-
3	6R9	A	702[A]	-	-	0/13/31/31	0/3/3/3
5	EDO	A	707	-	-	0/1/1/1	-
3	6R9	B	702[B]	-	-	2/13/31/31	0/3/3/3
5	EDO	B	706	-	-	0/1/1/1	-
5	EDO	C	704	-	-	0/1/1/1	-
2	ATP	B	701[A]	-	-	3/22/38/38	0/3/3/3
5	EDO	A	704	-	-	0/1/1/1	-
5	EDO	A	706	-	-	0/1/1/1	-
2	ATP	A	701[B]	4	-	6/22/38/38	0/3/3/3
5	EDO	B	705	-	-	0/1/1/1	-
3	6R9	C	702[A]	-	-	3/13/31/31	0/3/3/3
5	EDO	C	705	-	-	0/1/1/1	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702[A]	6R9	O14-C13	8.72	1.62	1.42
3	B	702[B]	6R9	O14-C13	8.71	1.62	1.42
3	C	702[A]	6R9	O14-C13	8.69	1.62	1.42
3	B	702[B]	6R9	O14-C10	-6.39	1.30	1.45
3	A	702[A]	6R9	O14-C10	-6.37	1.30	1.45
3	C	702[A]	6R9	O14-C10	-6.37	1.30	1.45
3	C	702[A]	6R9	C12-C13	-5.94	1.34	1.53
3	A	702[A]	6R9	C12-C13	-5.91	1.34	1.53
3	B	702[B]	6R9	C12-C13	-5.88	1.35	1.53
3	B	702[B]	6R9	C23-N24	4.29	1.45	1.34
3	A	702[A]	6R9	C23-N24	4.29	1.45	1.34
3	C	702[A]	6R9	C23-N24	4.25	1.45	1.34
3	B	702[B]	6R9	P05-O04	2.97	1.66	1.60
3	C	702[A]	6R9	P05-O04	2.93	1.65	1.60
3	A	702[A]	6R9	P05-O04	2.91	1.65	1.60
3	A	702[A]	6R9	C16-N15	-2.91	1.32	1.37
3	C	702[A]	6R9	C16-N15	-2.89	1.32	1.37
3	B	702[B]	6R9	C16-N15	-2.85	1.32	1.37
3	C	702[A]	6R9	C18-N17	-2.31	1.34	1.39
3	A	702[A]	6R9	C18-N17	-2.30	1.34	1.39
3	B	702[B]	6R9	C18-N17	-2.26	1.35	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702[A]	6R9	C18-C19-N20	-5.11	119.68	126.72
3	B	702[B]	6R9	C18-C19-N20	-5.06	119.75	126.72
3	C	702[A]	6R9	C18-C19-N20	-5.03	119.79	126.72
3	A	702[A]	6R9	O14-C13-N15	-4.38	99.67	108.09
3	B	702[B]	6R9	O14-C13-N15	-4.27	99.88	108.09
3	C	702[A]	6R9	N22-C21-N20	-4.20	122.23	128.58
3	B	702[B]	6R9	N22-C21-N20	-4.18	122.25	128.58
3	A	702[A]	6R9	N22-C21-N20	-4.16	122.28	128.58
3	C	702[A]	6R9	O14-C13-N15	-4.15	100.13	108.09
3	A	702[A]	6R9	N20-C19-N15	3.66	133.39	127.17
3	C	702[A]	6R9	N20-C19-N15	3.63	133.34	127.17
3	B	702[B]	6R9	N20-C19-N15	3.61	133.30	127.17
3	B	702[B]	6R9	C21-N20-C19	3.45	120.26	111.83
3	A	702[A]	6R9	C21-N20-C19	3.45	120.25	111.83
3	C	702[A]	6R9	C21-N20-C19	3.44	120.23	111.83
3	A	702[A]	6R9	C12-C13-N15	3.31	121.52	113.30
3	B	702[B]	6R9	C12-C13-N15	3.29	121.49	113.30
3	C	702[A]	6R9	C12-C13-N15	3.20	121.25	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702[B]	6R9	C19-C18-N17	-3.04	107.11	110.58
3	C	702[A]	6R9	C19-C18-N17	-3.01	107.14	110.58
3	A	702[A]	6R9	C19-C18-N17	-3.00	107.15	110.58
3	C	702[A]	6R9	N15-C16-N17	-2.97	109.73	113.94
3	C	702[A]	6R9	C18-N17-C16	2.91	108.02	103.45
3	B	702[B]	6R9	C18-N17-C16	2.88	107.97	103.45
3	B	702[B]	6R9	N15-C16-N17	-2.85	109.89	113.94
3	A	702[A]	6R9	C18-N17-C16	2.84	107.91	103.45
3	A	702[A]	6R9	N15-C16-N17	-2.83	109.92	113.94
3	C	702[A]	6R9	C19-N15-C16	2.38	108.24	105.74
3	A	702[A]	6R9	C19-N15-C16	2.24	108.09	105.74
3	B	702[B]	6R9	C19-N15-C16	2.23	108.08	105.74

There are no chirality outliers.

All (22) torsion outliers are listed below:

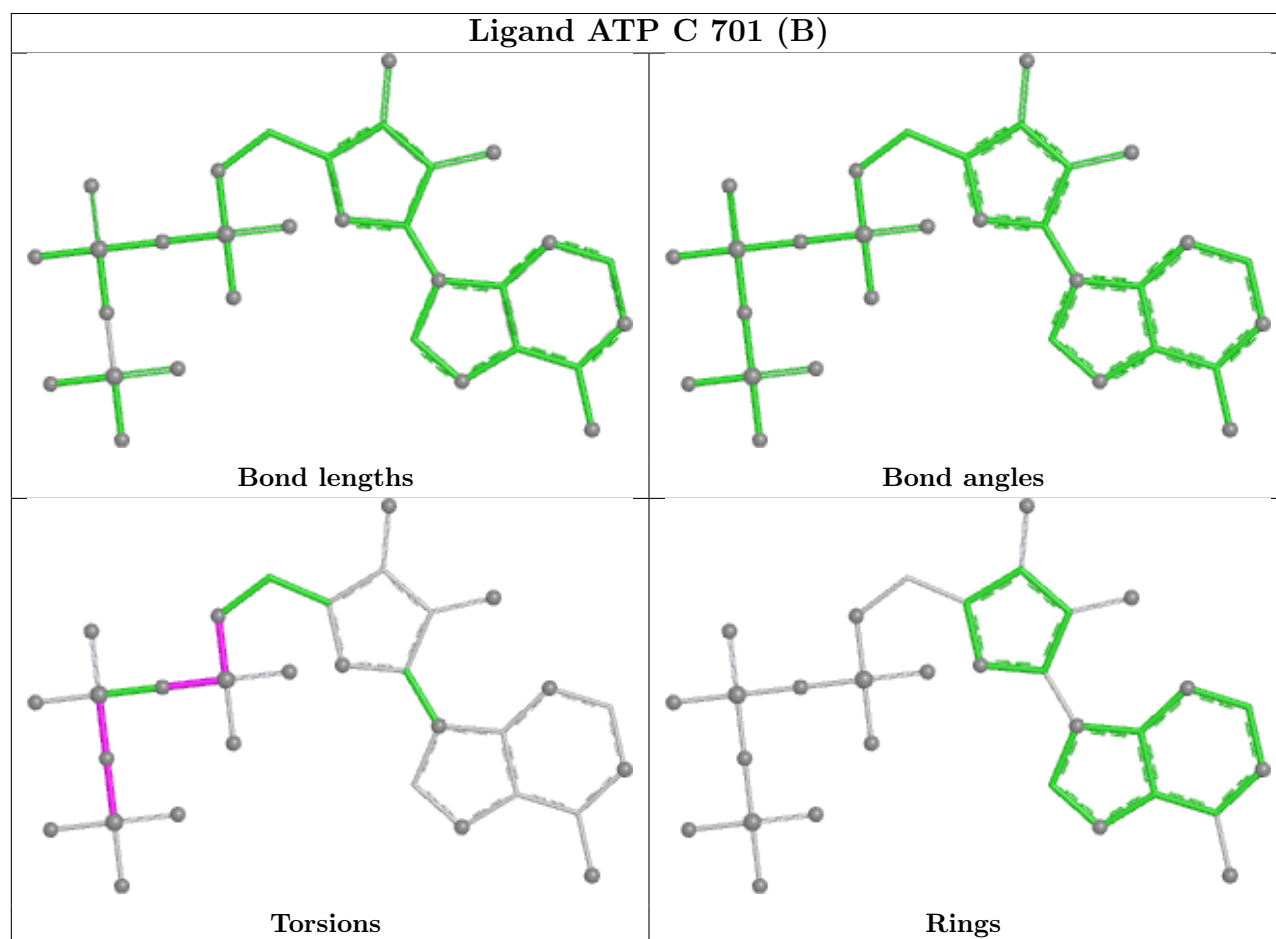
Mol	Chain	Res	Type	Atoms
2	A	701[B]	ATP	C5'-O5'-PA-O1A
2	A	701[B]	ATP	C5'-O5'-PA-O3A
2	C	701[B]	ATP	C5'-O5'-PA-O1A
2	C	701[B]	ATP	C5'-O5'-PA-O3A
3	C	702[A]	6R9	O08-C09-C10-C11
2	B	701[A]	ATP	PB-O3A-PA-O1A
2	A	701[B]	ATP	PB-O3A-PA-O5'
2	B	701[A]	ATP	PB-O3A-PA-O5'
2	C	701[B]	ATP	PB-O3A-PA-O5'
2	A	701[B]	ATP	C5'-O5'-PA-O2A
2	C	701[B]	ATP	C5'-O5'-PA-O2A
3	B	702[B]	6R9	C02-O04-P05-O08
3	C	702[A]	6R9	C02-O04-P05-O08
3	C	702[A]	6R9	O08-C09-C10-O14
3	B	702[B]	6R9	C02-O04-P05-O06
2	C	701[B]	ATP	PB-O3B-PG-O1G
2	A	701[B]	ATP	PB-O3A-PA-O1A
2	C	701[B]	ATP	PG-O3B-PB-O2B
2	C	701[B]	ATP	PB-O3A-PA-O1A
2	A	701[B]	ATP	PB-O3A-PA-O2A
2	B	701[A]	ATP	PG-O3B-PB-O2B
2	C	701[B]	ATP	PB-O3A-PA-O2A

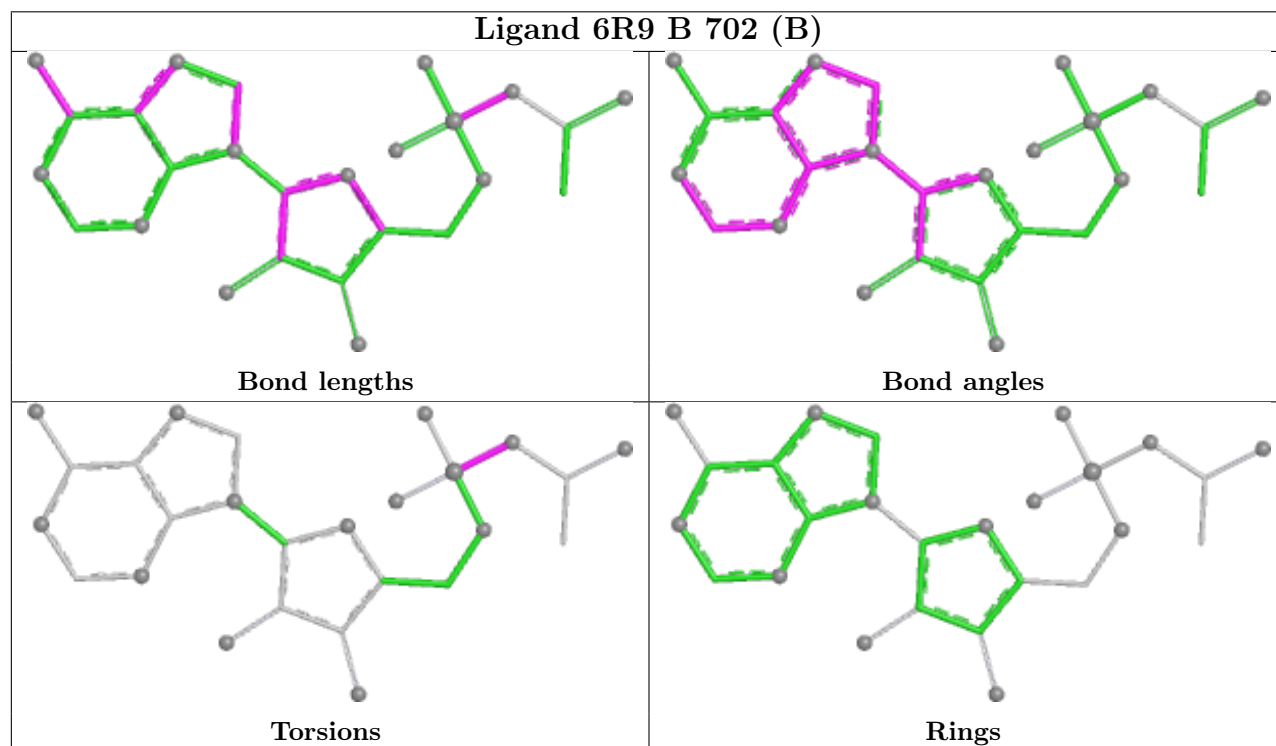
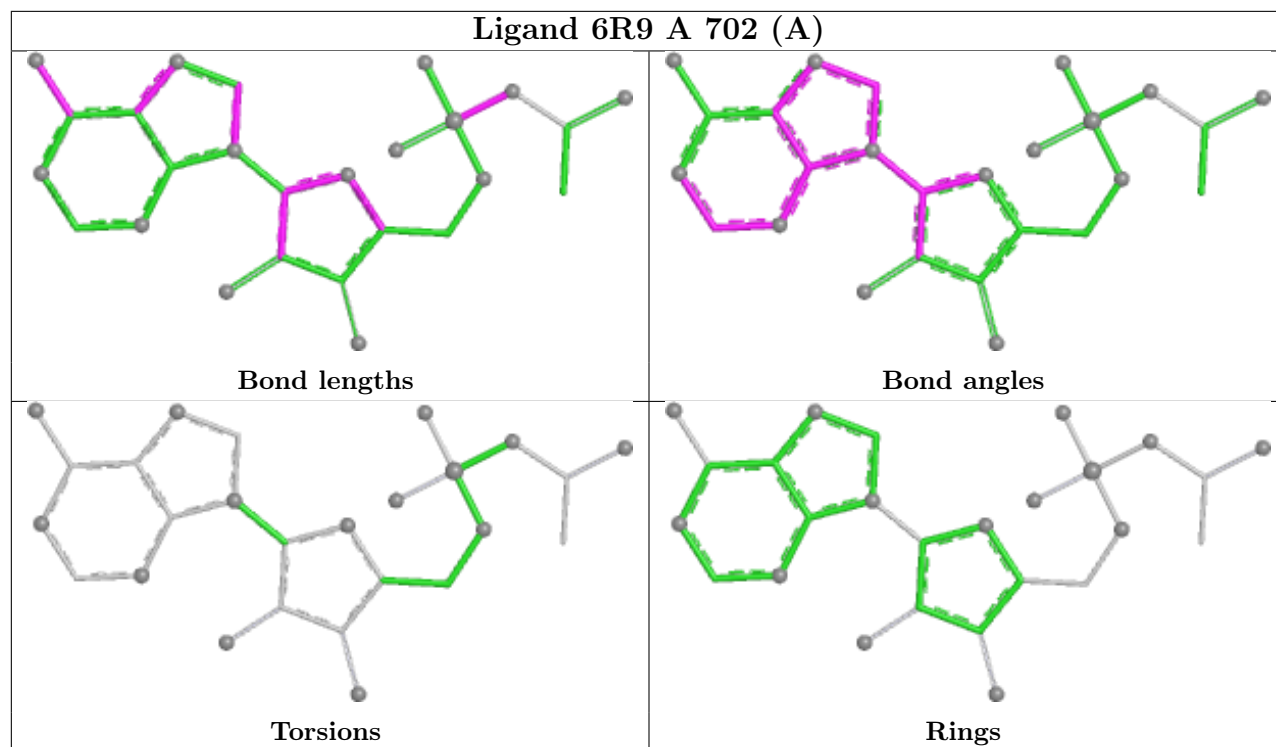
There are no ring outliers.

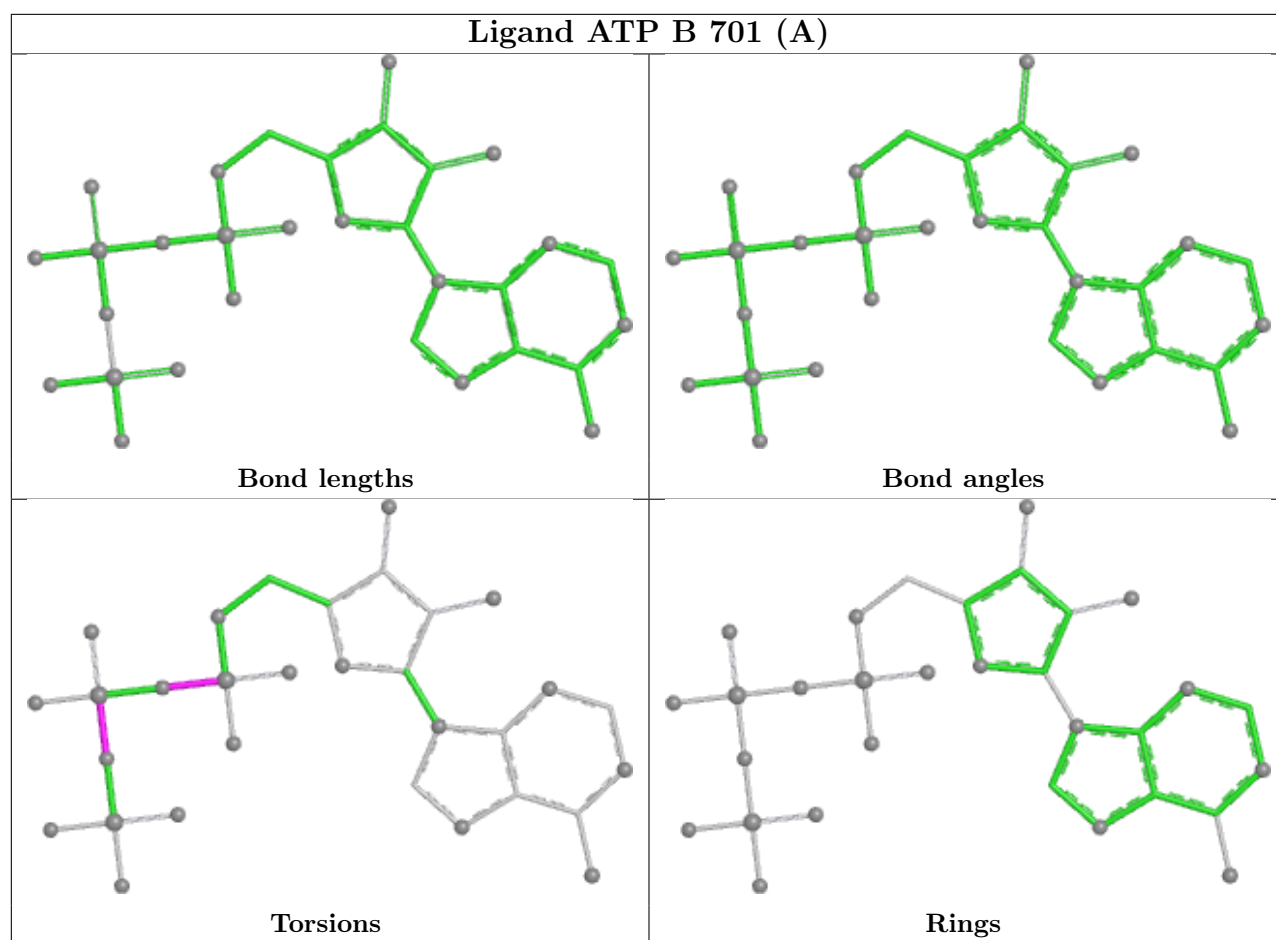
5 monomers are involved in 5 short contacts:

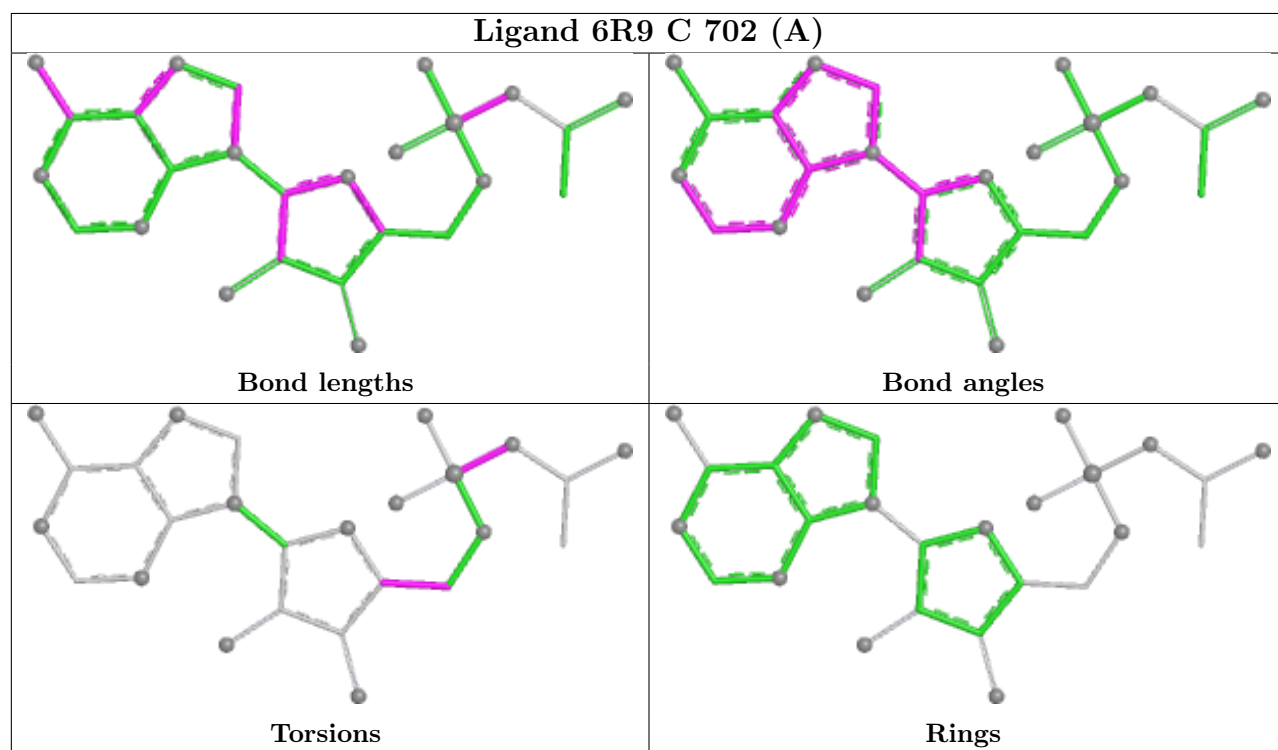
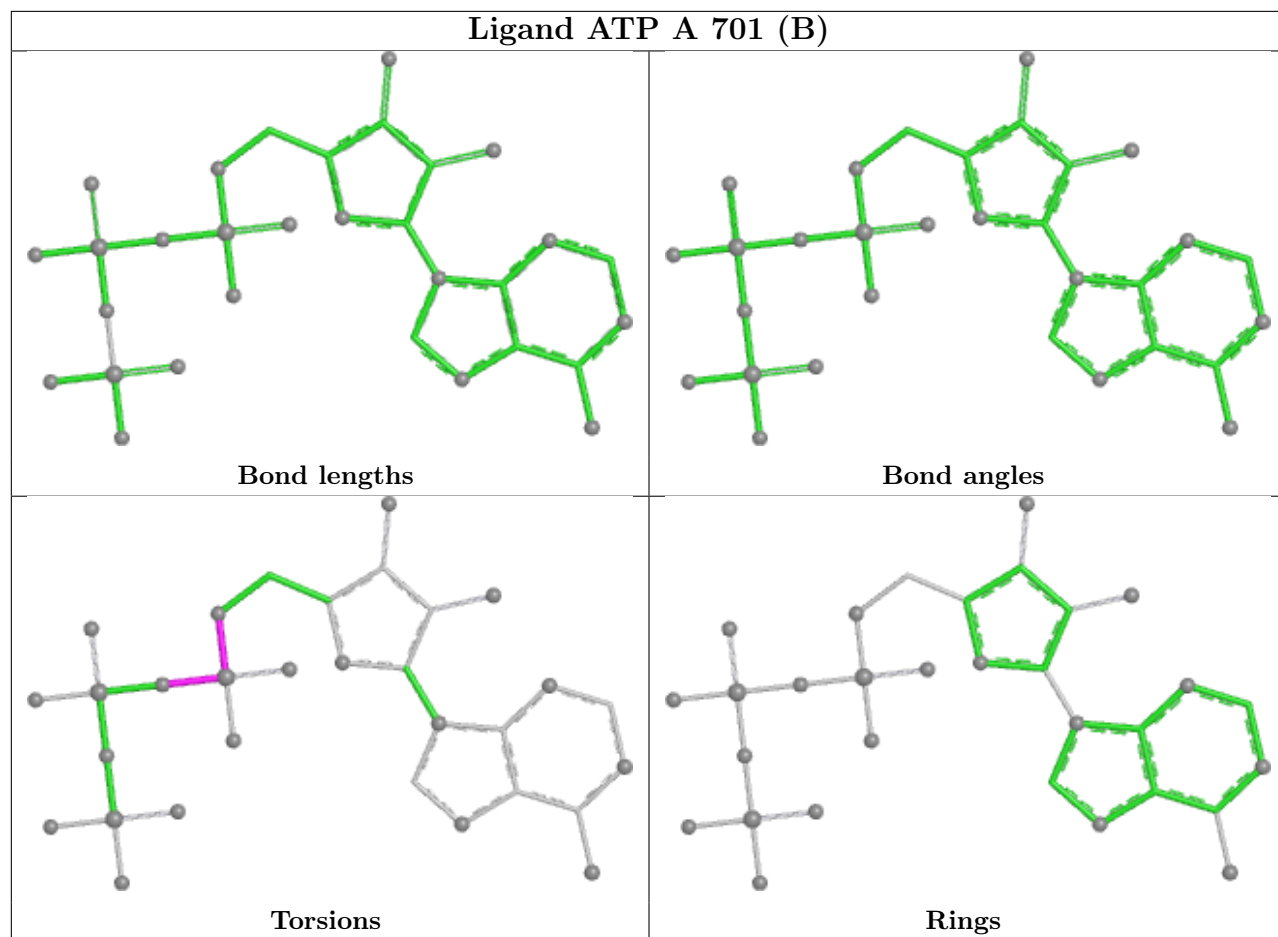
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701[B]	ATP	1	0
5	C	704	EDO	1	0
2	B	701[A]	ATP	1	0
3	C	702[A]	6R9	1	0
5	C	705	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	656/694 (94%)	-0.30	8 (1%) 76 78	16, 40, 90, 120	5 (0%)
1	B	655/694 (94%)	-0.02	8 (1%) 76 78	17, 56, 97, 120	4 (0%)
1	C	651/694 (93%)	-0.07	8 (1%) 76 78	23, 53, 92, 128	7 (1%)
All	All	1962/2082 (94%)	-0.13	24 (1%) 76 78	16, 48, 94, 128	16 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	SER	3.5
1	B	670	PRO	3.5
1	A	295	LYS	3.2
1	A	292	SER	3.0
1	A	291	GLY	3.0
1	C	38	GLY	2.8
1	B	399	ASN	2.8
1	B	601	THR	2.7
1	C	290	SER	2.7
1	C	681	THR	2.6
1	A	296	PRO	2.5
1	C	640[A]	LYS	2.4
1	B	595	GLU	2.3
1	B	570	ALA	2.3
1	B	605	ASP	2.3
1	C	582	THR	2.2
1	C	595	GLU	2.2
1	A	670	PRO	2.2
1	A	681	THR	2.2
1	A	638	SER	2.1
1	B	598	LEU	2.1
1	B	600	ALA	2.1
1	C	581	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	579	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.

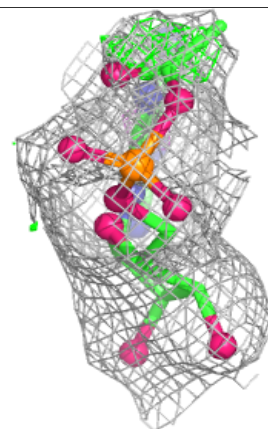
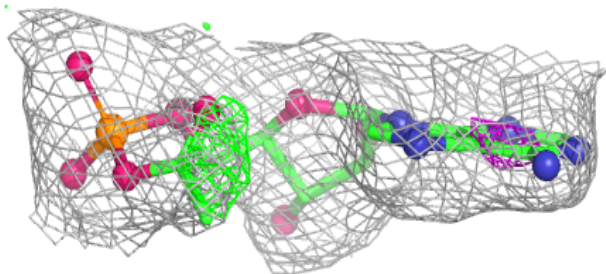
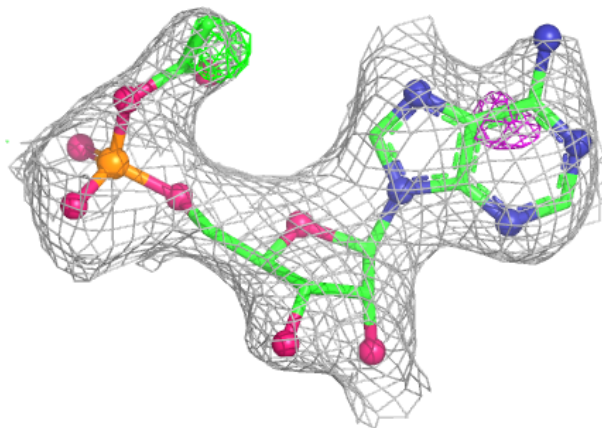
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	703[B]	1/1	0.72	0.12	48,48,48,48	1
4	MG	B	703[B]	1/1	0.73	0.21	64,64,64,64	1
5	EDO	A	707	4/4	0.77	0.19	42,46,47,47	0
3	6R9	B	702[B]	26/26	0.81	0.14	49,58,60,60	26
4	MG	C	703[B]	1/1	0.82	0.11	50,50,50,50	1
5	EDO	B	706	4/4	0.85	0.15	54,55,57,58	0
6	PO4	C	707	5/5	0.86	0.10	64,70,77,80	0
3	6R9	C	702[A]	26/26	0.89	0.11	41,46,48,48	26
2	ATP	B	701[A]	31/31	0.89	0.10	53,59,75,85	31
5	EDO	A	705	4/4	0.89	0.18	37,38,41,47	0
5	EDO	C	704	4/4	0.90	0.12	34,39,39,39	0
5	EDO	C	705	4/4	0.90	0.15	64,65,67,67	0
5	EDO	B	705	4/4	0.90	0.15	36,37,41,42	0
4	MG	C	706	1/1	0.91	0.07	56,56,56,56	0
3	6R9	A	702[A]	26/26	0.92	0.09	32,37,40,42	26
5	EDO	B	704	4/4	0.93	0.08	36,37,43,44	0
5	EDO	A	706	4/4	0.93	0.12	29,34,35,35	0
2	ATP	C	701[B]	31/31	0.93	0.08	44,47,54,56	31
2	ATP	A	701[B]	31/31	0.94	0.08	34,38,59,68	31
5	EDO	A	704	4/4	0.95	0.14	36,36,37,39	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.

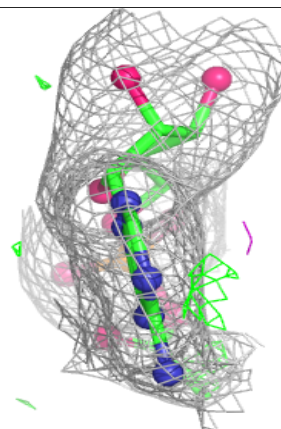
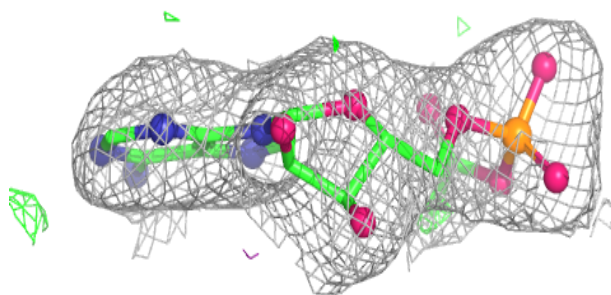
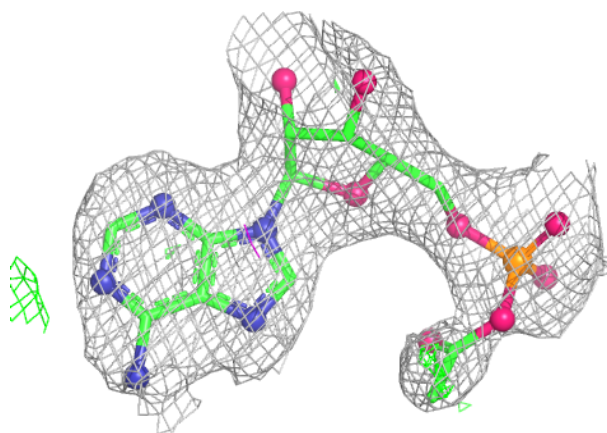
Electron density around 6R9 B 702 (B):

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

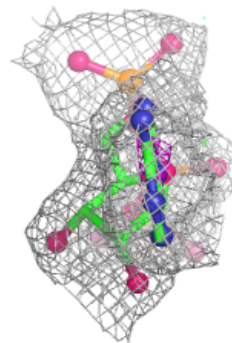
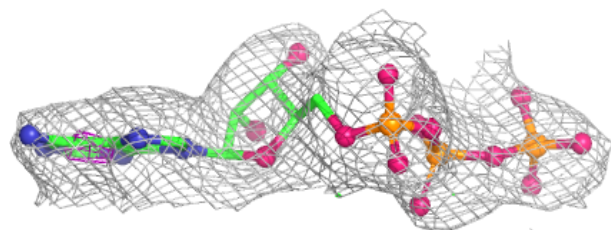
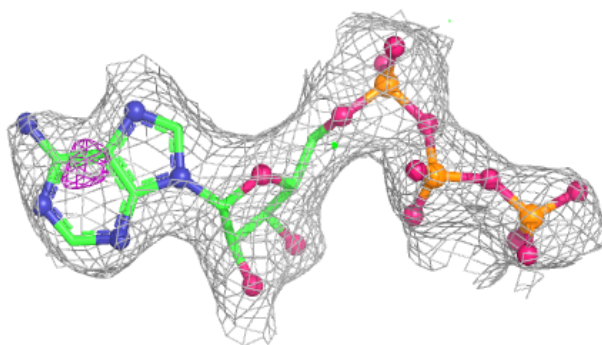


Electron density around 6R9 C 702 (A):

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

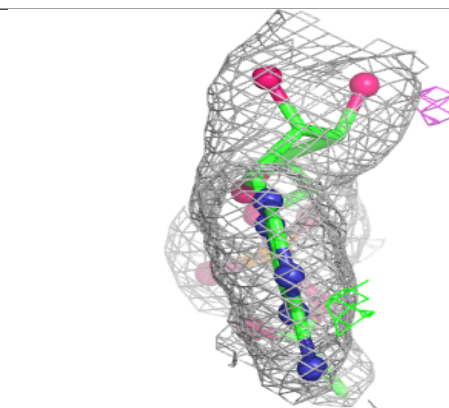
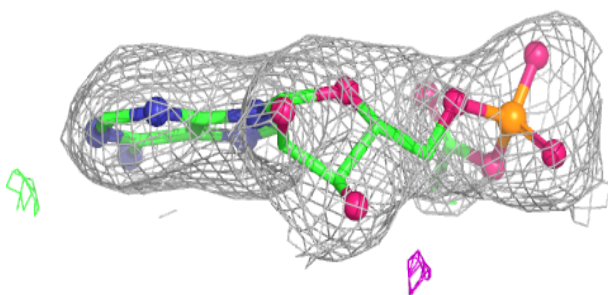
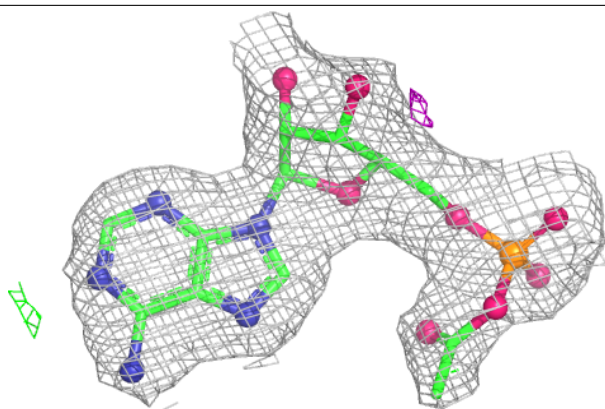
**Electron density around ATP B 701 (A):**

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

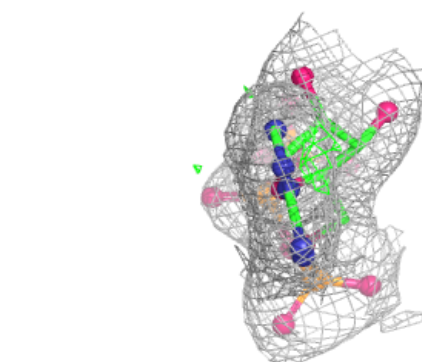
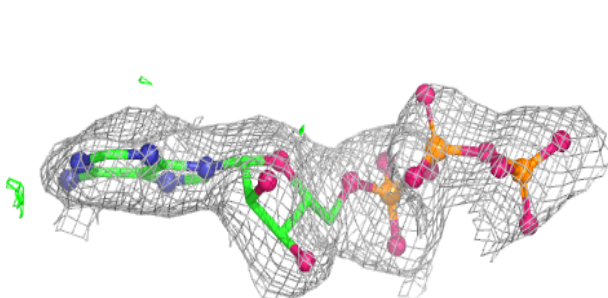
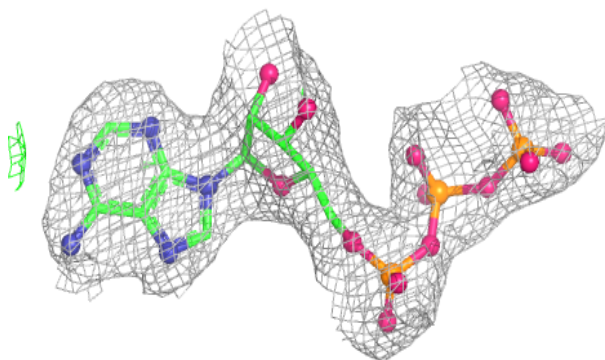


Electron density around 6R9 A 702 (A):

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

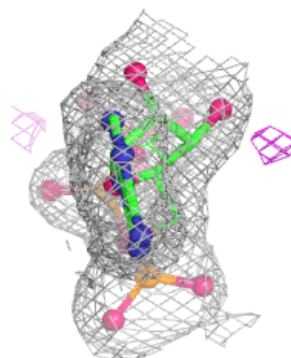
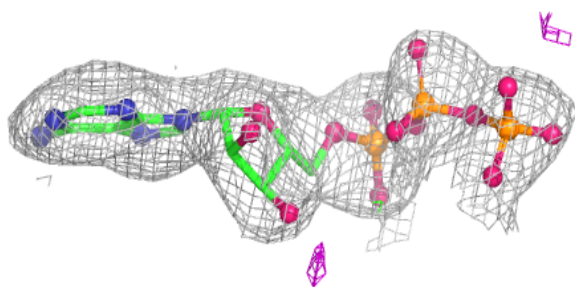
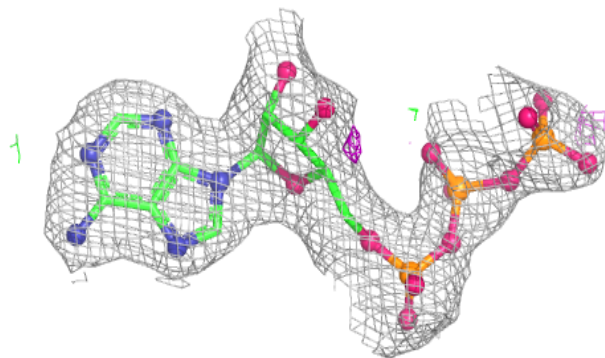
**Electron density around ATP C 701 (B):**

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



Electron density around ATP A 701 (B):

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.