Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 06:55 AM EDT

PDB ID	:	5K8F
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:

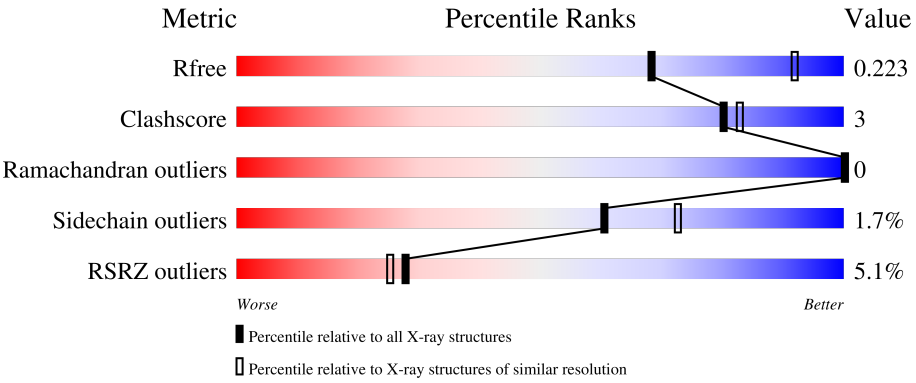
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	694	4% 86% 8% • 5%
1	B	694	8% 87% 7% 6%
1	C	694	3% 87% 7% 6%

2 Entry composition (i)

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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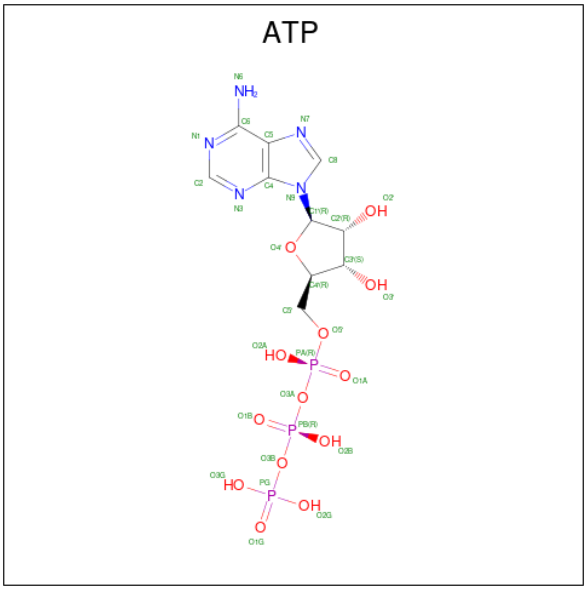
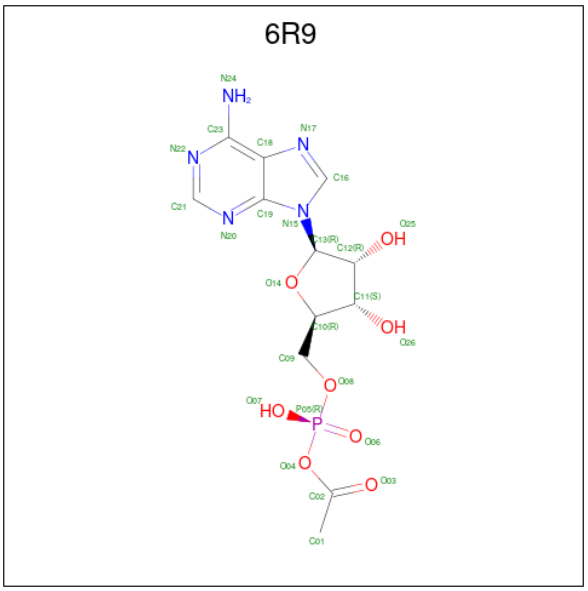
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP J9VFT1
B	-4	GLU	-	expression tag	UNP J9VFT1
B	-3	ASN	-	expression tag	UNP J9VFT1
B	-2	LEU	-	expression tag	UNP J9VFT1
B	-1	TYR	-	expression tag	UNP J9VFT1
B	0	PHE	-	expression tag	UNP J9VFT1
B	1	GLN	-	expression tag	UNP J9VFT1
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 (three-letter code: 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 (three-letter code: 6R9) (formula: $C_{12}H_{16}N_5O_8P$) (labeled as "Ligand of Interest" by depositor).

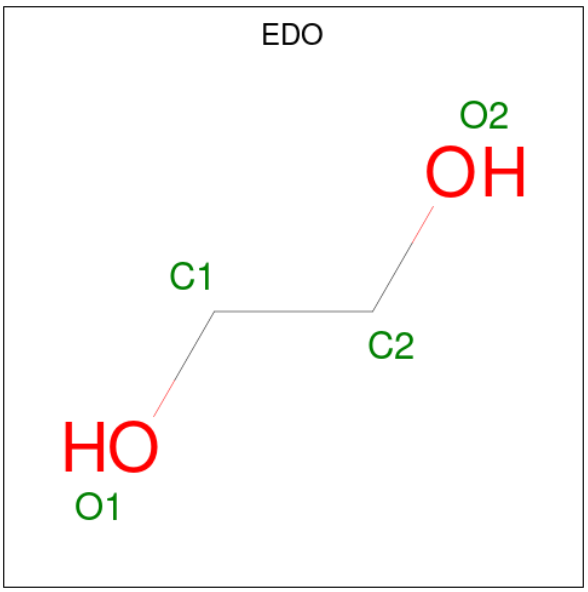


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			26	12	5	8	1		
3	B	1	Total	C	N	O	P	0	1
			26	12	5	8	1		
3	C	1	Total	C	N	O	P	0	1
			26	12	5	8	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

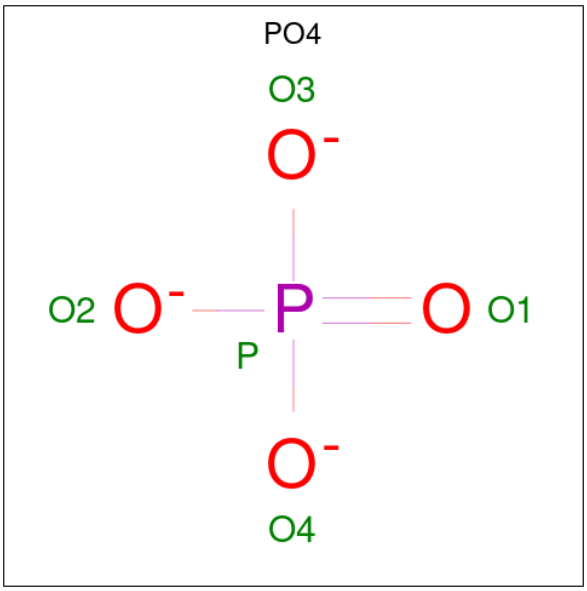
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	1
			1	1		
4	B	1	Total	Mg	0	1
			1	1		
4	C	2	Total	Mg	0	1
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: 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 (three-letter code: PO4) (formula: O_4P).



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

- Molecule 7 is water.

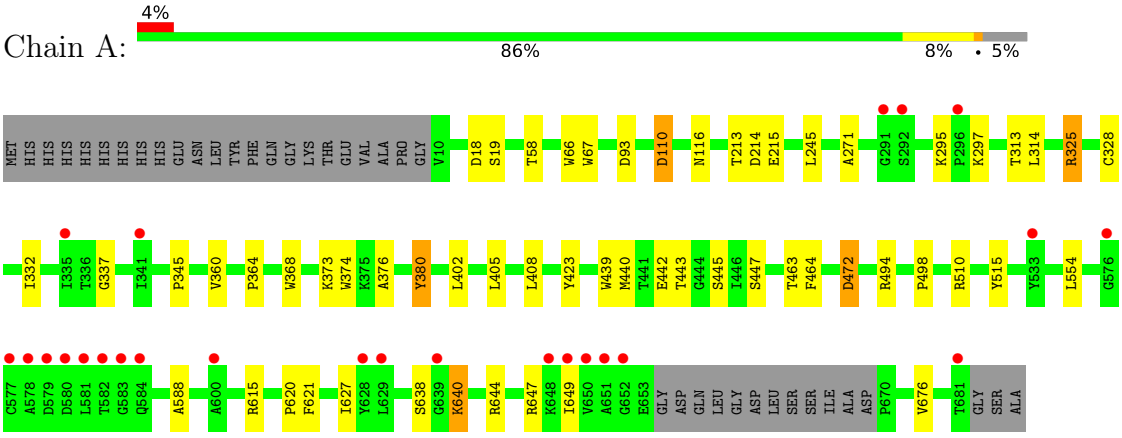
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	188	Total O 190 190	0	3
7	B	85	Total O 87 87	0	2
7	C	98	Total O 100 100	0	2

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.

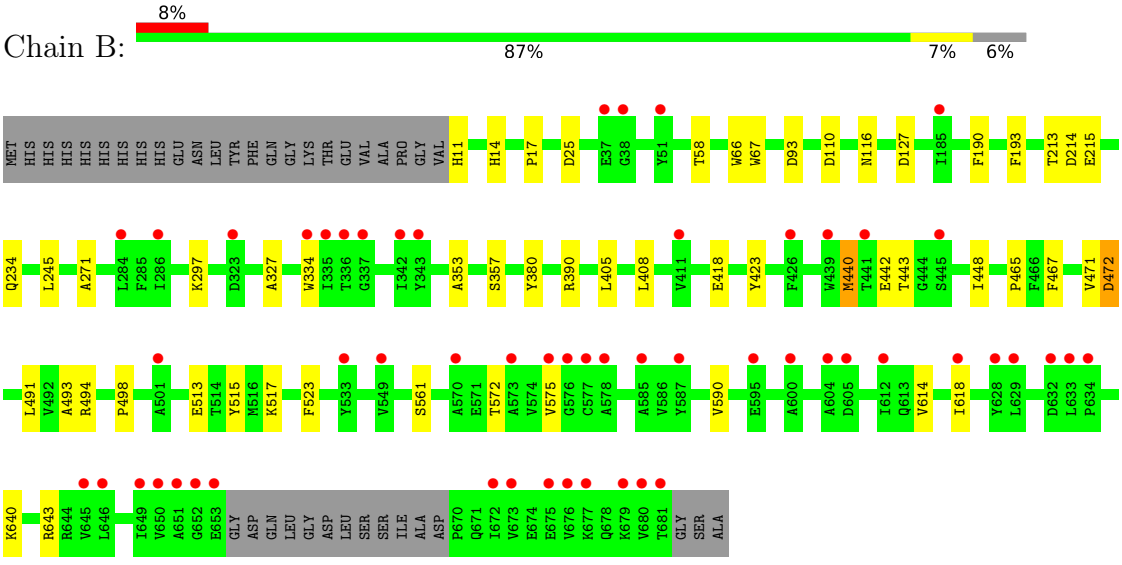
• Molecule 1: Acetyl-coenzyme A synthetase

Chain A:



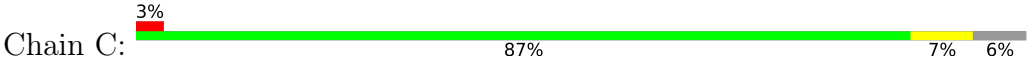
• Molecule 1: Acetyl-coenzyme A synthetase

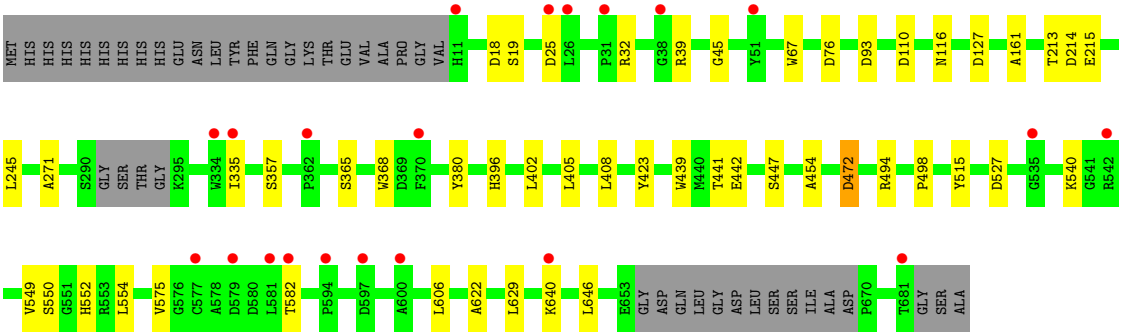
Chain B:



• Molecule 1: Acetyl-coenzyme A synthetase

Chain C:




MET HIS HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY LYS THR GLU VAL ALA PRO GLY VAL H11 D18 S19 D25 L26 P31 R32 G38 R39 G45 Y51 W67 D76 D93 D110 N116 D127 A161 T213 D214 E215
L245 A271 S290 GLY SER THR GLY K296 W334 I335 S357 P362 S365 W368 D369 F370 Y380 H396 L402 L405 L408 Y423 W439 M440 T441 E442 S447 A454 D472 R494 P498 Y515 D527 G536 K540 G541 R542
V549 S550 G551 H552 R553 L554 V575 G576 C577 A578 D579 D580 L581 T582 P594 D597 A600 L606 A622 L629 K640 L646 E653 GLY ASP GLN LEU GLY ASP LEU SER SER ILE ALA ASP P670 T681 GLY SER ALA

4 Data and refinement statistics (i)

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 47.48 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.6 (26.62-2.45) 98.6 (47.48-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.19rc4_4035	Depositor
R, R_{free}	0.188 , 0.224 0.186 , 0.223	Depositor DCC
R_{free} test set	2000 reflections (2.59%)	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)	0.32 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 6R9, ATP, PO4, 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	0.24	0/5202	0.48	0/7101
1	B	0.24	0/5135	0.47	0/7018
1	C	0.24	0/5148	0.47	0/7033
All	All	0.24	0/15485	0.47	0/21152

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5054	0	4776	29	0
1	B	4985	0	4657	27	0
1	C	4992	0	4699	25	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
3	B	26	0	0	0	0
3	C	26	0	0	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	78	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 (78) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:550:SER:N	1:C:582:THR:O	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

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
All	All	1964/2082 (94%)	1910 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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%)	503 (98%)	9 (2%)	59	71
1	B	492/576 (85%)	482 (98%)	10 (2%)	55	67
1	C	498/576 (86%)	491 (99%)	7 (1%)	67	77
All	All	1502/1728 (87%)	1476 (98%)	26 (2%)	60	73

All (26) 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	380	TYR
1	A	423	TYR
1	A	472	ASP
1	A	640	LYS
1	B	25	ASP
1	B	110	ASP
1	B	116	ASN
1	B	234	GLN
1	B	297	LYS
1	B	380	TYR
1	B	423	TYR
1	B	440	MET
1	B	472	ASP
1	B	640	LYS
1	C	25	ASP
1	C	76	ASP
1	C	110	ASP
1	C	116	ASN
1	C	380	TYR
1	C	423	TYR
1	C	472	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	566	HIS
1	C	348	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 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	0.46	0	2,2,2	0.32	0
2	ATP	C	701[B]	4	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
5	EDO	A	707	-	3,3,3	0.48	0	2,2,2	0.25	0
5	EDO	B	705	-	3,3,3	0.45	0	2,2,2	0.34	0
6	PO4	C	707	-	4,4,4	0.91	0	6,6,6	0.42	0
5	EDO	C	704	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	B	706	-	3,3,3	0.46	0	2,2,2	0.34	0
2	ATP	B	701[A]	-	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
5	EDO	A	706	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	C	705	-	3,3,3	0.45	0	2,2,2	0.38	0
3	6R9	C	702[A]	-	24,28,28	4.36	5 (20%)	26,42,42	1.30	3 (11%)
5	EDO	B	704	-	3,3,3	0.46	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	6R9	B	702[B]	-	24,28,28	4.36	5 (20%)	26,42,42	1.31	4 (15%)
2	ATP	A	701[B]	4	26,33,33	0.61	0	31,52,52	0.74	2 (6%)
3	6R9	A	702[A]	-	24,28,28	4.37	5 (20%)	26,42,42	1.25	3 (11%)
5	EDO	A	704	-	3,3,3	0.45	0	2,2,2	0.33	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	-	7/18/38/38	0/3/3/3
5	EDO	A	707	-	-	0/1/1/1	-
5	EDO	B	705	-	-	0/1/1/1	-
5	EDO	C	704	-	-	0/1/1/1	-
5	EDO	B	706	-	-	0/1/1/1	-
2	ATP	B	701[A]	-	-	3/18/38/38	0/3/3/3
5	EDO	A	706	-	-	0/1/1/1	-
5	EDO	C	705	-	-	0/1/1/1	-
3	6R9	C	702[A]	-	-	4/9/31/31	0/3/3/3
5	EDO	B	704	-	-	0/1/1/1	-
3	6R9	B	702[B]	-	-	2/9/31/31	0/3/3/3
2	ATP	A	701[B]	4	-	5/18/38/38	0/3/3/3
3	6R9	A	702[A]	-	-	0/9/31/31	0/3/3/3
5	EDO	A	704	-	-	0/1/1/1	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702[A]	6R9	O14-C13	15.10	1.62	1.41
3	B	702[B]	6R9	O14-C13	15.09	1.62	1.41
3	C	702[A]	6R9	O14-C13	15.06	1.62	1.41
3	C	702[A]	6R9	C12-C13	-12.49	1.34	1.53
3	A	702[A]	6R9	C12-C13	-12.43	1.34	1.53
3	B	702[B]	6R9	C12-C13	-12.37	1.35	1.53
3	B	702[B]	6R9	O14-C10	-6.36	1.30	1.45
3	A	702[A]	6R9	O14-C10	-6.34	1.30	1.45
3	C	702[A]	6R9	O14-C10	-6.34	1.30	1.45
3	B	702[B]	6R9	C23-N24	3.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702[A]	6R9	C23-N24	3.05	1.45	1.34
3	C	702[A]	6R9	C23-N24	3.02	1.45	1.34
3	B	702[B]	6R9	P05-O04	2.62	1.66	1.60
3	C	702[A]	6R9	P05-O04	2.58	1.65	1.60
3	A	702[A]	6R9	P05-O04	2.56	1.65	1.60

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	702[A]	6R9	N20-C21-N22	-4.13	122.23	128.68
3	B	702[B]	6R9	N20-C21-N22	-4.11	122.25	128.68
3	A	702[A]	6R9	N20-C21-N22	-4.09	122.28	128.68
3	C	702[A]	6R9	C11-C12-C13	2.82	105.23	100.98
3	B	702[B]	6R9	C11-C12-C13	2.72	105.07	100.98
3	A	702[A]	6R9	C11-C12-C13	2.44	104.64	100.98
2	C	701[B]	ATP	C5-C6-N6	2.31	123.87	120.35
2	B	701[A]	ATP	C5-C6-N6	2.26	123.79	120.35
2	A	701[B]	ATP	C5-C6-N6	2.26	123.79	120.35
3	B	702[B]	6R9	C19-C18-N17	-2.20	107.11	109.40
3	C	702[A]	6R9	C19-C18-N17	-2.17	107.14	109.40
3	A	702[A]	6R9	C19-C18-N17	-2.16	107.15	109.40
2	B	701[A]	ATP	PB-O3B-PG	2.11	140.07	132.83
2	C	701[B]	ATP	PB-O3B-PG	2.04	139.83	132.83
3	B	702[B]	6R9	O04-P05-O08	2.03	108.85	102.92
2	A	701[B]	ATP	PB-O3B-PG	2.03	139.78	132.83

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701[B]	ATP	C5'-O5'-PA-O1A
2	C	701[B]	ATP	C5'-O5'-PA-O1A
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'
3	B	702[B]	6R9	C02-O04-P05-O08
3	C	702[A]	6R9	C02-O04-P05-O08
2	A	701[B]	ATP	C5'-O5'-PA-O3A
2	B	701[A]	ATP	C5'-O5'-PA-O3A
2	C	701[B]	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
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-O06
3	C	702[A]	6R9	O08-C09-C10-O14
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
3	C	702[A]	6R9	C09-O08-P05-O06

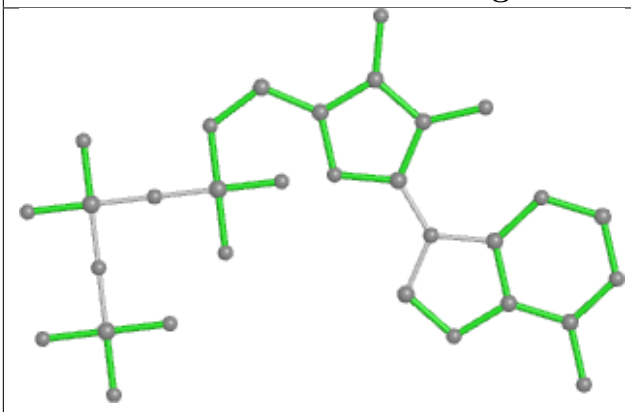
There are no ring outliers.

5 monomers are involved in 5 short contacts:

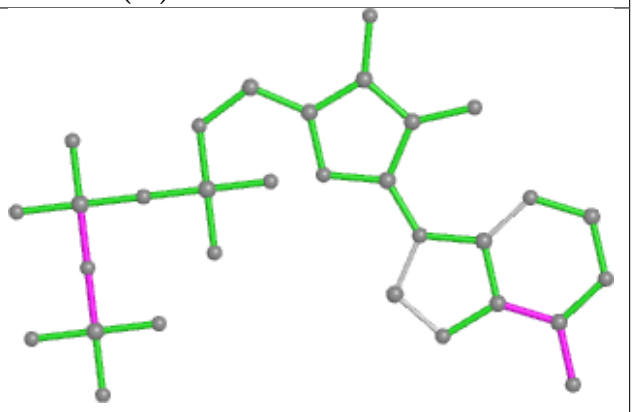
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701[B]	ATP	1	0
5	C	704	EDO	1	0
2	B	701[A]	ATP	1	0
5	C	705	EDO	1	0
3	C	702[A]	6R9	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

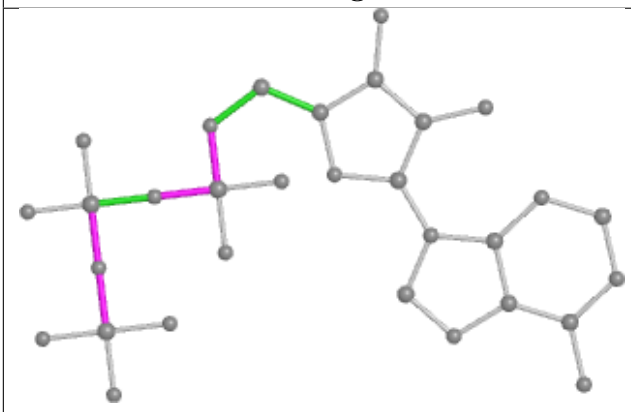
Ligand ATP C 701 (B)



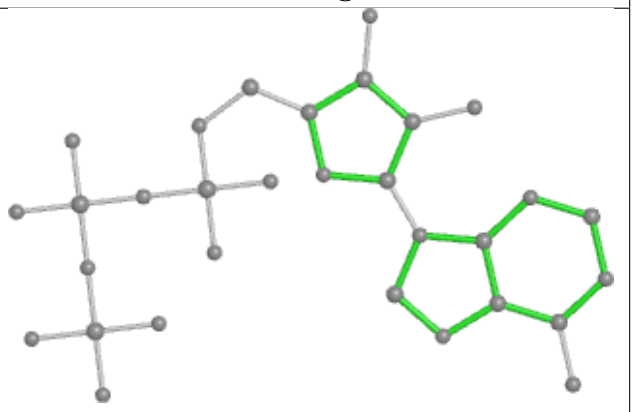
Bond lengths



Bond angles

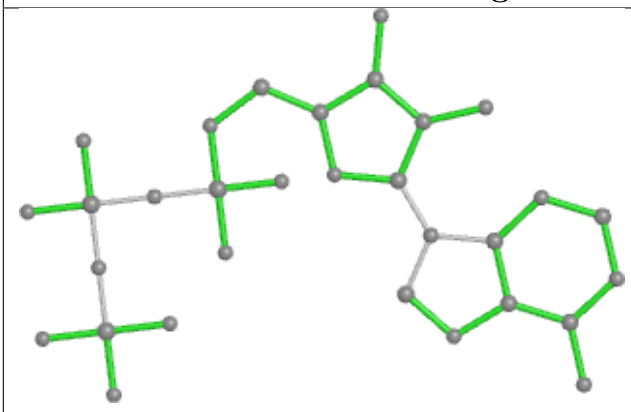


Torsions

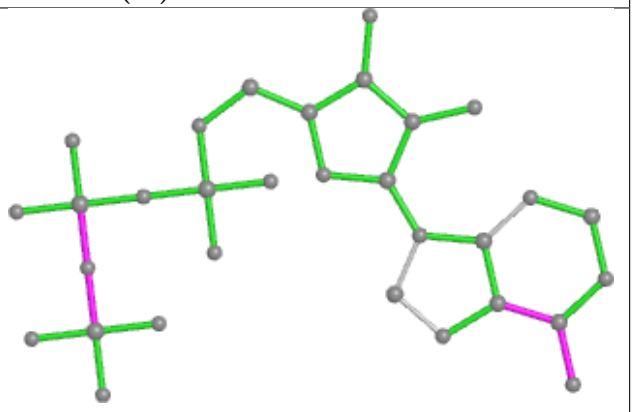


Rings

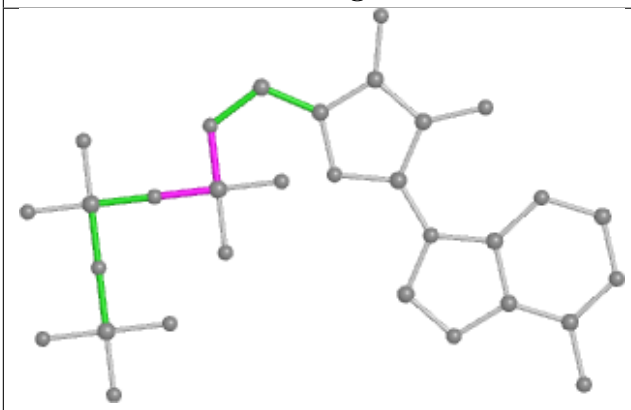
Ligand ATP B 701 (A)



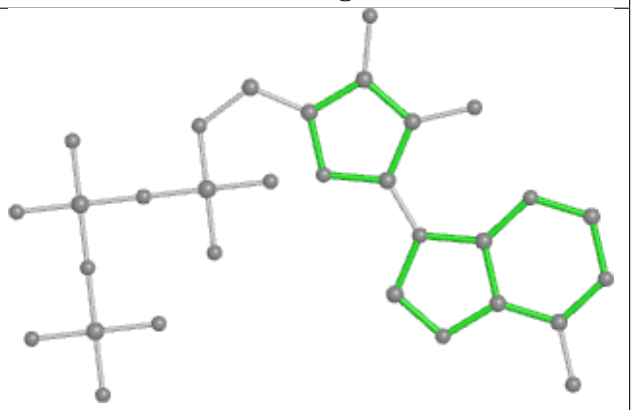
Bond lengths



Bond angles

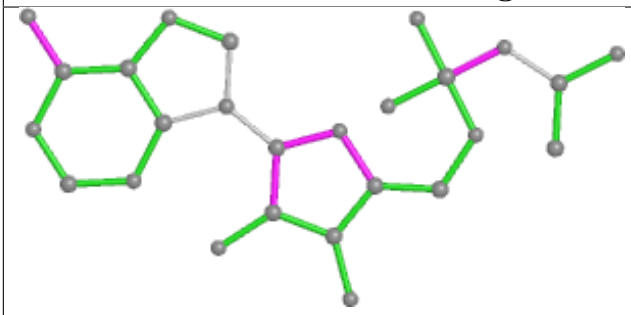


Torsions

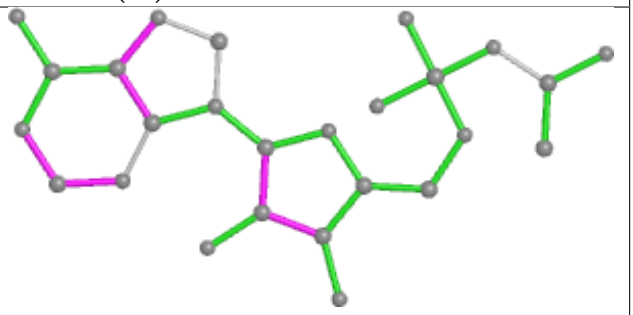


Rings

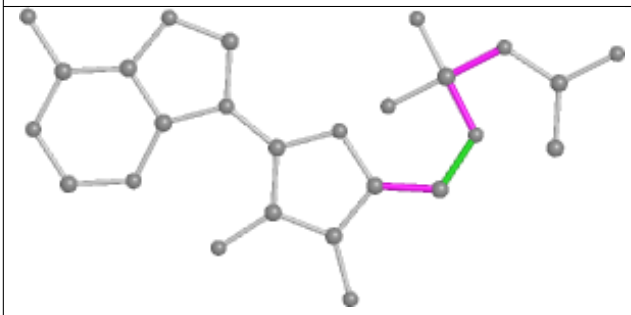
Ligand 6R9 C 702 (A)



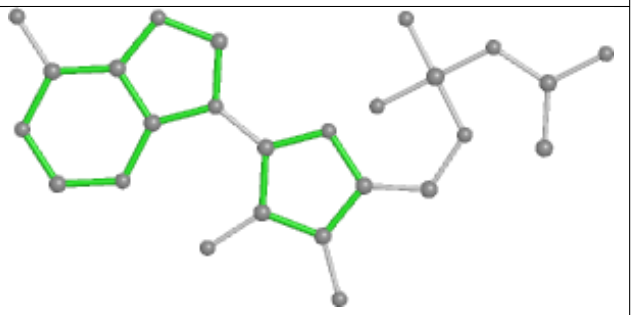
Bond lengths



Bond angles

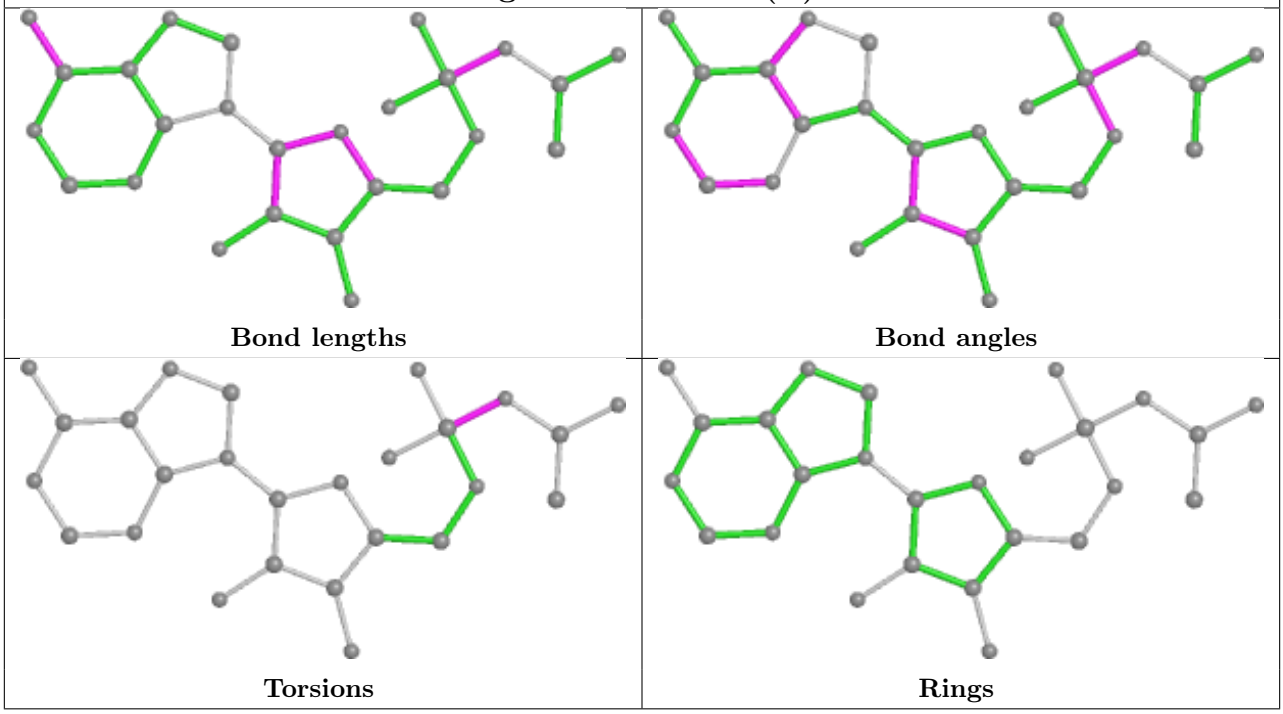


Torsions

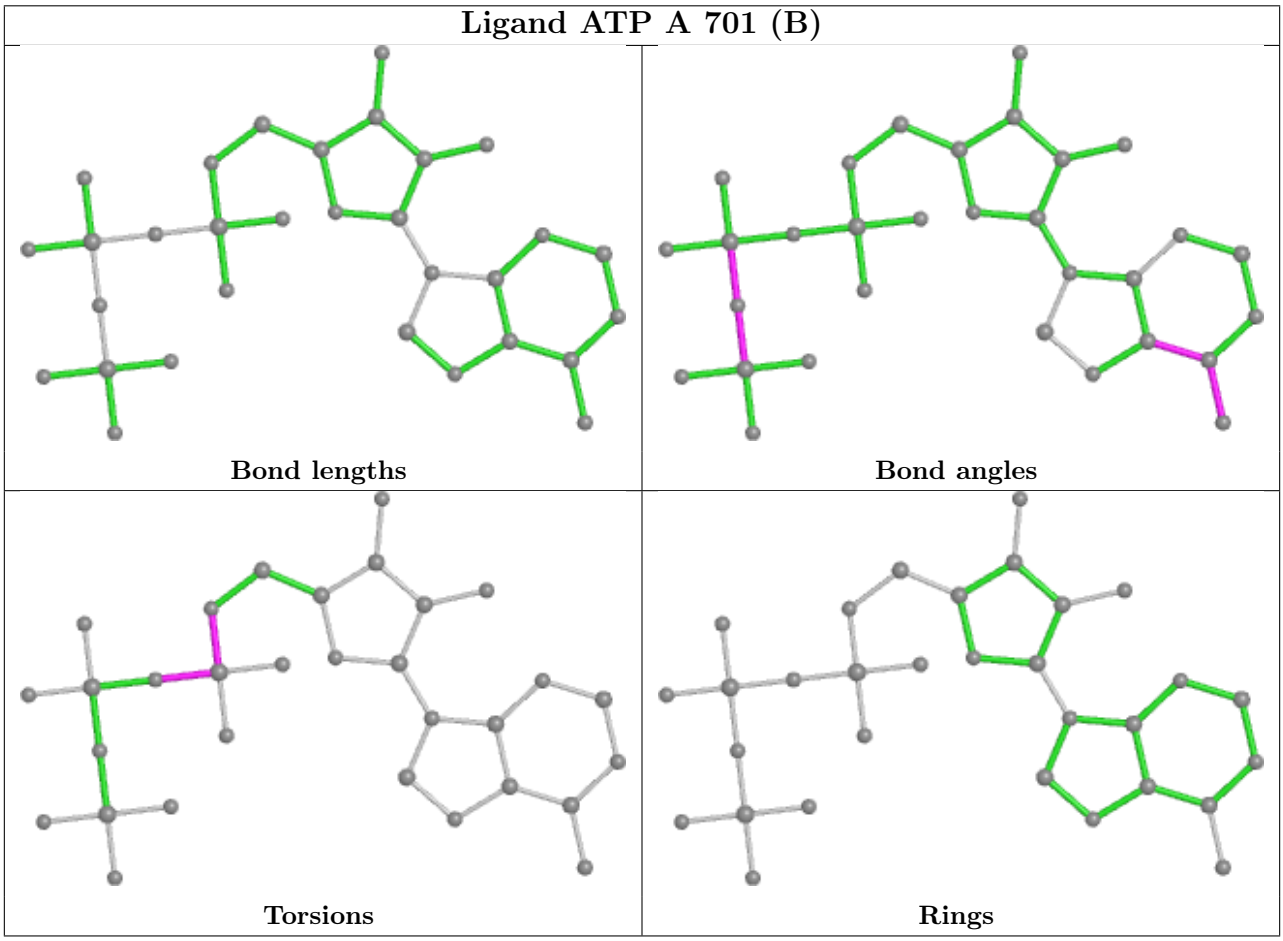


Rings

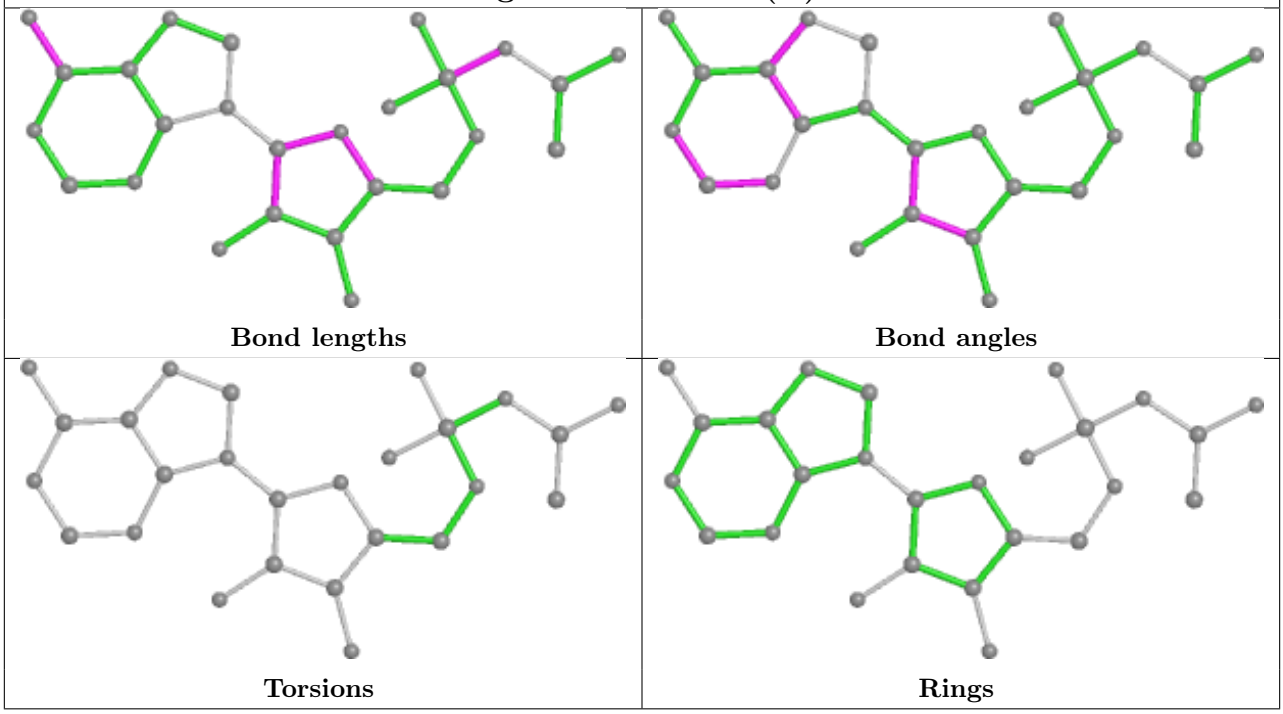
Ligand 6R9 B 702 (B)



Ligand ATP A 701 (B)



Ligand 6R9 A 702 (A)



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	656/694 (94%)	-0.08	25 (3%)	40	37	24, 41, 90, 120	0
1	B	655/694 (94%)	0.31	55 (8%)	11	8	28, 56, 97, 120	0
1	C	651/694 (93%)	0.04	21 (3%)	47	44	29, 54, 92, 128	0
All	All	1962/2082 (94%)	0.09	101 (5%)	28	25	24, 49, 94, 128	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	ALA	6.6
1	A	577	CYS	6.1
1	B	676	VAL	6.1
1	A	578	ALA	5.6
1	B	334[A]	TRP	5.6
1	C	38	GLY	5.3
1	B	681	THR	4.9
1	C	334[A]	TRP	4.8
1	B	578	ALA	4.6
1	B	673	VAL	4.4
1	B	604	ALA	4.1
1	A	581	LEU	4.1
1	A	652	GLY	4.1
1	B	652	GLY	4.1
1	B	628	TYR	4.1
1	B	577	CYS	3.9
1	B	650	VAL	3.8
1	B	646	LEU	3.8
1	A	579	ASP	3.8
1	B	335	ILE	3.7
1	B	675	GLU	3.6
1	A	628	TYR	3.5
1	C	582	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	291	GLY	3.4
1	A	296	PRO	3.4
1	B	634	PRO	3.4
1	B	645	VAL	3.4
1	B	680	VAL	3.4
1	B	618	ILE	3.4
1	C	577	CYS	3.3
1	C	640[A]	LYS	3.2
1	A	651	ALA	3.2
1	B	651	ALA	3.2
1	A	629	LEU	3.1
1	B	633	LEU	3.1
1	B	587	TYR	3.1
1	B	38	GLY	3.1
1	C	31	PRO	3.0
1	B	679	LYS	3.0
1	B	632	ASP	3.0
1	B	605	ASP	3.0
1	A	650	VAL	2.9
1	B	649	ILE	2.9
1	B	570	ALA	2.9
1	B	576	GLY	2.9
1	B	575	VAL	2.9
1	A	335	ILE	2.9
1	B	439	TRP	2.8
1	B	549	VAL	2.8
1	B	533	TYR	2.8
1	B	677	LYS	2.7
1	C	535	GLY	2.7
1	B	51	TYR	2.7
1	C	51	TYR	2.7
1	B	343	TYR	2.6
1	B	336	THR	2.6
1	C	597	ASP	2.6
1	B	672	ILE	2.6
1	A	533	TYR	2.6
1	A	649	ILE	2.5
1	C	542[A]	ARG	2.4
1	C	11	HIS	2.4
1	A	580	ASP	2.4
1	A	582	THR	2.4
1	B	573	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	583	GLY	2.3
1	A	648	LYS	2.3
1	B	653	GLU	2.3
1	B	445	SER	2.3
1	B	342	ILE	2.3
1	B	411	VAL	2.3
1	C	600	ALA	2.3
1	B	595	GLU	2.3
1	B	612	ILE	2.3
1	C	335	ILE	2.3
1	C	681	THR	2.3
1	A	341	ILE	2.2
1	B	284	LEU	2.2
1	C	25	ASP	2.2
1	C	362	PRO	2.2
1	B	629	LEU	2.2
1	B	37	GLU	2.2
1	C	370	PHE	2.2
1	A	292	SER	2.2
1	A	600	ALA	2.2
1	C	579	ASP	2.1
1	A	584	GLN	2.1
1	C	26	LEU	2.1
1	A	639	GLY	2.1
1	A	681	THR	2.1
1	C	594	PRO	2.1
1	B	286	ILE	2.1
1	B	501	ALA	2.1
1	B	185	ILE	2.1
1	B	585	ALA	2.1
1	B	426	PHE	2.1
1	B	323	ASP	2.0
1	B	441	THR	2.0
1	A	576	GLY	2.0
1	B	337	GLY	2.0
1	C	581	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

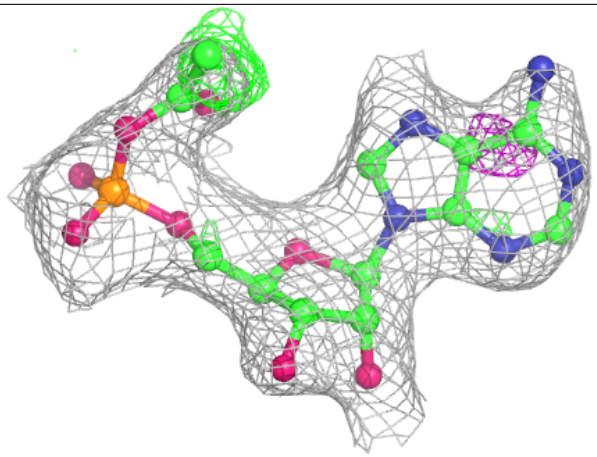
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

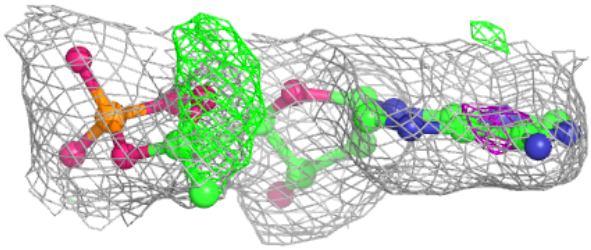
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	703[B]	1/1	0.73	0.14	48,48,48,48	1
5	EDO	A	707	4/4	0.79	0.24	42,46,47,47	0
4	MG	B	703[B]	1/1	0.86	0.70	64,64,64,64	1
3	6R9	B	702[B]	26/26	0.87	0.22	49,58,60,60	26
5	EDO	C	705	4/4	0.90	0.18	64,65,67,67	0
6	PO4	C	707	5/5	0.90	0.15	64,70,77,80	0
2	ATP	B	701[A]	31/31	0.92	0.20	53,59,75,85	31
4	MG	C	706	1/1	0.92	0.12	56,56,56,56	0
5	EDO	A	705	4/4	0.92	0.28	37,38,41,47	0
5	EDO	C	704	4/4	0.93	0.14	34,39,39,39	0
4	MG	C	703[B]	1/1	0.93	0.48	50,50,50,50	1
5	EDO	B	705	4/4	0.93	0.32	36,37,41,42	0
3	6R9	C	702[A]	26/26	0.94	0.24	41,46,48,48	26
3	6R9	A	702[A]	26/26	0.94	0.21	32,37,40,42	26
5	EDO	B	706	4/4	0.94	0.09	54,55,57,58	0
5	EDO	A	706	4/4	0.95	0.15	29,34,35,35	0
5	EDO	A	704	4/4	0.95	0.25	36,36,37,39	0
5	EDO	B	704	4/4	0.95	0.14	36,37,43,44	0
2	ATP	C	701[B]	31/31	0.95	0.22	44,47,54,56	31
2	ATP	A	701[B]	31/31	0.97	0.18	34,38,59,68	31

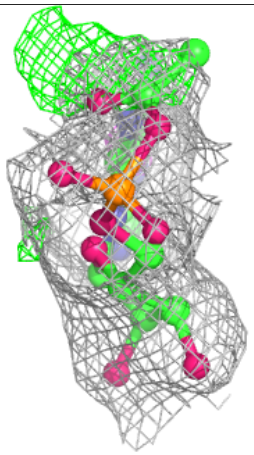
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

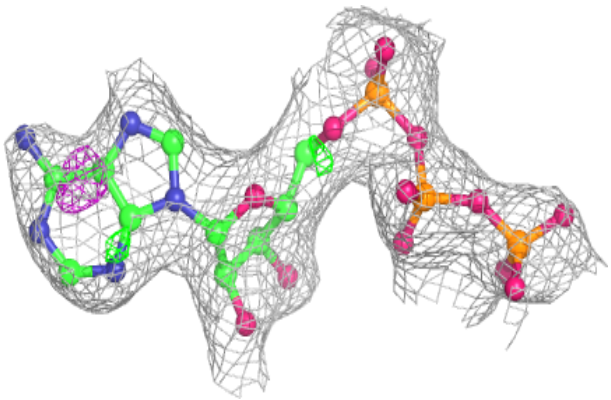


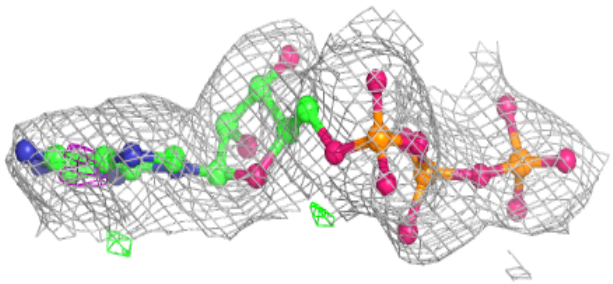


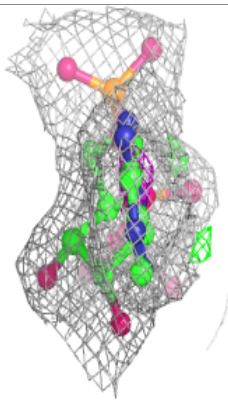


Electron density around ATP B 701 (A):

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

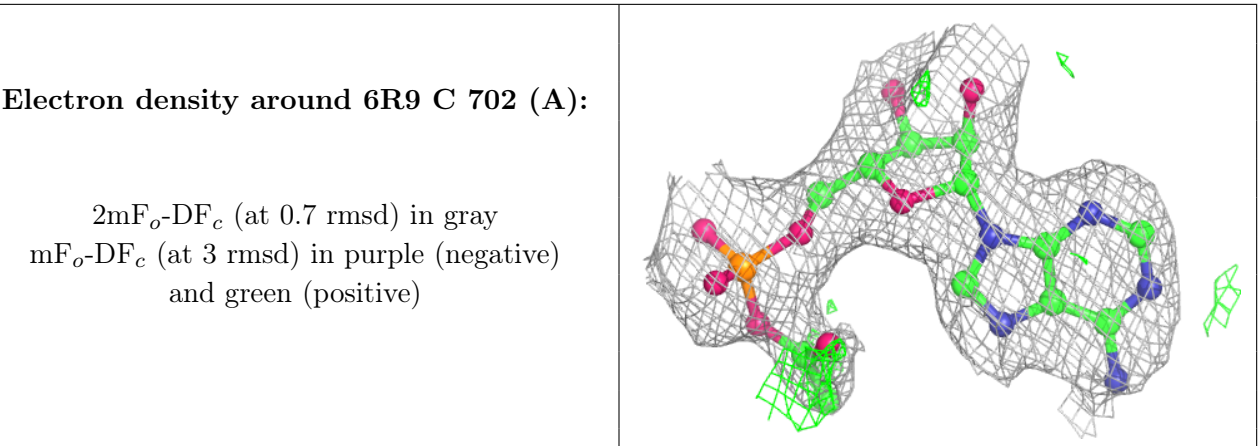






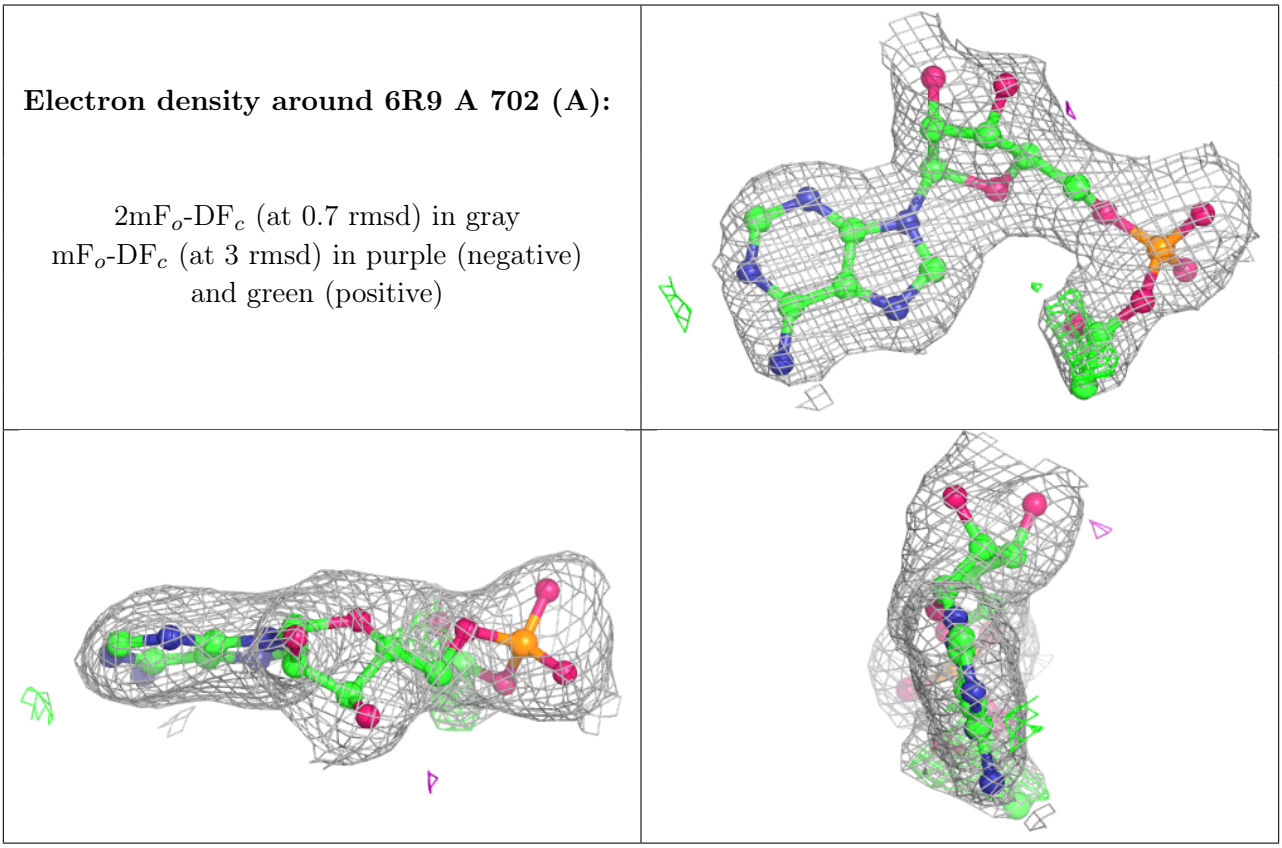
Electron density around 6R9 C 702 (A):

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



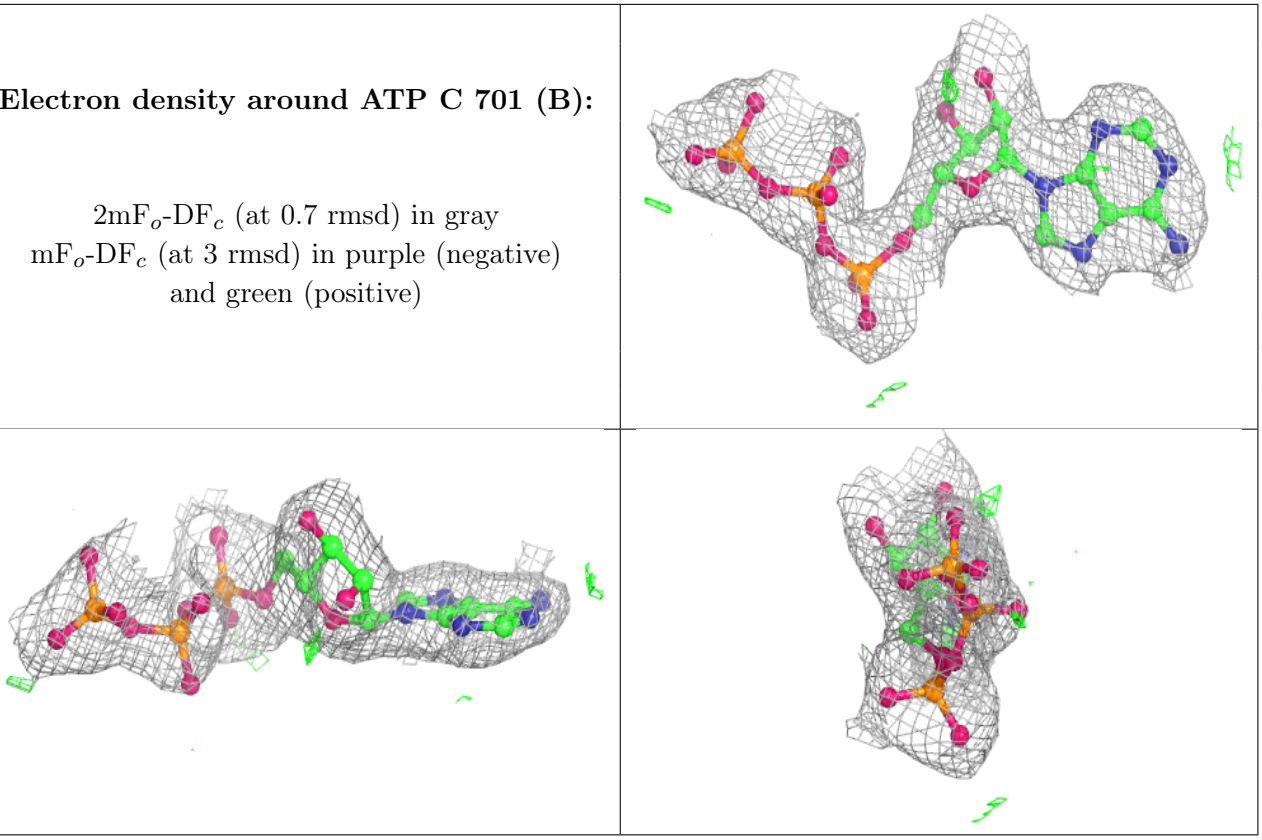
Electron density around 6R9 A 702 (A):

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



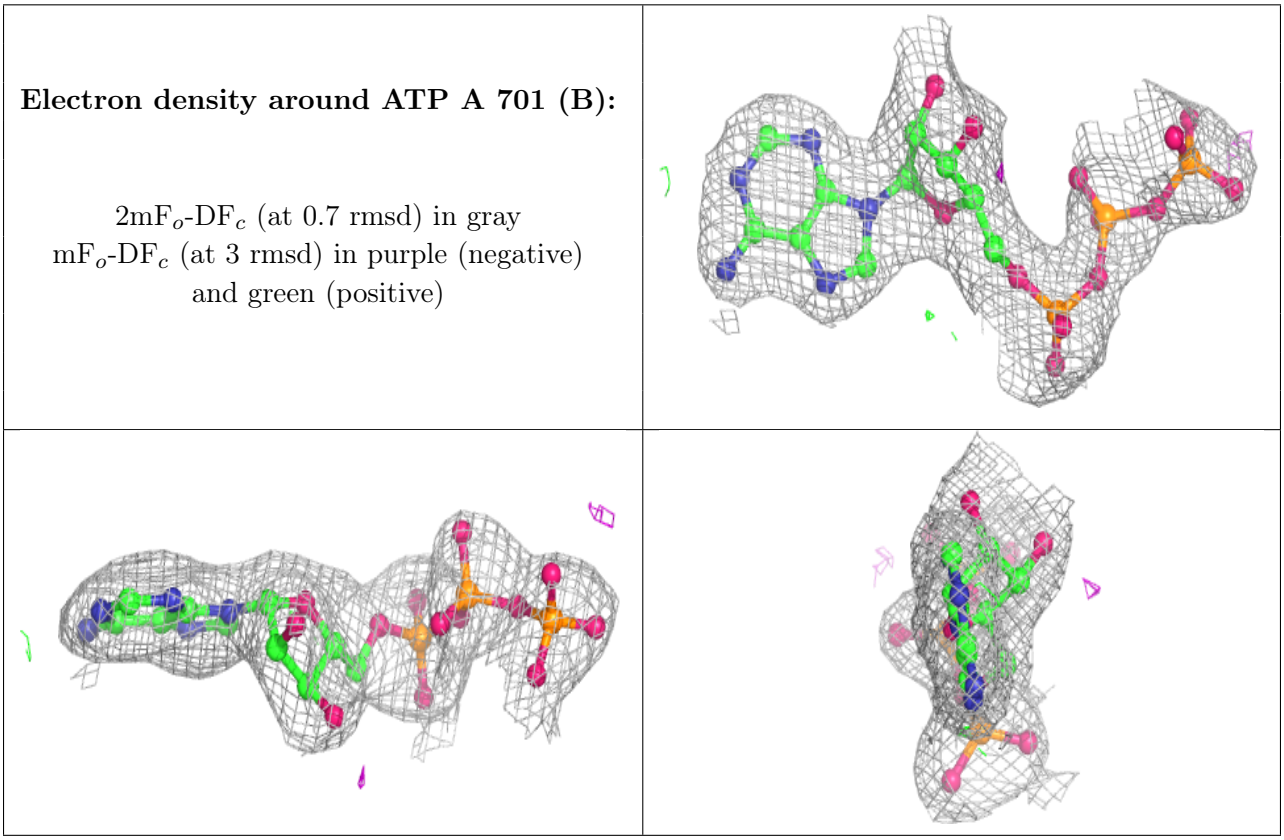
Electron density around ATP C 701 (B):

$2mF_o$-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.