



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:12 PM EDT

PDB ID : 3QX9 / pdb_00003qx9
Title : Crystal structure of MID domain from hAGO2 in complex with ATP
Authors : Frank, F.; Fabian, M.R.; Stepinski, J.; Jemielity, J.; Darzynkiewicz, E.; Sonnenberg, N.; Nagar, B.
Deposited on : 2011-03-01
Resolution : 2.00 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

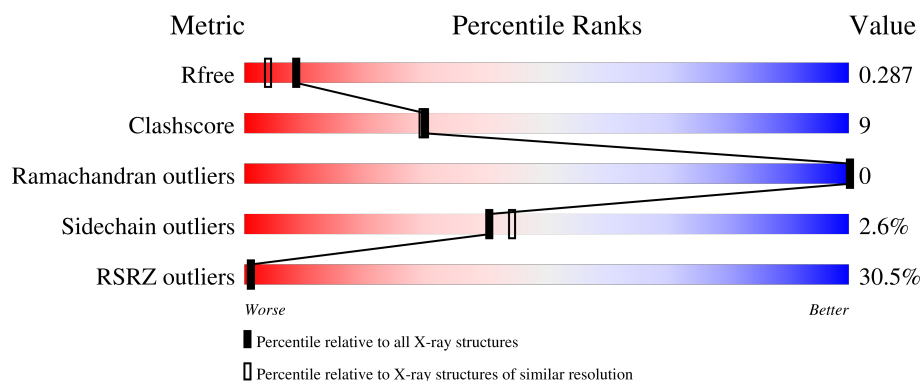
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	138	18% 80% 17% ..
1	B	138	53% 69% 24% ..
1	C	138	17% 80% 16% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3429 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.

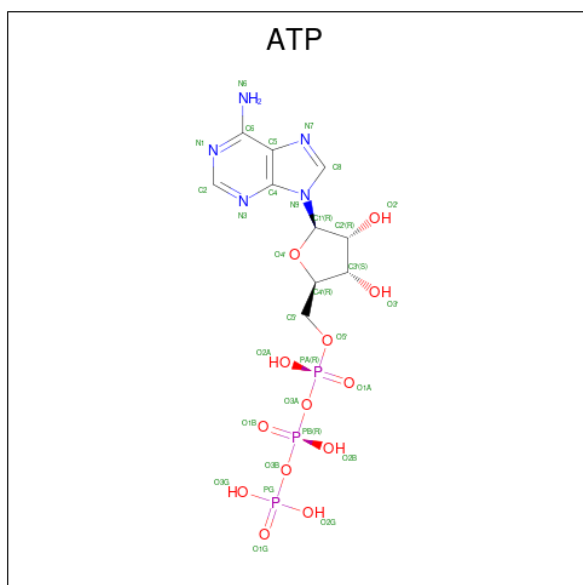
- Molecule 1 is a protein called Protein argonaute-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1047	666	187	184	10			
1	B	132	Total	C	N	O	S	0	0	0
			1027	653	183	181	10			
1	C	133	Total	C	N	O	S	0	0	0
			1036	659	185	182	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	SER	-	expression tag	UNP Q9UKV8
B	438	SER	-	expression tag	UNP Q9UKV8
C	438	SER	-	expression tag	UNP Q9UKV8

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

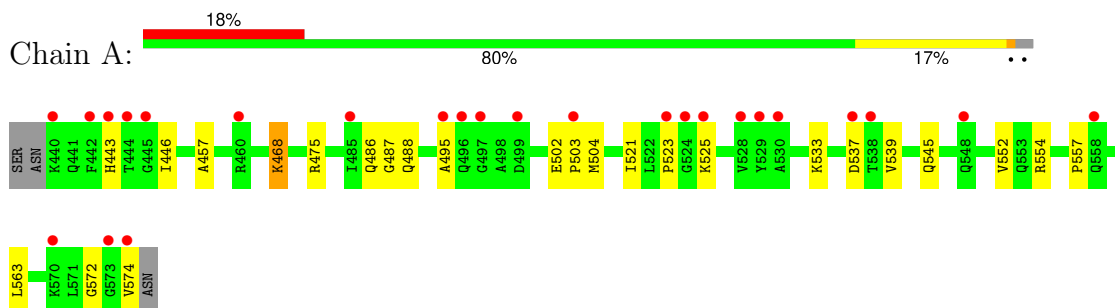
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	54	Total	O	0	0
			54	54		
3	C	70	Total	O	0	0
			70	70		

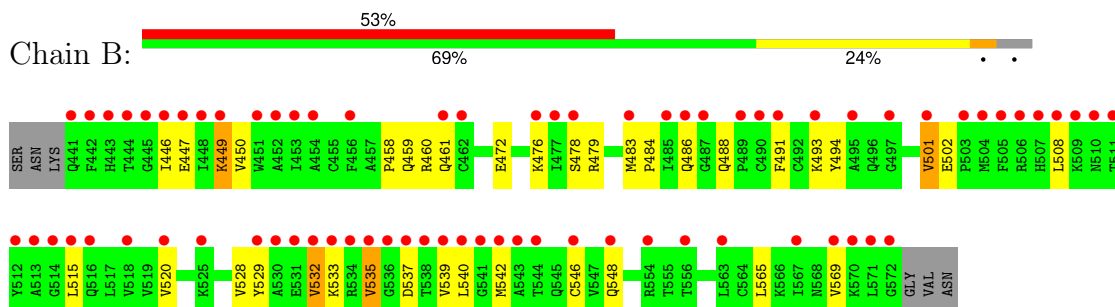
3 Residue-property plots [i](#)

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.

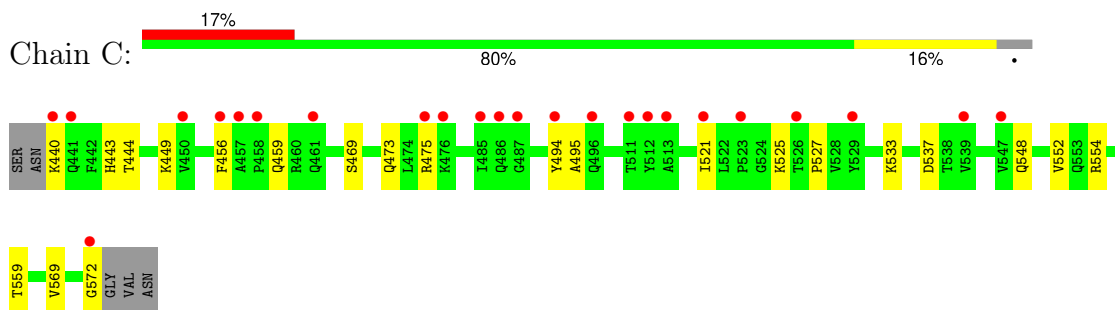
• Molecule 1: Protein argonaute-2



• Molecule 1: Protein argonaute-2



• Molecule 1: Protein argonaute-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.49Å 46.51Å 65.82Å 87.14° 73.56° 84.56°	Depositor
Resolution (Å)	28.70 – 2.00 28.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	84.8 (28.70-2.00) 56.7 (28.70-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 1.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.197 , 0.250 0.269 , 0.287	Depositor DCC
R_{free} test set	2776 reflections (5.92%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3429	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.93	2/1066 (0.2%)	1.07	1/1440 (0.1%)
1	B	1.08	3/1046 (0.3%)	1.18	5/1414 (0.4%)
1	C	0.98	2/1055 (0.2%)	1.07	1/1425 (0.1%)
All	All	1.00	7/3167 (0.2%)	1.11	7/4279 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	475	ARG	C-N	-6.34	1.25	1.33
1	B	449	LYS	C-N	6.05	1.40	1.33
1	A	488	GLN	C-N	5.59	1.40	1.33
1	B	461	GLN	C-N	5.33	1.40	1.33
1	B	447	GLU	C-N	5.26	1.41	1.33
1	A	486	GLN	C-N	-5.14	1.27	1.33
1	C	559	THR	CA-CB	5.08	1.61	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	501	VAL	N-CA-C	11.58	121.41	110.53
1	A	539	VAL	N-CA-C	7.86	118.32	111.56
1	B	458	PRO	CA-C-N	6.26	129.00	120.54
1	B	458	PRO	C-N-CA	6.26	129.00	120.54
1	B	535	VAL	N-CA-C	6.26	116.37	110.30
1	C	527	PRO	N-CA-C	-6.08	106.55	114.03
1	B	501	VAL	CB-CA-C	-5.23	105.16	112.02

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	1047	0	1089	15	0
1	B	1027	0	1064	29	0
1	C	1036	0	1077	12	0
2	A	31	0	12	1	0
2	B	31	0	12	5	0
2	C	31	0	12	2	0
3	A	102	0	0	0	0
3	B	54	0	0	1	0
3	C	70	0	0	0	0
All	All	3429	0	3266	55	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 9.

All (55) 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:B:548:GLN:HE22	2:B:1:ATP:H8	1.11	0.95
1:C:440:LYS:HE3	1:C:443:HIS:NE2	1.99	0.76
1:B:548:GLN:NE2	2:B:1:ATP:H8	1.86	0.74
1:B:548:GLN:HE21	2:B:1:ATP:H1'	1.54	0.71
1:B:548:GLN:NE2	2:B:1:ATP:C8	2.59	0.70
1:B:533:LYS:O	1:B:537:ASP:HB2	1.91	0.69
1:B:548:GLN:NE2	2:B:1:ATP:H1'	2.09	0.67
1:C:548:GLN:HE21	2:C:1:ATP:H1'	1.62	0.65
1:A:533:LYS:O	1:A:537:ASP:HB2	1.98	0.63
1:B:491:PHE:CD2	1:B:508:LEU:HD21	2.34	0.63
1:A:443:HIS:CE1	1:A:574:VAL:HB	2.36	0.61
1:A:521:ILE:HD13	1:A:552:VAL:HG21	1.84	0.60
1:B:446:ILE:O	1:B:484:PRO:HD2	2.02	0.60
1:B:450:VAL:HG12	1:B:515:LEU:HA	1.85	0.58
1:B:529:TYR:CE1	1:B:533:LYS:HD2	2.39	0.57
1:C:548:GLN:NE2	2:C:1:ATP:H1'	2.22	0.55
1:B:460:ARG:NH2	3:B:139:HOH:O	2.42	0.53
1:A:443:HIS:HE1	1:A:574:VAL:HB	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:GLN:HG2	1:B:488:GLN:H	1.72	0.53
1:B:502:GLU:HG3	1:B:535:VAL:HG22	1.89	0.52
1:B:478:SER:HB2	1:B:483:MET:O	2.10	0.51
1:A:502:GLU:N	1:A:503:PRO:CD	2.75	0.50
1:B:459:GLN:HG3	1:B:494:TYR:CZ	2.46	0.50
1:B:483:MET:O	1:B:483:MET:HG3	2.11	0.50
1:C:440:LYS:HE2	1:C:569:VAL:HA	1.94	0.49
1:B:565:LEU:O	1:B:569:VAL:HG23	2.12	0.49
1:C:533:LYS:O	1:C:537:ASP:HB2	2.11	0.49
1:B:539:VAL:HG12	1:B:540:LEU:CD1	2.42	0.49
1:B:459:GLN:HA	1:B:494:TYR:CE1	2.47	0.49
1:A:495:ALA:HB2	1:A:504:MET:CE	2.44	0.48
1:A:495:ALA:HB2	1:A:504:MET:HE3	1.96	0.47
1:A:457:ALA:HA	1:A:523:PRO:HG3	1.96	0.45
1:A:525:LYS:HA	2:A:1:ATP:C2	2.51	0.45
1:C:521:ILE:HD12	1:C:552:VAL:HG21	1.98	0.45
1:A:502:GLU:N	1:A:503:PRO:HD2	2.32	0.45
1:B:539:VAL:HG12	1:B:540:LEU:HD13	1.99	0.44
1:C:456:PHE:HA	1:C:495:ALA:O	2.17	0.44
1:A:475:ARG:HD3	1:A:487:GLY:HA3	1.99	0.44
1:B:476:LYS:HB3	1:B:476:LYS:HE2	1.88	0.44
1:C:443:HIS:CD2	1:C:572:GLY:HA3	2.53	0.43
1:C:459:GLN:HA	1:C:494:TYR:CE1	2.54	0.43
1:A:446:ILE:HD11	1:A:572:GLY:HA2	2.00	0.43
1:B:472:GLU:HG2	1:C:444:THR:HG23	1.99	0.43
1:B:449:LYS:HD2	1:B:486:GLN:OE1	2.19	0.43
1:A:533:LYS:HD3	1:A:533:LYS:HA	1.73	0.42
1:B:450:VAL:CG1	1:B:515:LEU:HA	2.50	0.42
1:B:540:LEU:HB3	1:B:542:MET:HG3	2.02	0.42
1:B:491:PHE:CZ	1:B:493:LYS:HG3	2.55	0.42
1:C:440:LYS:CE	1:C:443:HIS:NE2	2.77	0.41
1:C:469:SER:O	1:C:473:GLN:HG3	2.20	0.41
1:B:501:VAL:HG11	1:B:532:VAL:HA	2.02	0.41
1:A:545:GLN:CG	1:A:563:LEU:HD11	2.50	0.41
1:B:520:VAL:O	1:B:546:CYS:HA	2.21	0.41
1:A:468:LYS:HA	1:A:468:LYS:HD2	1.46	0.40
1:B:491:PHE:CG	1:B:508:LEU:HD21	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	133/138 (96%)	130 (98%)	3 (2%)	0	100	100
1	B	130/138 (94%)	124 (95%)	6 (5%)	0	100	100
1	C	131/138 (95%)	128 (98%)	3 (2%)	0	100	100
All	All	394/414 (95%)	382 (97%)	12 (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	116/119 (98%)	113 (97%)	3 (3%)	40	44
1	B	114/119 (96%)	111 (97%)	3 (3%)	40	44
1	C	115/119 (97%)	112 (97%)	3 (3%)	40	44
All	All	345/357 (97%)	336 (97%)	9 (3%)	40	44

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	LYS
1	A	554	ARG
1	A	557	PRO
1	B	479	ARG
1	B	528	VAL

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Mol	Chain	Res	Type
1	B	532	VAL
1	C	449	LYS
1	C	525	LYS
1	C	554	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	443	HIS
1	A	473	GLN
1	A	486	GLN
1	B	441	GLN
1	B	496	GLN
1	B	507	HIS
1	B	548	GLN
1	C	548	GLN
1	C	551	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](#)

3 ligands are modelled in this entry.

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	B	1	-	32,33,33	1.46	4 (12%)	48,52,52	1.70	7 (14%)
2	ATP	C	1	-	32,33,33	1.43	4 (12%)	48,52,52	1.79	8 (16%)
2	ATP	A	1	-	32,33,33	1.40	5 (15%)	48,52,52	1.71	8 (16%)

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	B	1	-	-	5/22/38/38	0/3/3/3
2	ATP	C	1	-	-	4/22/38/38	0/3/3/3
2	ATP	A	1	-	-	6/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	ATP	C5-C4	5.16	1.48	1.39
2	B	1	ATP	C5-C4	5.02	1.48	1.39
2	A	1	ATP	C5-C4	4.69	1.47	1.39
2	B	1	ATP	C5-C6	2.82	1.48	1.41
2	A	1	ATP	C5-C6	2.75	1.48	1.41
2	C	1	ATP	C5-C6	2.69	1.48	1.41
2	B	1	ATP	C5-N7	-2.49	1.34	1.39
2	A	1	ATP	C8-N7	2.34	1.36	1.31
2	C	1	ATP	C5-N7	-2.34	1.34	1.39
2	C	1	ATP	C8-N7	2.31	1.36	1.31
2	B	1	ATP	C8-N7	2.28	1.36	1.31
2	A	1	ATP	PB-O3B	2.23	1.61	1.59
2	A	1	ATP	C5-N7	-2.17	1.35	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	ATP	C5-C4-N3	-5.91	118.57	126.72
2	C	1	ATP	C5-C4-N3	-5.91	118.58	126.72
2	A	1	ATP	C5-C4-N3	-5.86	118.65	126.72
2	C	1	ATP	N3-C4-N9	5.00	135.66	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	ATP	N3-C4-N9	4.66	135.09	127.17
2	A	1	ATP	N3-C4-N9	4.46	134.75	127.17
2	C	1	ATP	C2-N3-C4	3.80	121.11	111.83
2	A	1	ATP	C4-C5-N7	-3.70	106.35	110.58
2	A	1	ATP	C2-N3-C4	3.61	120.66	111.83
2	B	1	ATP	C2-N3-C4	3.51	120.42	111.83
2	C	1	ATP	N3-C2-N1	-3.37	123.48	128.58
2	C	1	ATP	O4'-C1'-N9	3.34	114.50	108.09
2	A	1	ATP	N3-C2-N1	-3.04	123.97	128.58
2	B	1	ATP	C4-C5-N7	-3.03	107.11	110.58
2	B	1	ATP	N3-C2-N1	-2.93	124.15	128.58
2	B	1	ATP	O4'-C1'-N9	2.92	113.70	108.09
2	C	1	ATP	C4-C5-N7	-2.87	107.30	110.58
2	A	1	ATP	C5-N7-C8	2.68	107.66	103.45
2	C	1	ATP	C4-N9-C8	2.36	108.22	105.74
2	A	1	ATP	C4-N9-C8	2.34	108.20	105.74
2	A	1	ATP	C6-C5-N7	2.16	136.25	132.09
2	B	1	ATP	C5-N7-C8	2.13	106.80	103.45
2	C	1	ATP	C5-N7-C8	2.08	106.72	103.45

There are no chirality outliers.

All (15) torsion outliers are listed below:

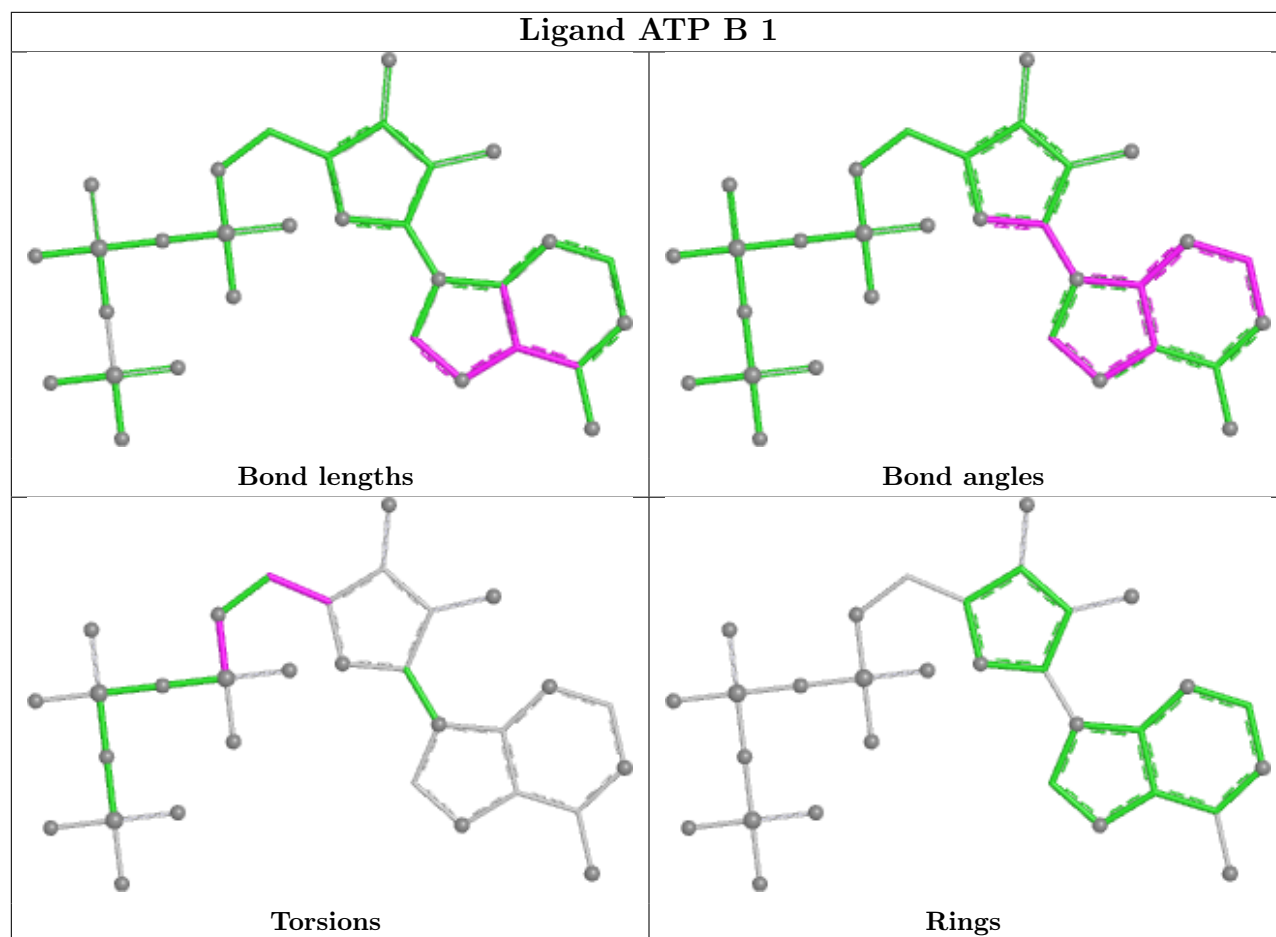
Mol	Chain	Res	Type	Atoms
2	A	1	ATP	C5'-O5'-PA-O1A
2	A	1	ATP	C5'-O5'-PA-O2A
2	A	1	ATP	C5'-O5'-PA-O3A
2	B	1	ATP	C5'-O5'-PA-O2A
2	C	1	ATP	C5'-O5'-PA-O3A
2	A	1	ATP	O4'-C4'-C5'-O5'
2	A	1	ATP	C3'-C4'-C5'-O5'
2	B	1	ATP	O4'-C4'-C5'-O5'
2	B	1	ATP	C3'-C4'-C5'-O5'
2	C	1	ATP	O4'-C4'-C5'-O5'
2	C	1	ATP	C3'-C4'-C5'-O5'
2	A	1	ATP	PA-O3A-PB-O1B
2	B	1	ATP	C5'-O5'-PA-O1A
2	B	1	ATP	C5'-O5'-PA-O3A
2	C	1	ATP	C5'-O5'-PA-O1A

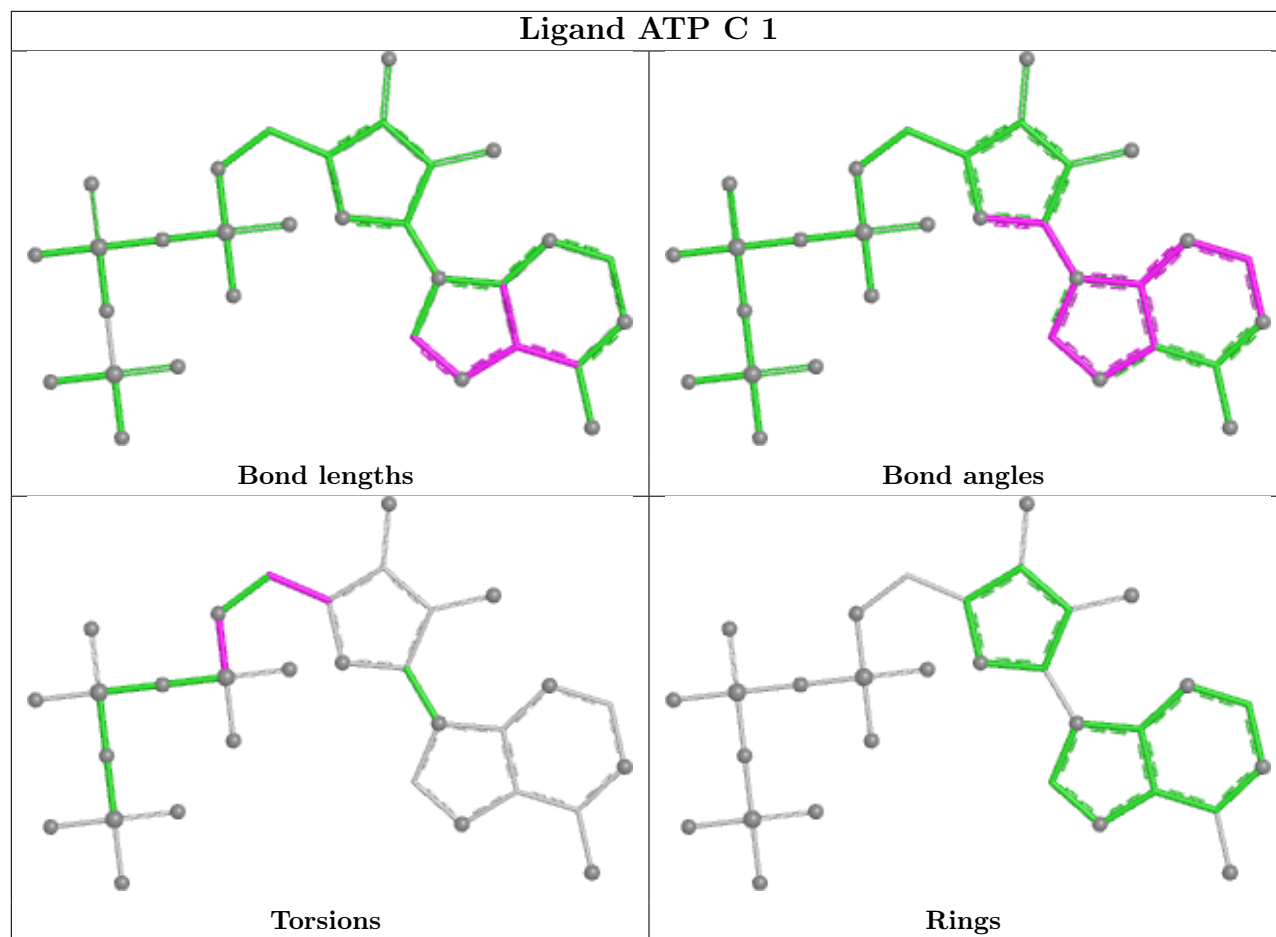
There are no ring outliers.

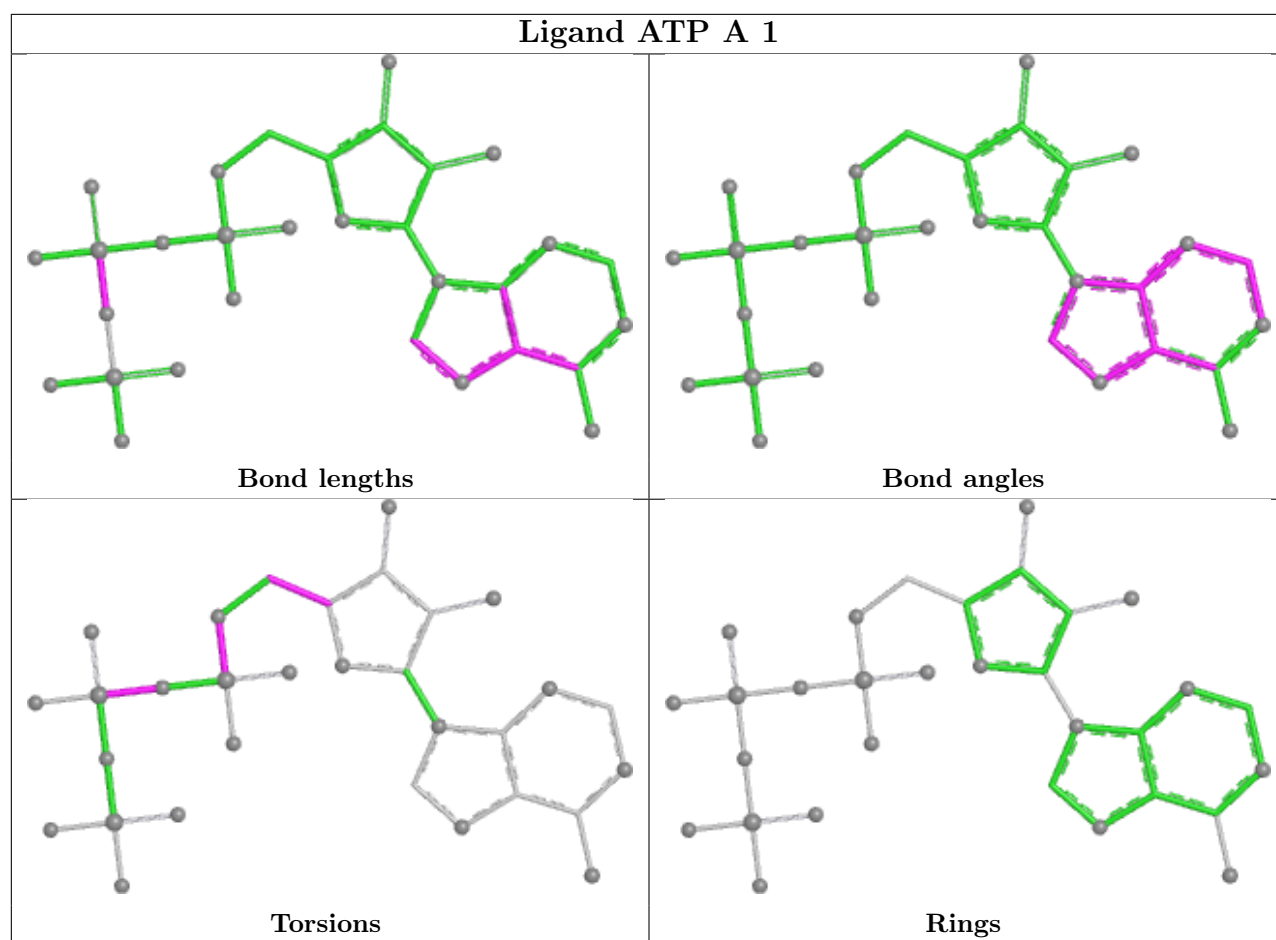
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	ATP	5	0
2	C	1	ATP	2	0
2	A	1	ATP	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	135/138 (97%)	1.29	25 (18%) 3 3	21, 30, 45, 76	0
1	B	132/138 (95%)	2.26	73 (55%) 0 0	25, 39, 58, 64	0
1	C	133/138 (96%)	1.40	24 (18%) 3 3	26, 34, 47, 61	0
All	All	400/414 (96%)	1.65	122 (30%) 1 1	21, 34, 55, 76	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	573	GLY	6.4
1	A	574	VAL	5.9
1	B	501	VAL	5.6
1	B	539	VAL	5.2
1	B	540	LEU	5.1
1	B	536	GLY	4.9
1	C	487	GLY	4.8
1	B	538	THR	4.5
1	B	505	PHE	4.4
1	B	491	PHE	4.4
1	B	452	ALA	4.1
1	C	496	GLN	4.1
1	A	444	THR	4.0
1	B	445	GLY	4.0
1	C	529	TYR	3.9
1	A	499	ASP	3.9
1	B	514	GLY	3.9
1	A	529	TYR	3.9
1	B	544	THR	3.8
1	B	530	ALA	3.8
1	B	512	TYR	3.7
1	B	542	MET	3.6
1	B	532	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	535	VAL	3.6
1	C	572	GLY	3.6
1	B	518	VAL	3.5
1	C	513	ALA	3.5
1	C	512	TYR	3.5
1	B	495	ALA	3.4
1	B	453	ILE	3.4
1	B	572	GLY	3.4
1	B	456	PHE	3.4
1	B	570	LYS	3.4
1	B	486	GLN	3.4
1	C	441	GLN	3.3
1	B	503	PRO	3.2
1	C	458	PRO	3.2
1	A	530	ALA	3.2
1	B	515	LEU	3.2
1	B	511	THR	3.2
1	A	445	GLY	3.2
1	B	569	VAL	3.2
1	B	543	ALA	3.2
1	C	456	PHE	3.1
1	B	449	LYS	3.0
1	B	504	MET	3.0
1	C	486	GLN	3.0
1	B	462	CYS	3.0
1	C	523	PRO	3.0
1	B	533	LYS	3.0
1	B	546	CYS	2.9
1	B	541	GLY	2.9
1	B	448	ILE	2.9
1	A	440	LYS	2.9
1	A	538	THR	2.9
1	C	450	VAL	2.8
1	B	485	ILE	2.8
1	C	485	ILE	2.8
1	B	537	ASP	2.8
1	B	513	ALA	2.8
1	B	529	TYR	2.8
1	B	563	LEU	2.8
1	A	525	LYS	2.8
1	C	526	THR	2.8
1	A	558	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	441	GLN	2.7
1	A	497	GLY	2.7
1	B	520	VAL	2.7
1	B	490	CYS	2.7
1	B	446	ILE	2.7
1	B	554	ARG	2.7
1	B	506	ARG	2.6
1	B	443	HIS	2.6
1	A	537	ASP	2.6
1	C	476	LYS	2.6
1	A	524	GLY	2.6
1	B	442	PHE	2.5
1	B	477	ILE	2.5
1	A	495	ALA	2.5
1	B	451	TRP	2.5
1	B	509	LYS	2.5
1	A	442	PHE	2.5
1	B	510	ASN	2.5
1	B	447	GLU	2.4
1	A	528	VAL	2.4
1	A	443	HIS	2.4
1	C	521	ILE	2.4
1	C	475	ARG	2.4
1	B	489	PRO	2.4
1	C	440	LYS	2.4
1	B	507	HIS	2.4
1	B	556	THR	2.4
1	C	539	VAL	2.3
1	C	494	TYR	2.3
1	B	454	ALA	2.3
1	B	508	LEU	2.3
1	B	567	ILE	2.3
1	B	478	SER	2.2
1	B	548	GLN	2.2
1	B	493	LYS	2.2
1	B	531	GLU	2.2
1	A	548	GLN	2.2
1	B	461	GLN	2.2
1	C	457	ALA	2.2
1	B	571	LEU	2.2
1	B	476	LYS	2.2
1	A	485	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	460	ARG	2.2
1	A	570	LYS	2.2
1	B	483	MET	2.2
1	A	496	GLN	2.1
1	C	547	VAL	2.1
1	A	523	PRO	2.1
1	B	516	GLN	2.1
1	B	534	ARG	2.1
1	B	525	LYS	2.1
1	A	503	PRO	2.0
1	B	487	GLY	2.0
1	C	461	GLN	2.0
1	B	444	THR	2.0
1	C	511	THR	2.0
1	B	497	GLY	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](#)

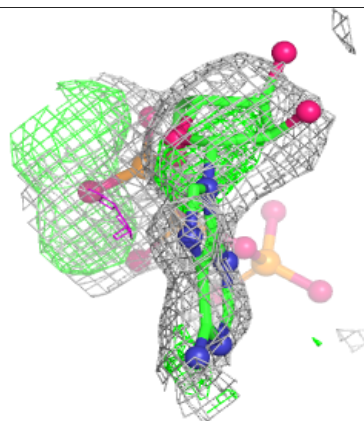
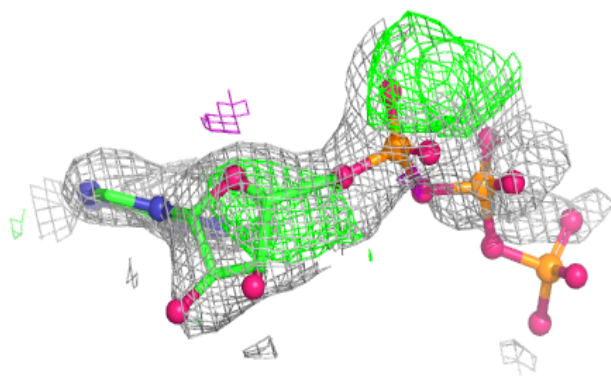
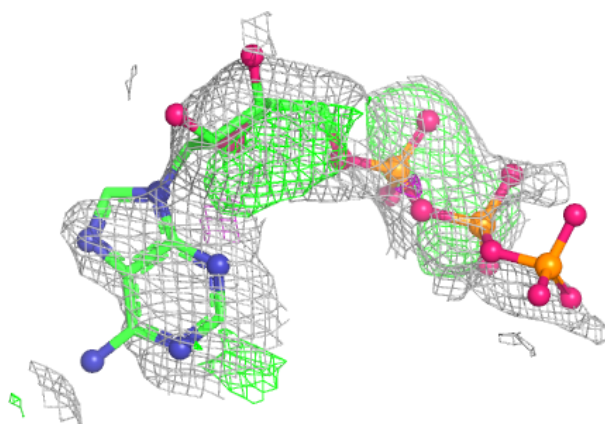
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	1	31/31	0.55	0.30	56,60,65,77	20
2	ATP	B	1	31/31	0.64	0.33	52,60,66,77	15
2	ATP	A	1	31/31	0.71	0.22	39,45,55,64	16

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.

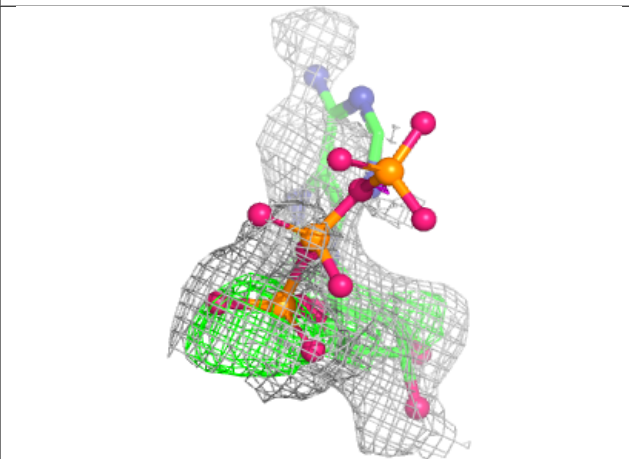
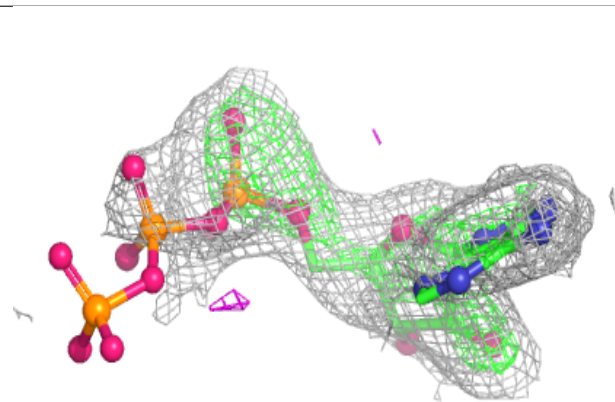
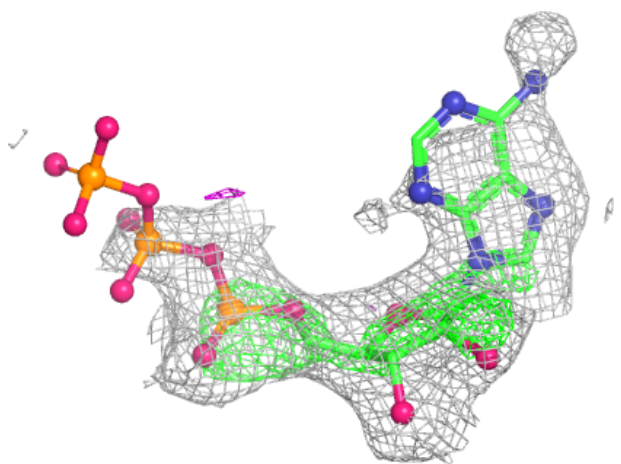
Electron density around ATP C 1:

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



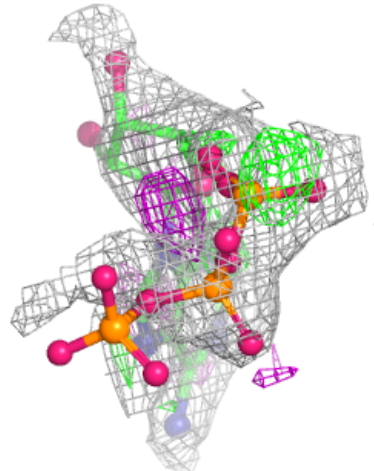
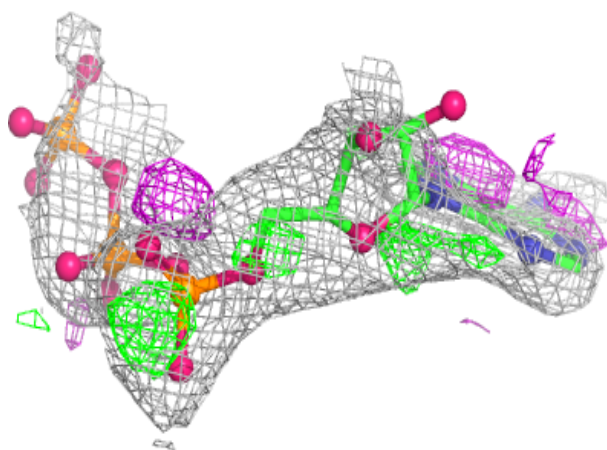
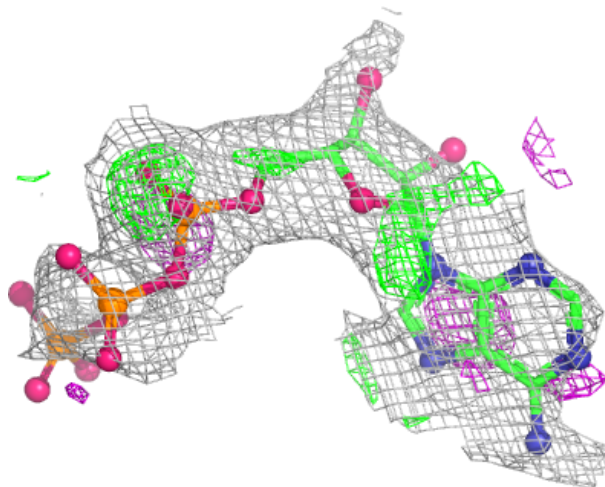
Electron density around ATP B 1:

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



Electron density around ATP A 1:

$2mF_o-DF_c$ (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.