



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:27 PM UTC

PDB ID : 2IXF / pdb_00002ixf
Title : Crystal structure of the ATPase domain of TAP1 with ATP (D645Q, Q678H mutant)
Authors : Procko, E.; Ferrin-O'Connell, I.; Ng, S.-L.; Gaudet, R.
Deposited on : 2006-07-08
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

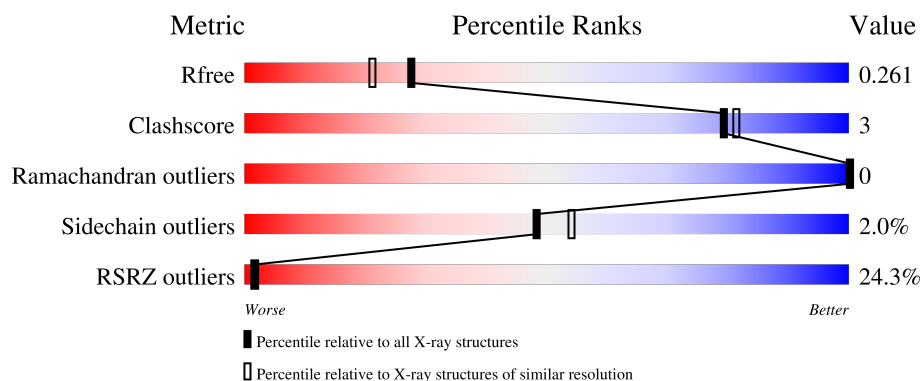
1 Overall quality at a glance

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	271	21% 86% 7% 6%
1	B	271	20% 87% 7% 6%
1	C	271	27% 86% 7% 7%
1	D	271	23% 86% 6% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8862 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 ANTIGEN PEPTIDE TRANSPORTER 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	3	0
			1933	1219	347	359	8			
1	B	255	Total	C	N	O	S	0	4	0
			1942	1227	345	362	8			
1	C	252	Total	C	N	O	S	0	5	0
			1931	1221	342	361	7			
1	D	250	Total	C	N	O	S	0	6	0
			1930	1220	346	357	7			

There are 48 discrepancies between the modelled and reference sequences:

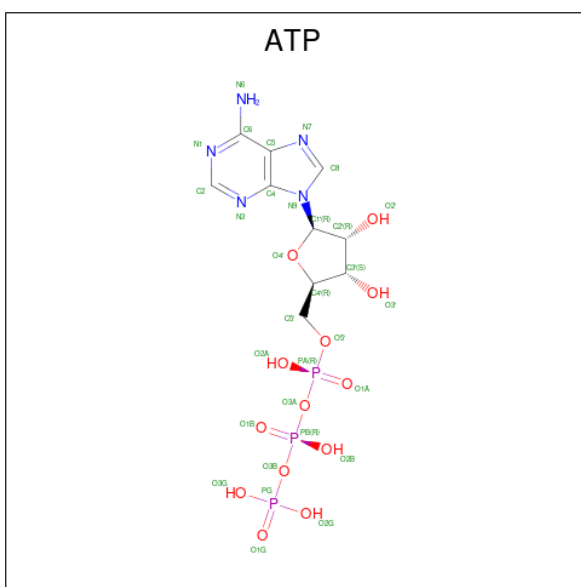
Chain	Residue	Modelled	Actual	Comment	Reference
A	464	MET	-	expression tag	UNP P36370
A	726	ALA	-	expression tag	UNP P36370
A	727	ALA	-	expression tag	UNP P36370
A	728	ALA	-	expression tag	UNP P36370
A	729	HIS	-	expression tag	UNP P36370
A	730	HIS	-	expression tag	UNP P36370
A	731	HIS	-	expression tag	UNP P36370
A	732	HIS	-	expression tag	UNP P36370
A	733	HIS	-	expression tag	UNP P36370
A	734	HIS	-	expression tag	UNP P36370
A	645	GLN	ASP	engineered mutation	UNP P36370
A	678	HIS	GLN	engineered mutation	UNP P36370
B	464	MET	-	expression tag	UNP P36370
B	726	ALA	-	expression tag	UNP P36370
B	727	ALA	-	expression tag	UNP P36370
B	728	ALA	-	expression tag	UNP P36370
B	729	HIS	-	expression tag	UNP P36370
B	730	HIS	-	expression tag	UNP P36370
B	731	HIS	-	expression tag	UNP P36370
B	732	HIS	-	expression tag	UNP P36370
B	733	HIS	-	expression tag	UNP P36370

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Chain	Residue	Modelled	Actual	Comment	Reference
B	734	HIS	-	expression tag	UNP P36370
B	645	GLN	ASP	engineered mutation	UNP P36370
B	678	HIS	GLN	engineered mutation	UNP P36370
C	464	MET	-	expression tag	UNP P36370
C	726	ALA	-	expression tag	UNP P36370
C	727	ALA	-	expression tag	UNP P36370
C	728	ALA	-	expression tag	UNP P36370
C	729	HIS	-	expression tag	UNP P36370
C	730	HIS	-	expression tag	UNP P36370
C	731	HIS	-	expression tag	UNP P36370
C	732	HIS	-	expression tag	UNP P36370
C	733	HIS	-	expression tag	UNP P36370
C	734	HIS	-	expression tag	UNP P36370
C	645	GLN	ASP	engineered mutation	UNP P36370
C	678	HIS	GLN	engineered mutation	UNP P36370
D	464	MET	-	expression tag	UNP P36370
D	726	ALA	-	expression tag	UNP P36370
D	727	ALA	-	expression tag	UNP P36370
D	728	ALA	-	expression tag	UNP P36370
D	729	HIS	-	expression tag	UNP P36370
D	730	HIS	-	expression tag	UNP P36370
D	731	HIS	-	expression tag	UNP P36370
D	732	HIS	-	expression tag	UNP P36370
D	733	HIS	-	expression tag	UNP P36370
D	734	HIS	-	expression tag	UNP P36370
D	645	GLN	ASP	engineered mutation	UNP P36370
D	678	HIS	GLN	engineered mutation	UNP P36370

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

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

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

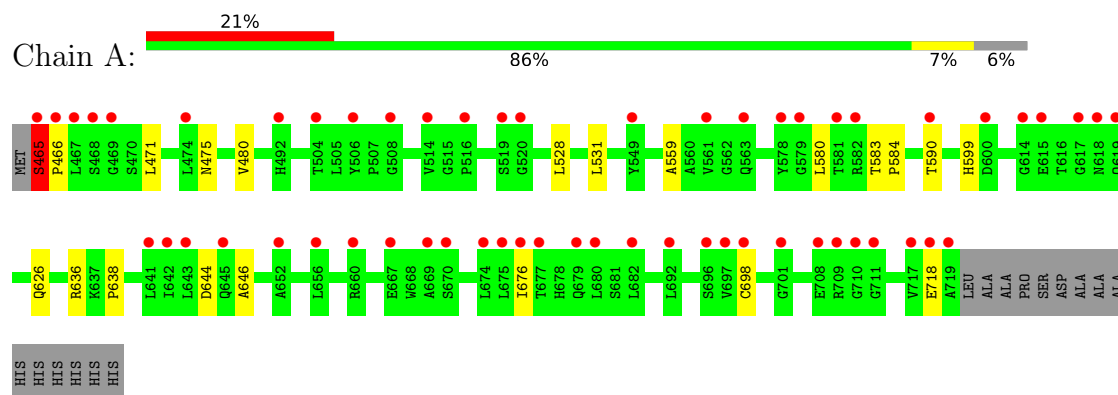
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	251	Total	O	0	0
			251	251		
5	B	262	Total	O	0	0
			262	262		
5	C	254	Total	O	0	0
			254	254		
5	D	201	Total	O	0	0
			201	201		

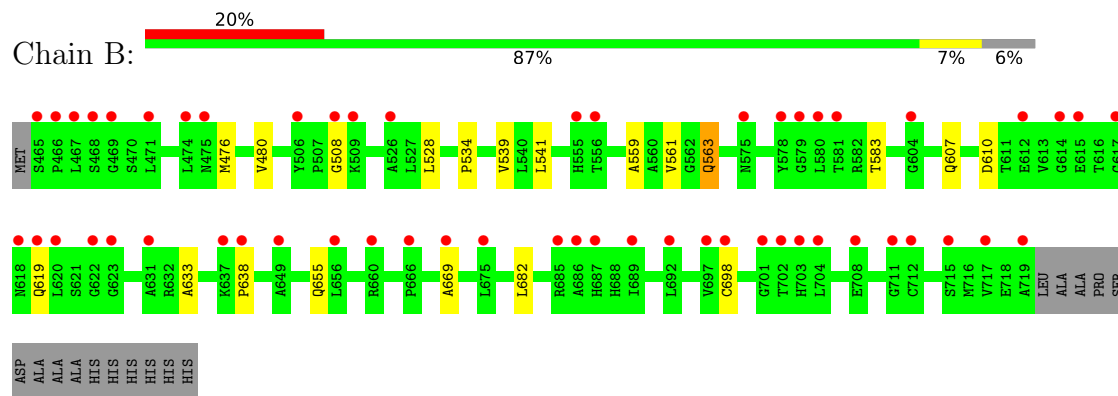
3 Residue-property plots

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.

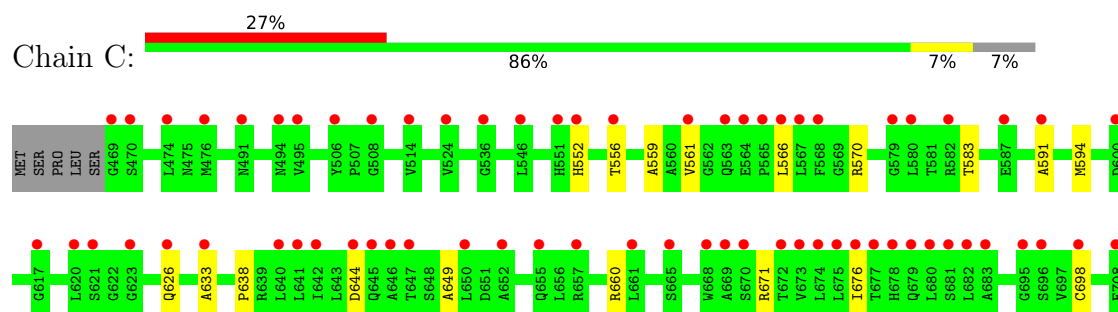
• Molecule 1: ANTIGEN PEPTIDE TRANSPORTER 1

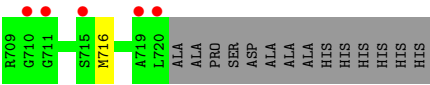


• Molecule 1: ANTIGEN PEPTIDE TRANSPORTER 1

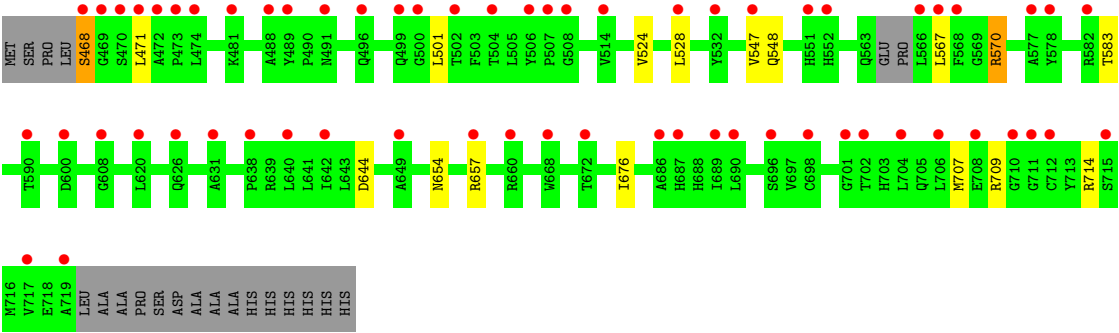
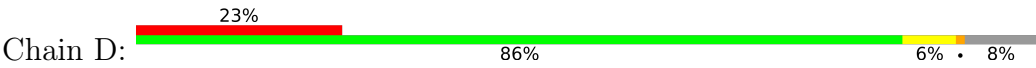


• Molecule 1: ANTIGEN PEPTIDE TRANSPORTER 1





● Molecule 1: ANTIGEN PEPTIDE TRANSPORTER 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.27Å 108.92Å 123.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.49 – 2.00 38.49 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.49-2.00) 98.9 (38.49-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.216 , 0.258 0.218 , 0.261	Depositor DCC
R_{free} test set	3776 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8862	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7772e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, ATP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/1981	0.68	1/2691 (0.0%)
1	B	0.48	0/1991	0.65	0/2706
1	C	0.48	0/1982	0.67	0/2693
1	D	0.46	0/1976	0.67	0/2681
All	All	0.47	0/7930	0.67	1/10771 (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	A	465	SER	N-CA-C	5.67	126.88	111.00

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	1933	0	1912	12	0
1	B	1942	0	1923	10	0
1	C	1931	0	1910	11	0
1	D	1930	0	1915	9	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	12	0	0
2	D	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	2	0
4	B	12	0	16	1	0
4	C	6	0	8	1	0
4	D	6	0	8	1	0
5	A	251	0	0	1	0
5	B	262	0	0	1	0
5	C	254	0	0	2	0
5	D	201	0	0	0	0
All	All	8862	0	7748	42	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 (42) 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:476[B]:MET:HE3	1:B:541:LEU:HD11	1.55	0.89
1:C:698:CYS:SG	5:C:2250:HOH:O	2.45	0.74
1:A:583:THR:HG23	4:A:3:GOL:H31	1.72	0.71
1:B:698:CYS:SG	5:B:2236:HOH:O	2.27	0.70
1:A:698:CYS:SG	5:A:2250:HOH:O	2.54	0.66
1:D:524:VAL:O	1:D:528:LEU:HD13	1.97	0.64
1:C:591:ALA:HA	1:C:594:MET:HE3	1.83	0.59
1:D:468:SER:HB2	1:D:547[B]:VAL:HG12	1.84	0.58
1:A:580:LEU:HD11	1:A:636:ARG:HG3	1.87	0.57
1:C:716:MET:SD	5:C:2052:HOH:O	2.58	0.56
1:A:583:THR:HG23	4:A:3:GOL:C3	2.34	0.56
1:B:559:ALA:HB3	1:B:638:PRO:HG3	1.89	0.53
1:B:563:GLN:HE21	1:B:563:GLN:N	2.06	0.52
1:A:559:ALA:HB3	1:A:638:PRO:HG3	1.94	0.50
1:C:626:GLN:CD	1:C:649:ALA:HB3	2.37	0.50
1:D:583:THR:HG23	4:D:3:GOL:O2	2.12	0.50
1:B:508:GLY:HA2	1:B:669:ALA:O	2.13	0.48
1:D:471:LEU:HD22	1:D:548:GLN:HB3	1.95	0.48
1:D:567:LEU:HB3	1:D:570:ARG:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:HIS:O	1:C:556:THR:HG23	2.16	0.46
1:C:638:PRO:O	1:C:671:ARG:HD3	2.15	0.46
1:D:644:ASP:HA	1:D:676:ILE:HB	1.98	0.46
1:B:583:THR:HG23	4:B:3:GOL:O2	2.16	0.45
1:A:590:THR:HG23	1:A:599:HIS:CE1	2.51	0.45
1:B:480:VAL:HG11	1:B:528:LEU:HD21	1.99	0.44
1:D:707:MET:HE3	1:D:714:ARG:HH11	1.82	0.44
1:A:626:GLN:CG	1:A:646:ALA:O	2.66	0.44
1:B:561:VAL:HG22	1:B:633:ALA:HB2	2.00	0.44
1:C:626:GLN:OE1	1:C:649:ALA:HB3	2.18	0.44
1:A:465:SER:N	1:A:466:PRO:HD3	2.33	0.43
1:C:583:THR:HG23	4:C:3:GOL:O2	2.18	0.43
1:C:559:ALA:HB3	1:C:638:PRO:HG3	1.99	0.43
1:B:655:GLN:NE2	1:B:682:LEU:HD11	2.33	0.43
1:A:480:VAL:HG11	1:A:528:LEU:HD21	2.00	0.43
1:D:468:SER:HB2	1:D:547[A]:VAL:HG22	2.00	0.43
1:C:561:VAL:HG22	1:C:633:ALA:HB2	2.01	0.42
1:B:534:PRO:HG3	1:B:539:VAL:HG23	2.02	0.41
1:C:644:ASP:HA	1:C:676:ILE:HB	2.03	0.41
1:A:644:ASP:HA	1:A:676:ILE:HB	2.03	0.41
1:D:654:ASN:OD1	1:D:657:ARG:NH1	2.54	0.40
1:A:580:LEU:CD1	1:A:636:ARG:HG3	2.49	0.40
1:A:580:LEU:HD23	1:A:584:PRO:HG3	2.03	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	256/271 (94%)	254 (99%)	2 (1%)	0	100	100
1	B	257/271 (95%)	256 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	255/271 (94%)	254 (100%)	1 (0%)	0	100	100
1	D	252/271 (93%)	251 (100%)	1 (0%)	0	100	100
All	All	1020/1084 (94%)	1015 (100%)	5 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/219 (92%)	196 (98%)	5 (2%)	42	45
1	B	204/219 (93%)	200 (98%)	4 (2%)	48	54
1	C	202/219 (92%)	199 (98%)	3 (2%)	57	64
1	D	201/219 (92%)	196 (98%)	5 (2%)	42	45
All	All	808/876 (92%)	791 (98%)	17 (2%)	48	52

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	SER
1	A	471	LEU
1	A	475	ASN
1	A	531	LEU
1	A	718	GLU
1	B	563	GLN
1	B	607	GLN
1	B	610	ASP
1	B	619	GLN
1	C	566	LEU
1	C	570	ARG
1	C	660	ARG
1	D	468	SER
1	D	501	LEU

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Mol	Chain	Res	Type
1	D	570	ARG
1	D	709[A]	ARG
1	D	709[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	483	GLN
1	A	492	HIS
1	A	607	GLN
1	A	700	GLN
1	B	552	HIS
1	B	555	HIS
1	B	563	GLN
1	B	607	GLN
1	B	645	GLN
1	B	655	GLN
1	C	483	GLN
1	C	529	GLN
1	C	533	GLN
1	C	555	HIS
1	C	557	GLN
1	C	645	GLN
1	D	492	HIS
1	D	533	GLN
1	D	557	GLN
1	D	619	GLN
1	D	645	GLN
1	D	659	GLN
1	D	700	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	B	1	3	32,33,33	1.40	7 (21%)	48,52,52	1.78	12 (25%)
4	GOL	B	4	-	5,5,5	0.36	0	5,5,5	0.42	0
2	ATP	A	1	3	32,33,33	1.41	7 (21%)	48,52,52	1.86	12 (25%)
4	GOL	C	3	-	5,5,5	0.37	0	5,5,5	0.41	0
2	ATP	C	1	3	32,33,33	1.55	6 (18%)	48,52,52	1.82	11 (22%)
4	GOL	D	3	-	5,5,5	0.39	0	5,5,5	0.26	0
2	ATP	D	1	3	32,33,33	1.44	6 (18%)	48,52,52	1.80	10 (20%)
4	GOL	B	3	-	5,5,5	0.38	0	5,5,5	0.16	0
4	GOL	A	3	-	5,5,5	0.40	0	5,5,5	0.34	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
2	ATP	B	1	3	-	2/22/38/38	0/3/3/3
4	GOL	B	4	-	-	3/4/4/4	-
2	ATP	A	1	3	-	2/22/38/38	0/3/3/3
4	GOL	C	3	-	-	2/4/4/4	-
2	ATP	C	1	3	-	2/22/38/38	0/3/3/3
4	GOL	D	3	-	-	0/4/4/4	-
2	ATP	D	1	3	-	2/22/38/38	0/3/3/3
4	GOL	B	3	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	3	-	-	1/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	ATP	C5-C4	4.49	1.47	1.39
2	C	1	ATP	PB-O3B	4.34	1.64	1.59
2	C	1	ATP	C5-C4	4.20	1.46	1.39
2	A	1	ATP	C5-C4	4.17	1.46	1.39
2	B	1	ATP	C5-C4	4.01	1.46	1.39
2	D	1	ATP	PB-O3B	3.10	1.62	1.59
2	B	1	ATP	PB-O3B	3.00	1.62	1.59
2	C	1	ATP	PA-O3A	2.92	1.62	1.59
2	A	1	ATP	PA-O3A	2.58	1.62	1.59
2	C	1	ATP	C5-N7	-2.53	1.34	1.39
2	D	1	ATP	C5-N7	-2.52	1.34	1.39
2	D	1	ATP	C5-C6	2.48	1.47	1.41
2	A	1	ATP	C5-N7	-2.45	1.34	1.39
2	C	1	ATP	C4-N9	-2.42	1.32	1.37
2	B	1	ATP	C5-C6	2.35	1.47	1.41
2	A	1	ATP	C5-C6	2.31	1.47	1.41
2	B	1	ATP	C5-N7	-2.30	1.34	1.39
2	A	1	ATP	PB-O3A	2.29	1.62	1.59
2	B	1	ATP	C4-N9	-2.26	1.33	1.37
2	A	1	ATP	PB-O3B	2.26	1.61	1.59
2	A	1	ATP	C4-N9	-2.14	1.33	1.37
2	B	1	ATP	PA-O3A	2.13	1.61	1.59
2	C	1	ATP	C5-C6	2.12	1.46	1.41
2	B	1	ATP	PB-O3A	2.03	1.61	1.59
2	D	1	ATP	C4-N9	-2.01	1.33	1.37
2	D	1	ATP	C8-N7	2.01	1.35	1.31

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	ATP	C5-C4-N3	-5.59	119.03	126.72
2	A	1	ATP	C5-C4-N3	-5.28	119.44	126.72
2	C	1	ATP	C5-C4-N3	-5.19	119.57	126.72
2	B	1	ATP	C5-C4-N3	-5.03	119.79	126.72
2	D	1	ATP	N3-C4-N9	4.63	135.05	127.17
2	C	1	ATP	N3-C4-N9	4.59	134.97	127.17
2	A	1	ATP	N3-C4-N9	4.58	134.95	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	ATP	N3-C4-N9	4.37	134.59	127.17
2	C	1	ATP	N3-C2-N1	-4.20	122.23	128.58
2	A	1	ATP	N3-C2-N1	-4.08	122.40	128.58
2	B	1	ATP	N3-C2-N1	-4.02	122.50	128.58
2	D	1	ATP	N3-C2-N1	-3.94	122.61	128.58
2	D	1	ATP	C2-N3-C4	3.92	121.41	111.83
2	C	1	ATP	C2-N3-C4	3.84	121.21	111.83
2	A	1	ATP	C2-N3-C4	3.72	120.92	111.83
2	B	1	ATP	C2-N3-C4	3.70	120.87	111.83
2	C	1	ATP	C4-N9-C8	3.51	109.42	105.74
2	A	1	ATP	C4-N9-C8	3.46	109.38	105.74
2	B	1	ATP	C4-N9-C8	3.43	109.34	105.74
2	D	1	ATP	C4-C5-N7	-3.30	106.81	110.58
2	A	1	ATP	C4-C5-N7	-3.24	106.87	110.58
2	D	1	ATP	C4-N9-C8	3.00	108.88	105.74
2	B	1	ATP	C4-C5-N7	-2.92	107.24	110.58
2	A	1	ATP	C5-N7-C8	2.73	107.75	103.45
2	D	1	ATP	C5-N7-C8	2.72	107.73	103.45
2	C	1	ATP	C4-C5-N7	-2.62	107.58	110.58
2	C	1	ATP	N9-C8-N7	-2.56	110.30	113.94
2	A	1	ATP	O2A-PA-O3A	2.56	114.19	107.27
2	A	1	ATP	N9-C8-N7	-2.49	110.40	113.94
2	B	1	ATP	C5-N7-C8	2.46	107.31	103.45
2	B	1	ATP	N9-C8-N7	-2.43	110.48	113.94
2	C	1	ATP	C5-N7-C8	2.40	107.23	103.45
2	D	1	ATP	N9-C8-N7	-2.33	110.64	113.94
2	B	1	ATP	O2A-PA-O3A	2.32	113.55	107.27
2	A	1	ATP	C2-N1-C6	2.31	122.52	118.73
2	B	1	ATP	C6-C5-N7	2.31	136.54	132.09
2	D	1	ATP	C6-C5-N7	2.20	136.34	132.09
2	B	1	ATP	C2-N1-C6	2.19	122.33	118.73
2	B	1	ATP	O2B-PB-O3B	2.17	113.15	107.27
2	A	1	ATP	C6-C5-N7	2.15	136.23	132.09
2	C	1	ATP	C2-N1-C6	2.13	122.23	118.73
2	C	1	ATP	C6-C5-N7	2.11	136.16	132.09
2	D	1	ATP	O2B-PB-O3A	2.05	112.82	107.27
2	C	1	ATP	O2B-PB-O3B	2.05	112.81	107.27
2	A	1	ATP	O3A-PB-O1B	-2.00	104.67	110.70

There are no chirality outliers.

All (18) torsion outliers are listed below:

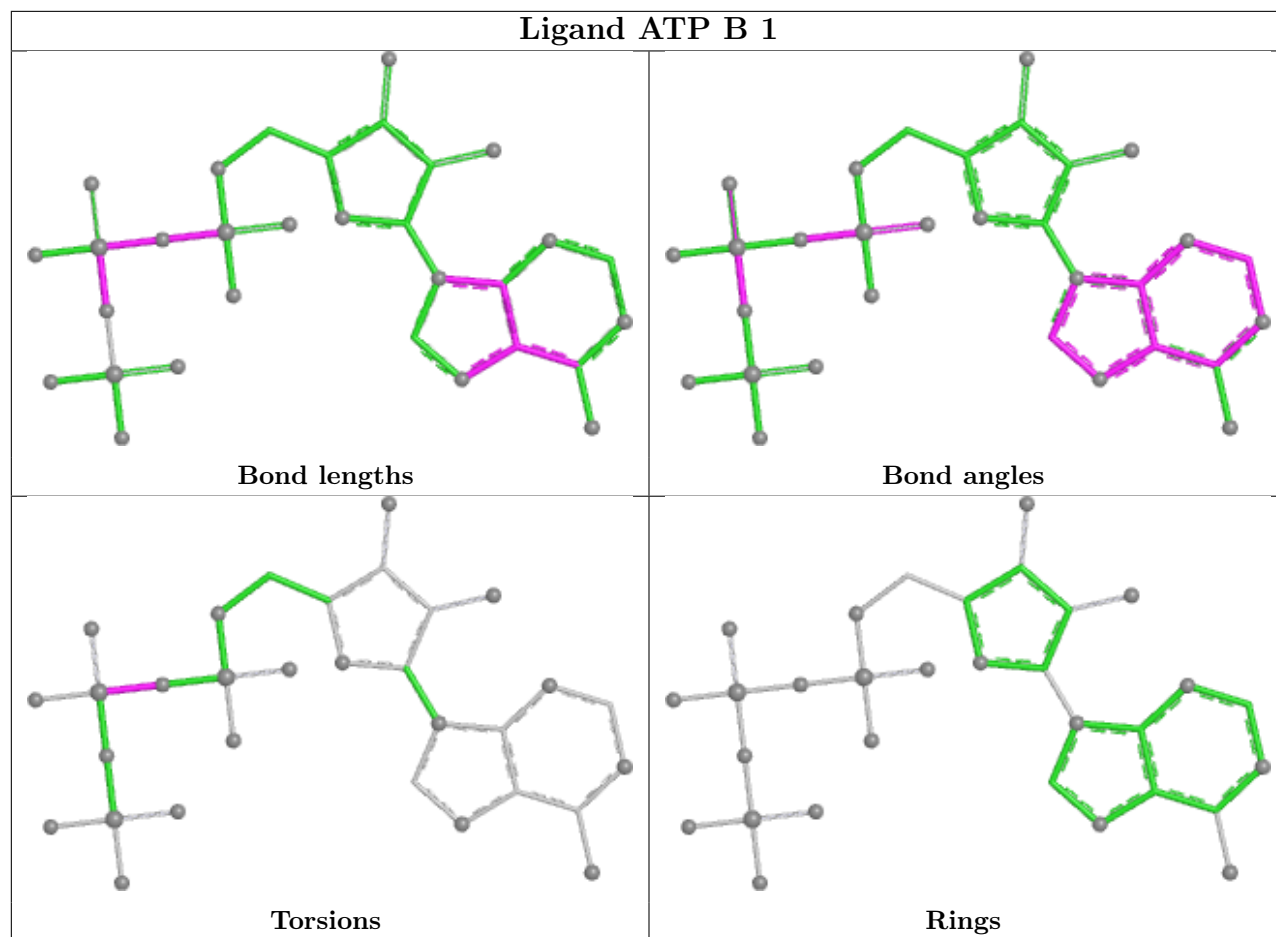
Mol	Chain	Res	Type	Atoms
4	B	3	GOL	C1-C2-C3-O3
4	B	3	GOL	O1-C1-C2-O2
4	B	3	GOL	O1-C1-C2-C3
4	B	4	GOL	C1-C2-C3-O3
4	C	3	GOL	C1-C2-C3-O3
4	B	3	GOL	O2-C2-C3-O3
4	A	3	GOL	C1-C2-C3-O3
2	B	1	ATP	PA-O3A-PB-O2B
2	C	1	ATP	PA-O3A-PB-O2B
2	D	1	ATP	PA-O3A-PB-O2B
4	C	3	GOL	O2-C2-C3-O3
2	A	1	ATP	PA-O3A-PB-O2B
4	B	4	GOL	O1-C1-C2-O2
4	B	4	GOL	O2-C2-C3-O3
2	A	1	ATP	PA-O3A-PB-O1B
2	B	1	ATP	PA-O3A-PB-O1B
2	C	1	ATP	PA-O3A-PB-O1B
2	D	1	ATP	PA-O3A-PB-O1B

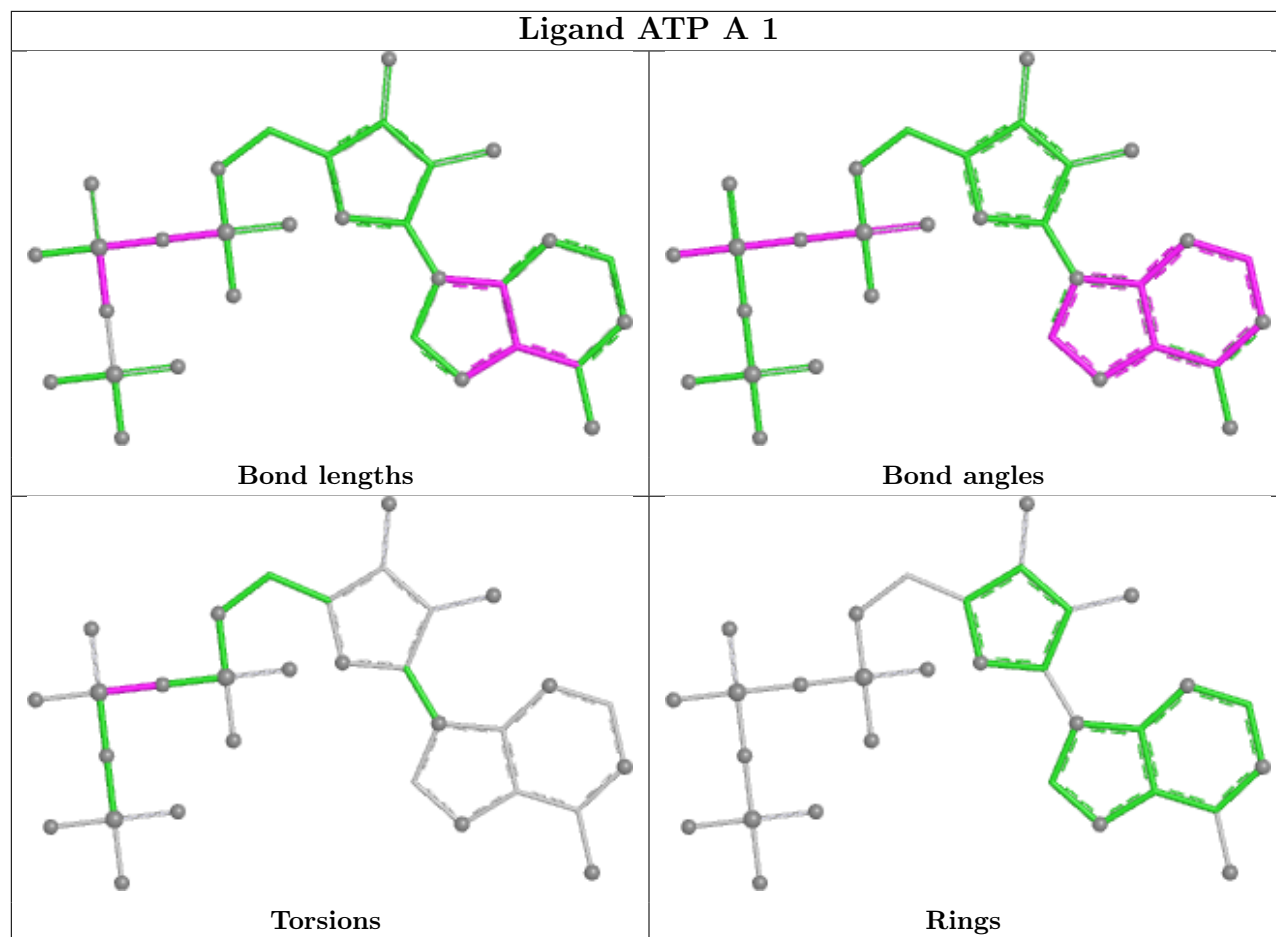
There are no ring outliers.

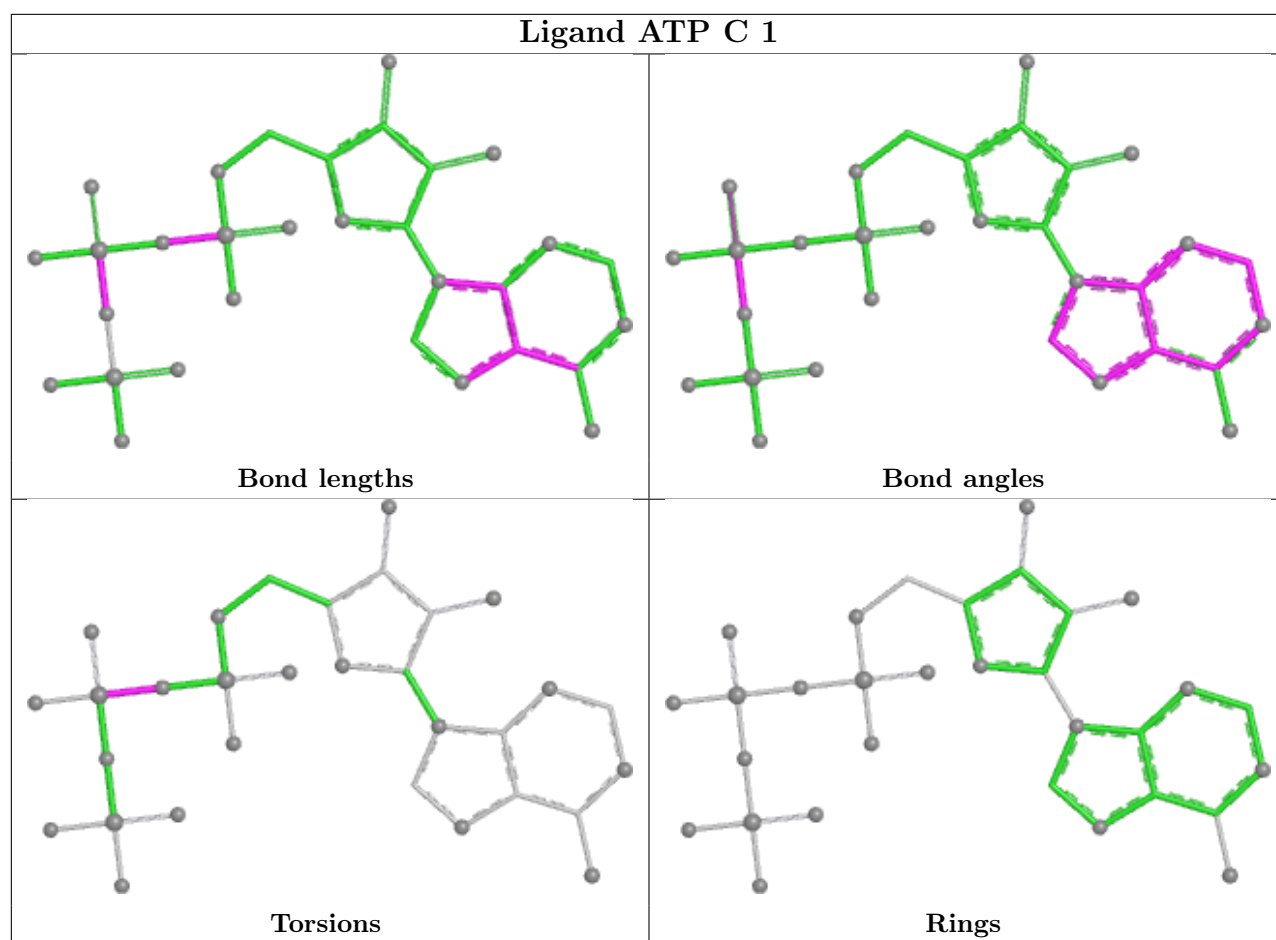
4 monomers are involved in 5 short contacts:

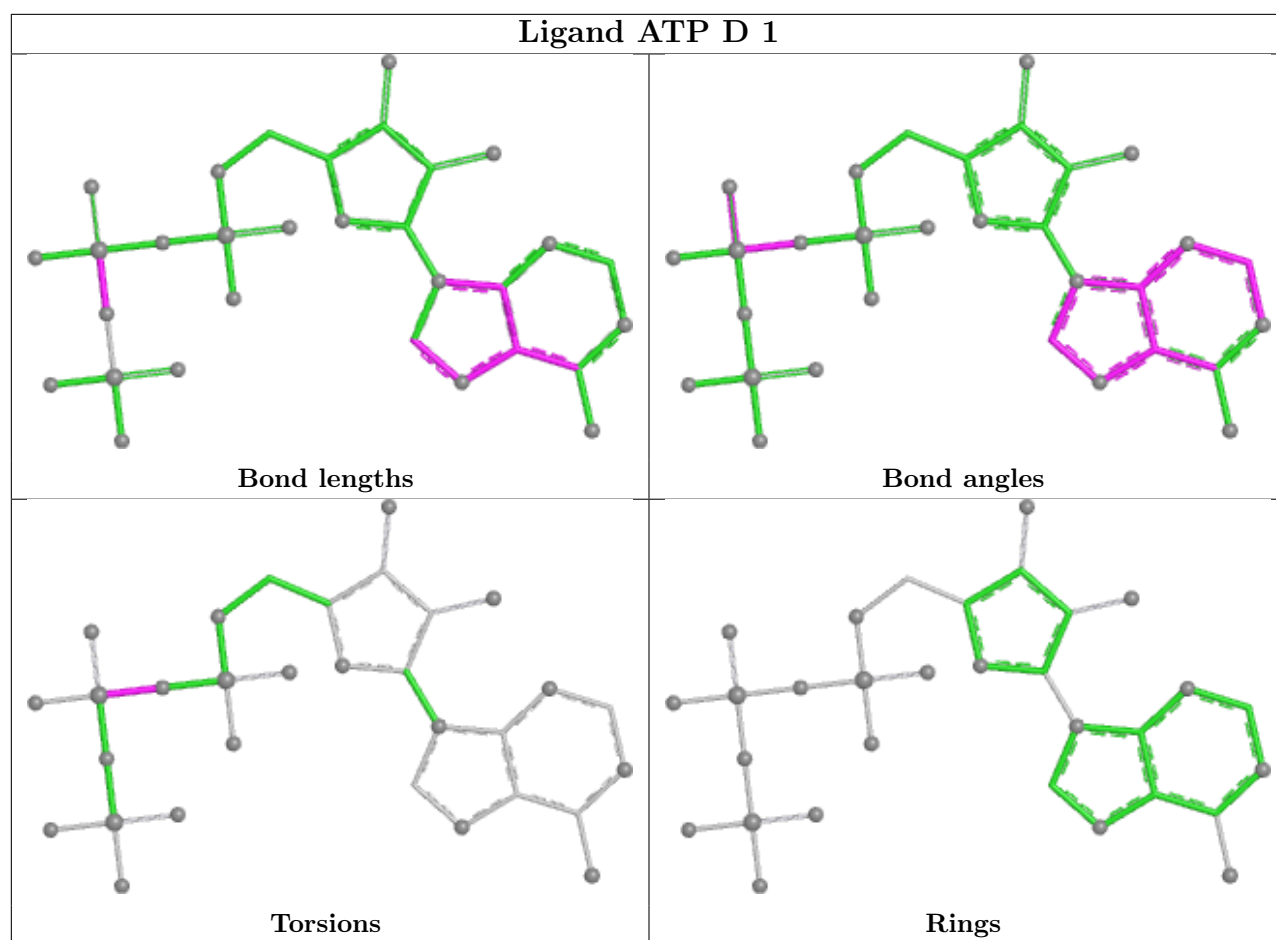
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3	GOL	1	0
4	D	3	GOL	1	0
4	B	3	GOL	1	0
4	A	3	GOL	2	0

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	255/271 (94%)	1.50	57 (22%) 2 2	21, 38, 43, 46	3 (1%)
1	B	255/271 (94%)	1.45	55 (21%) 2 2	20, 38, 44, 46	4 (1%)
1	C	252/271 (92%)	1.60	72 (28%) 1 1	19, 38, 43, 48	5 (1%)
1	D	250/271 (92%)	1.48	62 (24%) 2 1	19, 38, 43, 49	6 (2%)
All	All	1012/1084 (93%)	1.51	246 (24%) 2 1	19, 38, 43, 49	18 (1%)

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	SER	8.0
1	A	619	GLN	6.6
1	B	465	SER	6.3
1	B	619	GLN	5.9
1	C	469	GLY	5.8
1	C	674	LEU	5.2
1	B	685	ARG	5.0
1	C	720	LEU	4.8
1	C	677	THR	4.6
1	A	579	GLY	4.6
1	A	708	GLU	4.5
1	B	466	PRO	4.4
1	B	719	ALA	4.4
1	C	565	PRO	4.4
1	C	680	LEU	4.4
1	D	568	PHE	4.2
1	D	469	GLY	4.1
1	C	508	GLY	4.0
1	C	645	GLN	4.0
1	B	467	LEU	3.9
1	B	711	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	701	GLY	3.9
1	C	672	THR	3.9
1	A	508	GLY	3.9
1	C	676	ILE	3.8
1	C	470	SER	3.8
1	B	579	GLY	3.8
1	C	564	GLU	3.6
1	C	568	PHE	3.6
1	B	704	LEU	3.6
1	C	642	ILE	3.5
1	D	552	HIS	3.5
1	C	579	GLY	3.5
1	A	466	PRO	3.5
1	D	500	GLY	3.5
1	A	652	ALA	3.5
1	A	643	LEU	3.5
1	D	708	GLU	3.5
1	A	615	GLU	3.3
1	D	702	THR	3.3
1	C	683	ALA	3.3
1	C	675	LEU	3.3
1	A	614	GLY	3.3
1	D	471	LEU	3.3
1	A	467	LEU	3.2
1	B	660	ARG	3.1
1	B	615	GLU	3.1
1	B	556	THR	3.1
1	D	698	CYS	3.1
1	B	475	ASN	3.0
1	B	702	THR	3.0
1	C	640	LEU	3.0
1	B	468	SER	3.0
1	C	708	GLU	3.0
1	B	474	LEU	3.0
1	D	701	GLY	3.0
1	C	621	SER	3.0
1	D	567	LEU	3.0
1	A	578	TYR	2.9
1	D	668	TRP	2.9
1	A	468	SER	2.9
1	C	682	LEU	2.9
1	D	711	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	673	VAL	2.9
1	D	547[A]	VAL	2.9
1	B	689	ILE	2.9
1	D	468	SER	2.9
1	A	711	GLY	2.9
1	C	670	SER	2.9
1	A	719	ALA	2.9
1	A	692	LEU	2.8
1	D	474	LEU	2.8
1	D	551	HIS	2.8
1	D	608	GLY	2.8
1	D	649	ALA	2.8
1	B	578	TYR	2.8
1	D	508	GLY	2.8
1	A	514	VAL	2.8
1	C	668	TRP	2.8
1	C	678	HIS	2.7
1	C	474	LEU	2.7
1	C	551	HIS	2.7
1	A	641	LEU	2.7
1	D	473	PRO	2.7
1	A	676	ILE	2.7
1	D	719	ALA	2.7
1	D	672	THR	2.7
1	D	532	TYR	2.7
1	B	618	ASN	2.6
1	A	660	ARG	2.6
1	A	710	GLY	2.6
1	B	686	ALA	2.6
1	A	590	THR	2.6
1	D	566	LEU	2.6
1	B	715	SER	2.6
1	B	506	TYR	2.6
1	D	506	TYR	2.6
1	B	575	ASN	2.6
1	D	507	PRO	2.6
1	D	600	ASP	2.6
1	A	645	GLN	2.6
1	B	623	GLY	2.6
1	C	711	GLY	2.6
1	A	492	HIS	2.6
1	B	687	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	687	HIS	2.6
1	A	677	THR	2.6
1	C	646	ALA	2.6
1	A	696	SER	2.6
1	C	665	SER	2.6
1	C	587	GLU	2.5
1	A	717	VAL	2.5
1	D	578	TYR	2.5
1	C	582	ARG	2.5
1	D	502	THR	2.5
1	D	528	LEU	2.5
1	D	704	LEU	2.5
1	C	552	HIS	2.5
1	C	652	ALA	2.5
1	C	681	SER	2.5
1	D	696	SER	2.5
1	C	567	LEU	2.5
1	A	642	ILE	2.5
1	A	709	ARG	2.5
1	A	506	TYR	2.5
1	C	696	SER	2.5
1	B	656	LEU	2.5
1	D	620	LEU	2.5
1	A	701	GLY	2.5
1	D	489	TYR	2.4
1	A	679	GLN	2.4
1	A	718	GLU	2.4
1	D	715	SER	2.4
1	C	476	MET	2.4
1	C	647	THR	2.4
1	B	617	GLY	2.4
1	C	491	ASN	2.4
1	B	712	CYS	2.4
1	C	719	ALA	2.4
1	A	697	VAL	2.4
1	A	581	THR	2.4
1	D	638	PRO	2.4
1	B	675	LEU	2.3
1	D	706	LEU	2.3
1	B	469	GLY	2.3
1	B	717	VAL	2.3
1	C	561	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	504	THR	2.3
1	A	698	CYS	2.3
1	D	577	ALA	2.3
1	C	600	ASP	2.3
1	B	509	LYS	2.3
1	D	481	LYS	2.3
1	A	516	PRO	2.3
1	D	499	GLN	2.3
1	D	504	THR	2.3
1	D	491	ASN	2.3
1	A	474	LEU	2.3
1	A	549	TYR	2.3
1	A	682	LEU	2.3
1	B	692	LEU	2.3
1	C	650	LEU	2.3
1	B	708	GLU	2.3
1	C	715	SER	2.3
1	C	679	GLN	2.3
1	B	666	PRO	2.3
1	D	488	ALA	2.3
1	D	686	ALA	2.3
1	B	620	LEU	2.3
1	C	566	LEU	2.3
1	D	690	LEU	2.3
1	B	703	HIS	2.2
1	D	470	SER	2.2
1	B	697	VAL	2.2
1	D	717	VAL	2.2
1	A	669	ALA	2.2
1	B	614	GLY	2.2
1	A	656	LEU	2.2
1	C	546	LEU	2.2
1	B	555	HIS	2.2
1	C	626	GLN	2.2
1	D	657	ARG	2.2
1	B	581	THR	2.2
1	C	524	VAL	2.2
1	C	644	ASP	2.2
1	C	623	GLY	2.2
1	B	669	ALA	2.2
1	C	620	LEU	2.2
1	D	660	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	637	LYS	2.2
1	A	618	ASN	2.2
1	C	494	ASN	2.2
1	C	556	THR	2.2
1	D	642	ILE	2.2
1	A	520	GLY	2.2
1	C	655	GLN	2.2
1	D	626	GLN	2.2
1	A	675	LEU	2.2
1	A	680	LEU	2.2
1	C	580	LEU	2.2
1	C	641	LEU	2.2
1	B	638	PRO	2.1
1	A	667	GLU	2.1
1	B	612	GLU	2.1
1	C	495	VAL	2.1
1	A	563	GLN	2.1
1	B	622	GLY	2.1
1	C	695	GLY	2.1
1	C	633	ALA	2.1
1	B	580	LEU	2.1
1	D	712	CYS	2.1
1	A	561	VAL	2.1
1	B	508	GLY	2.1
1	C	536	GLY	2.1
1	C	617	GLY	2.1
1	D	514	VAL	2.1
1	A	582	ARG	2.1
1	D	582	ARG	2.1
1	C	669	ALA	2.1
1	D	640	LEU	2.1
1	D	590	THR	2.1
1	A	469	GLY	2.1
1	C	710	GLY	2.1
1	D	472	ALA	2.1
1	A	670	SER	2.1
1	D	496	GLN	2.1
1	C	506	TYR	2.1
1	A	617	GLY	2.1
1	D	689	ILE	2.1
1	C	514	VAL	2.1
1	B	526	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	631	ALA	2.1
1	C	591	ALA	2.1
1	B	471	LEU	2.0
1	C	661	LEU	2.0
1	A	600	ASP	2.0
1	B	698	CYS	2.0
1	C	698	CYS	2.0
1	B	604	GLY	2.0
1	D	710	GLY	2.0
1	A	519	SER	2.0
1	B	649	ALA	2.0
1	D	631	ALA	2.0
1	A	674	LEU	2.0
1	C	563	GLN	2.0
1	C	657	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

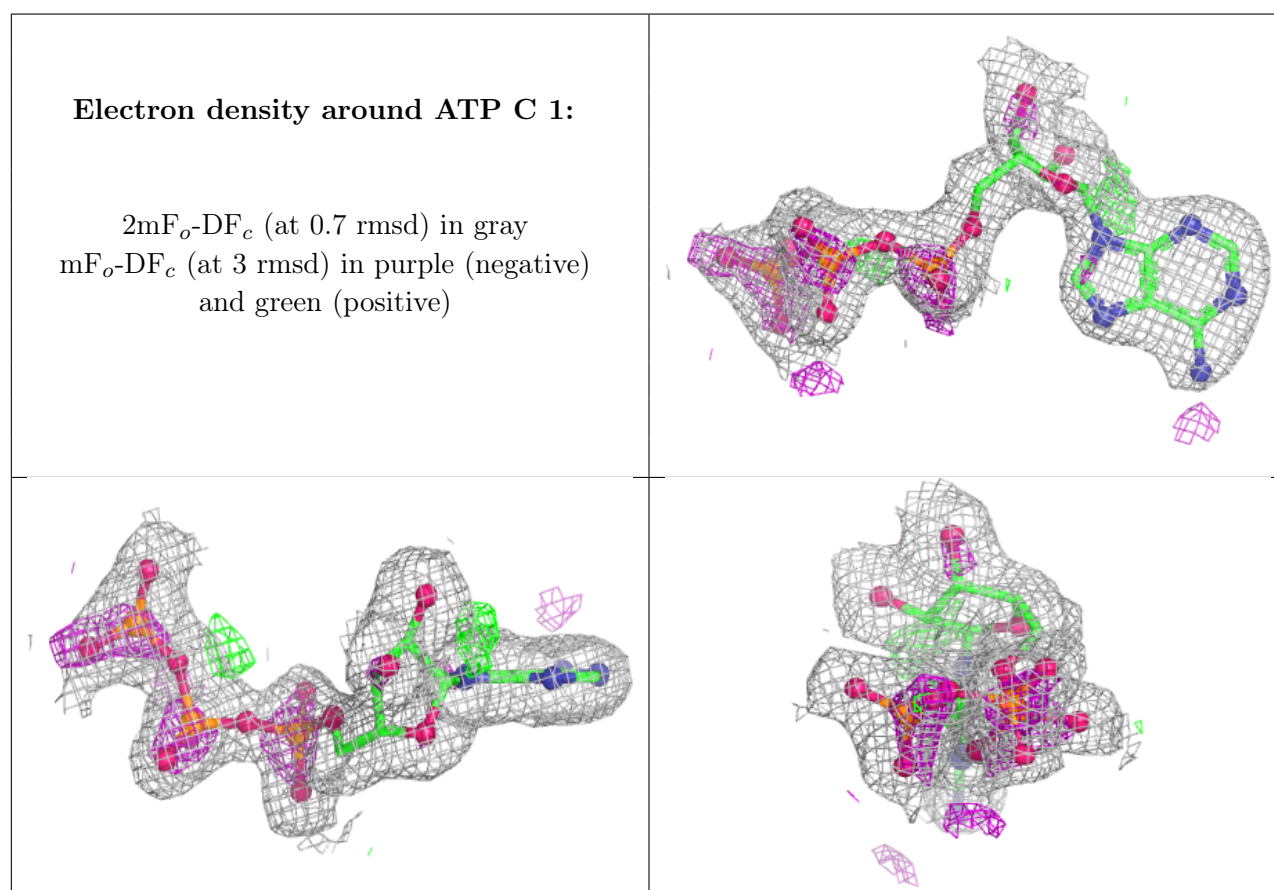
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	3	6/6	0.64	0.17	64,64,65,65	0
4	GOL	C	3	6/6	0.65	0.17	72,72,73,73	0
4	GOL	D	3	6/6	0.66	0.19	92,92,92,92	0
4	GOL	B	4	6/6	0.69	0.16	57,57,58,58	0
4	GOL	A	3	6/6	0.72	0.15	59,60,60,61	0
3	MG	C	2	1/1	0.92	0.19	34,34,34,34	0
3	MG	A	2	1/1	0.94	0.18	27,27,27,27	0
2	ATP	C	1	31/31	0.95	0.10	21,28,30,31	0

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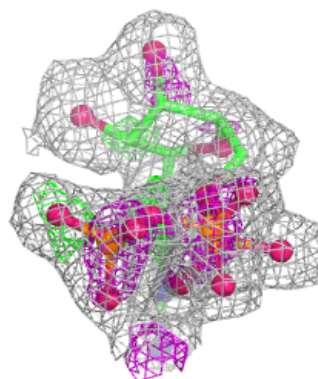
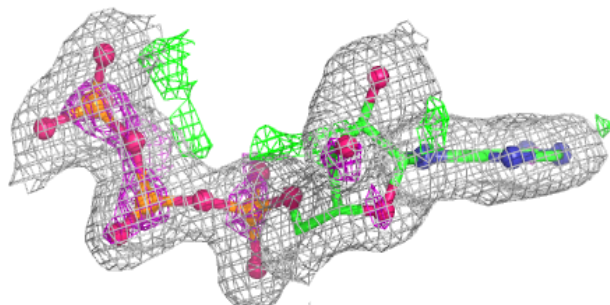
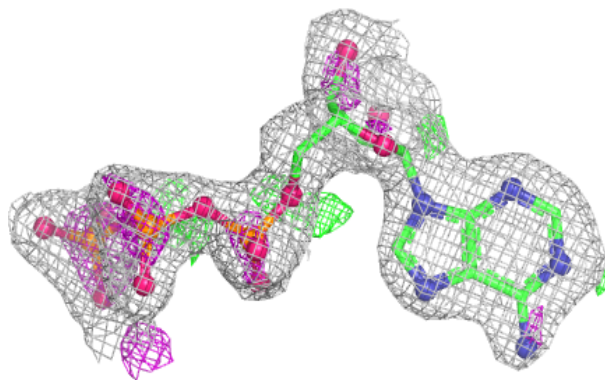
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ATP	D	1	31/31	0.95	0.10	25,30,32,33	0
2	ATP	A	1	31/31	0.95	0.10	19,25,29,29	0
3	MG	D	2	1/1	0.96	0.16	27,27,27,27	0
3	MG	B	2	1/1	0.96	0.25	30,30,30,30	0
2	ATP	B	1	31/31	0.96	0.09	21,26,28,29	0

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

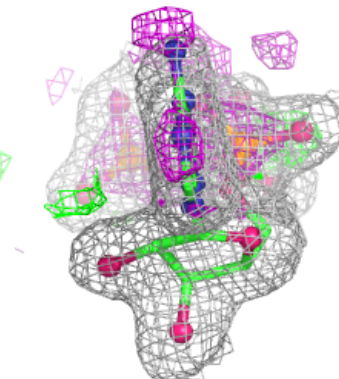
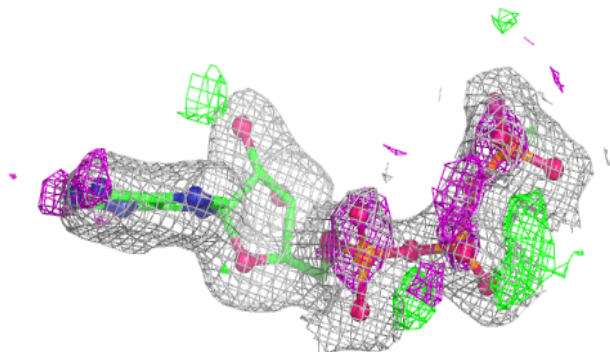
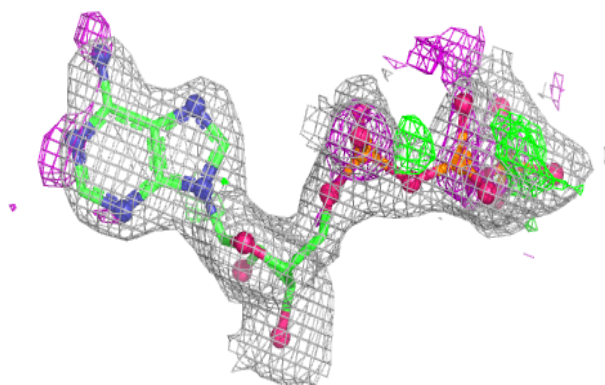


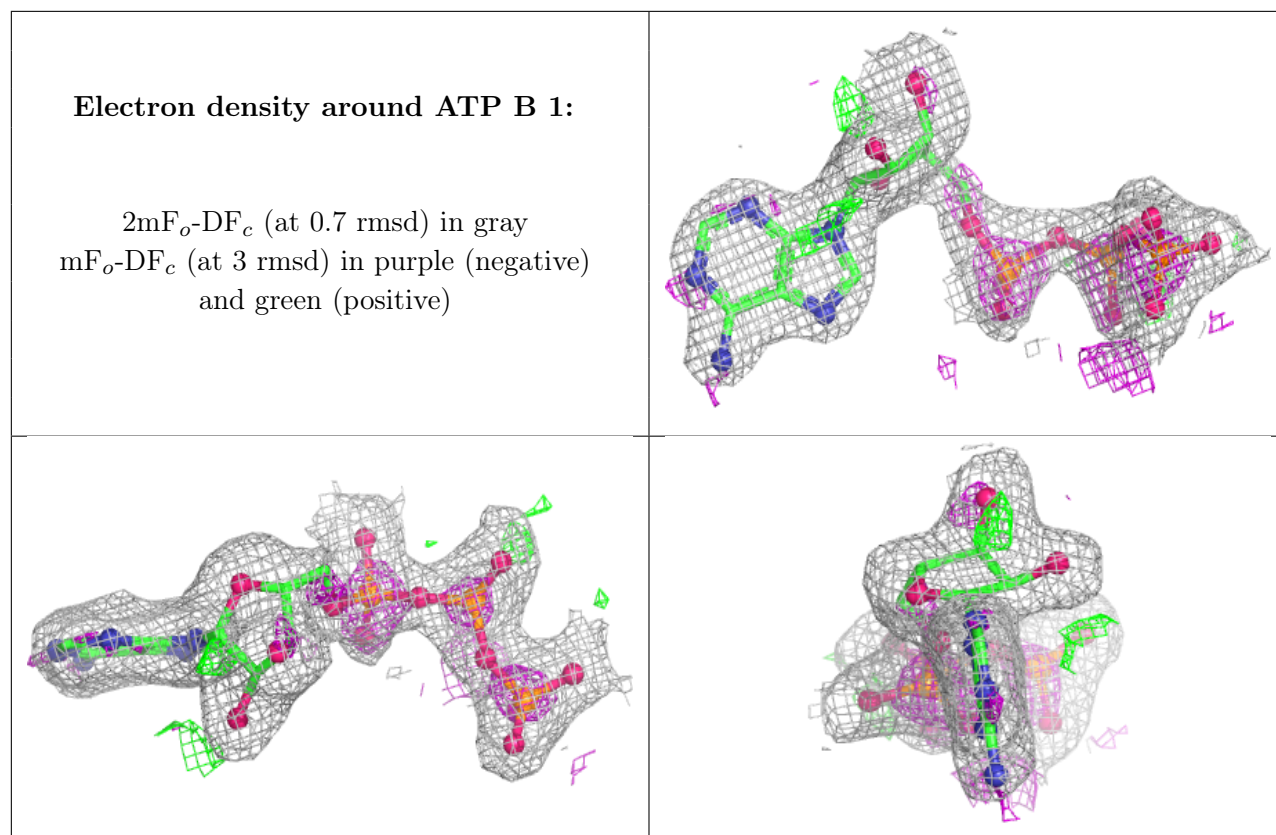
Electron density around ATP D 1:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.