



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 08:02 AM EDT

PDB ID : 2FGK
Title : Crystal structure of the ABC-cassette E631Q mutant of HlyB with bound ATP
Authors : Zaitseva, J.; Oswald, C.; Jumpertz, T.; Jenewein, S.; Holland, I.B.; Schmitt, L.
Deposited on : 2005-12-22
Resolution : 2.70 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 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	:	2.23.2
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)	:	2.23.2

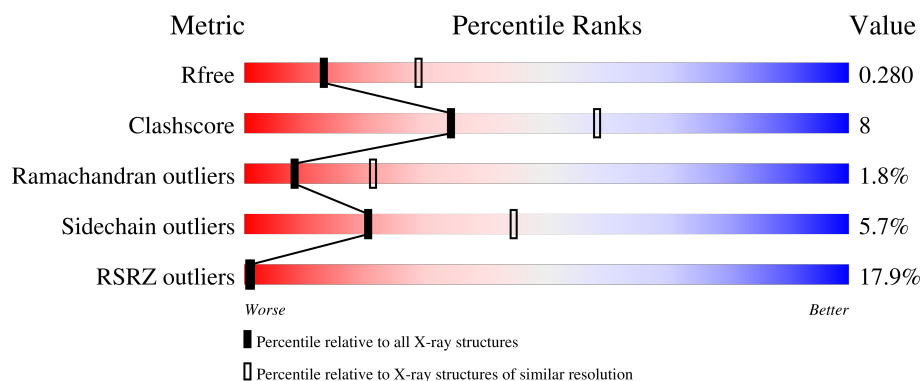
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	247	
1	B	247	
1	C	247	
1	D	247	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7848 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 Alpha-hemolysin translocation ATP-binding protein hlyB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1893	1194	342	352	5			
1	B	241	Total	C	N	O	S	0	0	0
			1893	1194	342	352	5			
1	C	241	Total	C	N	O	S	0	0	0
			1893	1194	342	352	5			
1	D	241	Total	C	N	O	S	0	0	0
			1893	1194	342	352	5			

There are 28 discrepancies between the modelled and reference sequences:

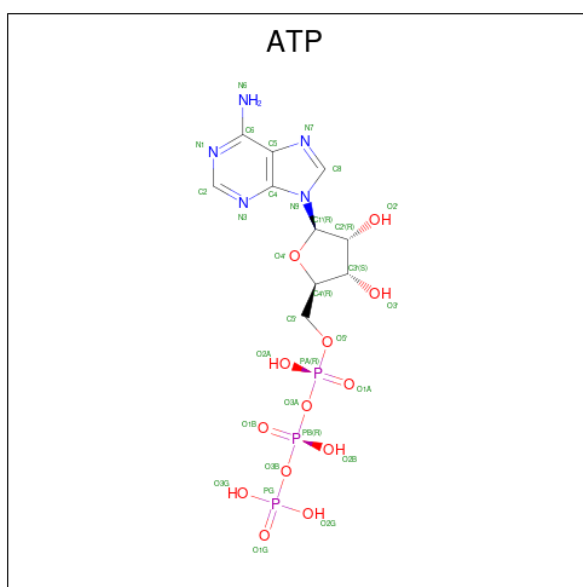
Chain	Residue	Modelled	Actual	Comment	Reference
A	461	HIS	-	expression tag	UNP P08716
A	462	HIS	-	expression tag	UNP P08716
A	463	HIS	-	expression tag	UNP P08716
A	464	HIS	-	expression tag	UNP P08716
A	465	HIS	-	expression tag	UNP P08716
A	466	HIS	-	expression tag	UNP P08716
A	631	GLN	GLU	engineered mutation	UNP P08716
B	461	HIS	-	expression tag	UNP P08716
B	462	HIS	-	expression tag	UNP P08716
B	463	HIS	-	expression tag	UNP P08716
B	464	HIS	-	expression tag	UNP P08716
B	465	HIS	-	expression tag	UNP P08716
B	466	HIS	-	expression tag	UNP P08716
B	631	GLN	GLU	engineered mutation	UNP P08716
C	461	HIS	-	expression tag	UNP P08716
C	462	HIS	-	expression tag	UNP P08716
C	463	HIS	-	expression tag	UNP P08716
C	464	HIS	-	expression tag	UNP P08716
C	465	HIS	-	expression tag	UNP P08716
C	466	HIS	-	expression tag	UNP P08716
C	631	GLN	GLU	engineered mutation	UNP P08716

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Chain	Residue	Modelled	Actual	Comment	Reference
D	461	HIS	-	expression tag	UNP P08716
D	462	HIS	-	expression tag	UNP P08716
D	463	HIS	-	expression tag	UNP P08716
D	464	HIS	-	expression tag	UNP P08716
D	465	HIS	-	expression tag	UNP P08716
D	466	HIS	-	expression tag	UNP P08716
D	631	GLN	GLU	engineered mutation	UNP P08716

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: 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 water.

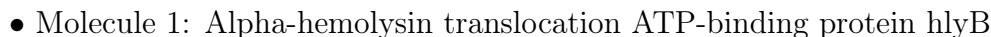
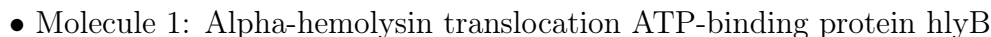
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		

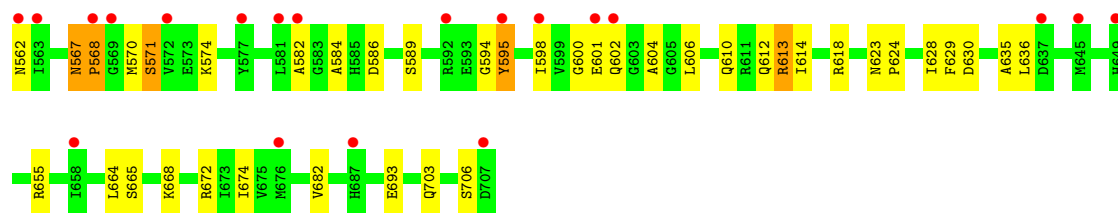
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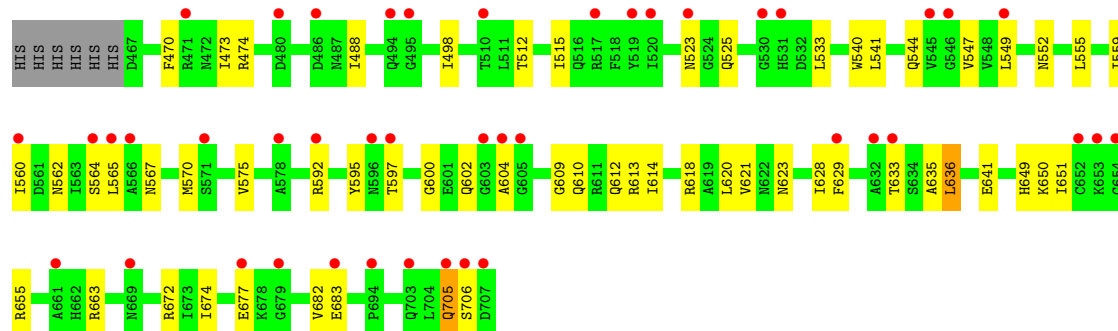
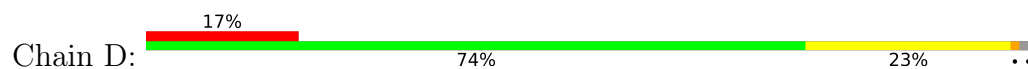
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	44	Total 44	O 44	0	0
3	C	32	Total 32	O 32	0	0
3	D	40	Total 40	O 40	0	0

- Molecule 1: Alpha-hemolysin translocation ATP-binding protein hlyB





● Molecule 1: Alpha-hemolysin translocation ATP-binding protein hlyB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.14Å 189.26Å 63.48Å 90.00° 111.87° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.70) 98.8 (20.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.53 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.223 , 0.280 0.222 , 0.280	Depositor DCC
R_{free} test set	1406 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.406 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7848	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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	1.27	8/1920 (0.4%)	0.68	4/2589 (0.2%)
1	B	0.41	0/1920	0.58	0/2589
1	C	0.73	8/1920 (0.4%)	0.67	4/2589 (0.2%)
1	D	0.41	0/1920	0.57	0/2589
All	All	0.79	16/7680 (0.2%)	0.63	8/10356 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	593	GLU	CD-OE2	43.26	1.73	1.25
1	A	593	GLU	CD-OE1	18.30	1.45	1.25
1	C	558	SER	CB-OG	14.44	1.61	1.42
1	A	595	TYR	CE2-CZ	13.03	1.55	1.38
1	C	595	TYR	CE2-CZ	12.90	1.55	1.38
1	A	557	ARG	NE-CZ	11.85	1.48	1.33
1	A	557	ARG	CZ-NH1	8.69	1.44	1.33
1	A	595	TYR	CG-CD2	8.64	1.50	1.39
1	C	589	SER	CB-OG	7.98	1.52	1.42
1	C	595	TYR	CG-CD2	7.36	1.48	1.39
1	C	557	ARG	CZ-NH1	7.19	1.42	1.33
1	A	589	SER	CB-OG	6.98	1.51	1.42
1	A	596	ASN	CG-OD1	5.95	1.37	1.24
1	C	558	SER	C-O	5.87	1.34	1.23
1	C	557	ARG	CD-NE	5.59	1.55	1.46
1	C	595	TYR	CG-CD1	5.32	1.46	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	557	ARG	NE-CZ-NH2	-10.21	115.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	557	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	A	593	GLU	OE1-CD-OE2	9.53	134.74	123.30
1	C	595	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	A	595	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	C	595	TYR	CG-CD2-CE2	-5.84	116.62	121.30
1	A	595	TYR	CG-CD2-CE2	-5.63	116.80	121.30
1	C	557	ARG	NE-CZ-NH1	5.63	123.11	120.30

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	1893	0	1949	29	0
1	B	1893	0	1949	36	0
1	C	1893	0	1949	31	0
1	D	1893	0	1949	37	0
2	A	31	0	12	0	0
2	B	31	0	12	1	0
2	C	31	0	12	0	0
2	D	31	0	12	0	0
3	A	36	0	0	5	0
3	B	44	0	0	2	0
3	C	32	0	0	3	0
3	D	40	0	0	1	0
All	All	7848	0	7844	130	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 8.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:GLU:CD	1:A:593:GLU:OE2	1.73	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:SER:HB2	1:C:574:LYS:HB2	1.36	1.06
1:B:612:GLN:HE22	1:B:635:ALA:H	1.13	0.90
1:C:560:ILE:HB	3:C:139:HOH:O	1.73	0.88
1:C:612:GLN:HE22	1:C:635:ALA:H	1.27	0.83
1:A:612:GLN:HE22	1:A:635:ALA:H	1.27	0.81
1:A:582:ALA:O	1:A:613:ARG:HG2	1.85	0.77
1:C:571:SER:CB	1:C:574:LYS:HB2	2.15	0.76
1:B:623:ASN:HD22	1:B:655:ARG:HH12	1.36	0.72
1:A:557:ARG:HB2	1:A:561:ASP:OD2	1.89	0.72
1:A:498:ILE:HD11	1:A:674:ILE:HG13	1.73	0.71
1:A:600:GLY:H	1:A:604:ALA:H	1.39	0.70
1:A:612:GLN:HE21	1:A:636:LEU:HD13	1.55	0.70
1:D:612:GLN:HE22	1:D:635:ALA:H	1.38	0.70
1:B:512:THR:HA	1:B:515:ILE:HD12	1.74	0.70
1:C:582:ALA:O	1:C:613:ARG:HG2	1.91	0.69
1:C:571:SER:HB2	1:C:574:LYS:CB	2.21	0.68
1:C:498:ILE:HD11	1:C:674:ILE:HG13	1.75	0.67
1:A:555:LEU:H	1:A:562:ASN:HD21	1.42	0.66
1:D:512:THR:HA	1:D:515:ILE:HD12	1.78	0.66
1:B:612:GLN:HE21	1:B:636:LEU:HD13	1.60	0.65
1:D:623:ASN:HD22	1:D:655:ARG:HH12	1.44	0.65
1:A:571:SER:HB2	1:A:574:LYS:HB2	1.78	0.65
1:D:592:ARG:HG2	3:D:9:HOH:O	1.95	0.65
1:C:595:TYR:HB3	3:C:139:HOH:O	1.96	0.64
1:C:612:GLN:HE21	1:C:636:LEU:HD13	1.62	0.64
1:D:609:GLY:O	1:D:613:ARG:HD3	1.98	0.63
1:B:609:GLY:O	1:B:613:ARG:HD3	1.97	0.63
1:D:549:LEU:H	1:D:552:ASN:HD21	1.44	0.63
1:B:612:GLN:NE2	1:B:635:ALA:H	1.92	0.62
1:D:623:ASN:ND2	1:D:655:ARG:HH12	2.00	0.60
1:A:561:ASP:HB3	1:C:561:ASP:OD1	2.01	0.59
1:A:558:SER:HB3	1:A:561:ASP:OD1	2.04	0.57
1:D:540:TRP:O	1:D:544:GLN:HG2	2.05	0.57
1:A:584:ALA:HB2	1:A:613:ARG:HB3	1.86	0.56
1:D:612:GLN:HE21	1:D:636:LEU:HD13	1.71	0.56
1:D:567:ASN:ND2	1:D:570:MET:HB2	2.19	0.56
1:D:641:GLU:OE2	1:D:663:ARG:HD2	2.05	0.56
1:B:623:ASN:ND2	1:B:655:ARG:HH12	2.02	0.55
1:D:555:LEU:H	1:D:562:ASN:HD21	1.54	0.55
1:B:540:TRP:O	1:B:544:GLN:HG2	2.08	0.54
1:B:641:GLU:OE2	1:B:663:ARG:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:ASN:HD22	1:D:570:MET:HB2	1.73	0.53
1:C:584:ALA:HB2	1:C:613:ARG:HB3	1.89	0.53
1:C:612:GLN:NE2	1:C:635:ALA:H	2.02	0.53
1:A:568:PRO:HD3	1:C:568:PRO:HD3	1.89	0.53
1:B:560:ILE:HG13	1:B:575:VAL:HG11	1.90	0.52
1:D:555:LEU:N	1:D:562:ASN:HD21	2.06	0.52
1:B:512:THR:HB	1:B:628:ILE:HD13	1.92	0.52
1:C:600:GLY:HA3	1:C:604:ALA:HB3	1.92	0.52
1:D:512:THR:HB	1:D:628:ILE:HD13	1.92	0.52
1:B:682:VAL:HG12	1:B:683:GLU:HG3	1.92	0.51
1:D:682:VAL:HG12	1:D:683:GLU:HG3	1.93	0.50
1:D:549:LEU:N	1:D:552:ASN:HD21	2.09	0.50
1:C:555:LEU:H	1:C:562:ASN:HD21	1.59	0.50
1:C:568:PRO:C	1:C:570:MET:N	2.64	0.50
1:A:498:ILE:HD12	3:A:142:HOH:O	2.12	0.49
1:C:703:GLN:HB3	3:C:14:HOH:O	2.12	0.49
1:B:474:ARG:HB3	1:B:523:ASN:HB3	1.95	0.49
1:D:600:GLY:HA3	1:D:604:ALA:O	2.13	0.48
1:B:592:ARG:HG2	3:B:150:HOH:O	2.12	0.48
1:B:550:GLN:HA	3:B:40:HOH:O	2.13	0.48
1:D:470:PHE:HD1	1:D:473:ILE:HG13	1.78	0.48
1:B:588:ILE:O	1:B:594:GLY:HA2	2.14	0.48
1:D:474:ARG:HB3	1:D:523:ASN:HB3	1.96	0.48
1:D:705:GLN:O	1:D:705:GLN:HG3	2.13	0.48
1:B:555:LEU:H	1:B:562:ASN:HD21	1.62	0.47
1:D:498:ILE:HD11	1:D:674:ILE:HG13	1.96	0.47
1:A:588:ILE:HA	1:A:591:LEU:HD12	1.95	0.47
1:B:705:GLN:O	1:B:705:GLN:HG3	2.13	0.47
1:C:512:THR:HB	1:C:628:ILE:HD13	1.97	0.47
1:A:468:ILE:HB	1:A:492:ILE:HB	1.97	0.47
1:B:567:ASN:ND2	1:B:570:MET:HB2	2.30	0.47
1:D:562:ASN:O	1:D:618:ARG:HG3	2.15	0.47
1:C:558:SER:HA	1:C:598:ILE:HA	1.97	0.47
1:D:633:THR:HA	1:D:636:LEU:HD22	1.96	0.47
1:A:603:GLY:O	1:A:605:GLY:N	2.48	0.46
1:B:470:PHE:HD1	1:B:473:ILE:HG13	1.80	0.46
1:C:623:ASN:ND2	1:C:655:ARG:HH22	2.13	0.46
1:A:512:THR:HB	1:A:628:ILE:HD13	1.96	0.46
1:A:548:VAL:O	1:A:630:ASP:HB3	2.16	0.46
1:A:478:LYS:HB3	1:A:479:PRO:HD2	1.97	0.46
1:B:649:HIS:CE1	1:B:650:LYS:HE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:ILE:HD11	1:B:674:ILE:CG1	2.46	0.46
1:C:468:ILE:HB	1:C:492:ILE:HB	1.99	0.45
1:B:588:ILE:HD11	1:B:614:ILE:CD1	2.46	0.45
1:B:498:ILE:HD11	1:B:674:ILE:HG13	1.98	0.45
1:B:555:LEU:N	1:B:562:ASN:HD21	2.14	0.45
1:D:560:ILE:HG13	1:D:575:VAL:HG11	1.98	0.45
1:B:599:VAL:HG11	1:B:606:LEU:HD21	1.98	0.45
1:B:599:VAL:CG1	1:B:606:LEU:HD21	2.47	0.45
1:B:572:VAL:HG12	1:B:576:ILE:HD13	1.99	0.45
1:C:478:LYS:HB3	1:C:479:PRO:HD2	1.98	0.44
1:D:559:ILE:HD12	1:D:597:THR:HB	1.98	0.44
1:A:476:ARG:HD3	1:A:481:SER:O	2.17	0.44
1:A:546:GLY:HA3	1:A:624:PRO:HG3	1.99	0.44
1:A:665:SER:HA	1:A:668:LYS:HG3	1.99	0.44
1:C:546:GLY:HA3	1:C:624:PRO:HG3	1.99	0.44
1:A:496:GLU:CD	3:A:142:HOH:O	2.55	0.44
1:D:498:ILE:HD11	1:D:674:ILE:CG1	2.47	0.44
1:D:549:LEU:H	1:D:552:ASN:ND2	2.14	0.44
1:D:620:LEU:HD21	1:D:651:ILE:HG23	2.00	0.44
1:D:610:GLN:O	1:D:614:ILE:HG12	2.18	0.43
1:C:568:PRO:C	1:C:570:MET:H	2.22	0.43
1:D:560:ILE:HB	1:D:595:TYR:HB3	2.00	0.43
1:B:633:THR:HA	1:B:636:LEU:HD22	2.00	0.43
1:C:548:VAL:O	1:C:630:ASP:HB3	2.18	0.43
1:C:476:ARG:HD3	1:C:481:SER:O	2.19	0.43
1:D:533:LEU:HD22	1:D:541:LEU:HD13	2.00	0.43
1:D:612:GLN:NE2	1:D:635:ALA:H	2.12	0.43
1:C:665:SER:HA	1:C:668:LYS:HG3	2.01	0.43
1:A:688:LYS:HE2	3:A:41:HOH:O	2.19	0.43
1:B:504:SER:HA	2:B:801:ATP:O2G	2.18	0.42
1:B:677:GLU:HB3	1:B:682:VAL:HG21	2.01	0.42
1:D:473:ILE:HB	1:D:488:ILE:HB	2.01	0.42
1:B:560:ILE:HB	1:B:595:TYR:HB3	2.01	0.42
1:C:610:GLN:O	1:C:614:ILE:HG12	2.18	0.42
1:A:618:ARG:HD2	3:A:63:HOH:O	2.19	0.42
1:C:567:ASN:HA	1:C:568:PRO:HD3	1.80	0.42
1:B:533:LEU:HD22	1:B:541:LEU:HD13	2.01	0.42
1:B:473:ILE:HB	1:B:488:ILE:HB	2.02	0.42
1:A:557:ARG:HH22	1:C:568:PRO:CB	2.33	0.41
1:A:492:ILE:HG23	3:A:142:HOH:O	2.20	0.41
1:A:584:ALA:HA	1:A:587:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:549:LEU:H	1:C:552:ASN:HD21	1.68	0.41
1:D:649:HIS:CE1	1:D:650:LYS:HE2	2.55	0.41
1:D:547:VAL:HG22	1:D:628:ILE:HB	2.03	0.41
1:D:677:GLU:HB3	1:D:682:VAL:HG21	2.02	0.41
1:B:516:GLN:CD	1:B:547:VAL:HG21	2.41	0.40
1:B:588:ILE:HD11	1:B:614:ILE:HD12	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	239/247 (97%)	223 (93%)	10 (4%)	6 (2%)	5	14
1	B	239/247 (97%)	226 (95%)	10 (4%)	3 (1%)	12	30
1	C	239/247 (97%)	222 (93%)	11 (5%)	6 (2%)	5	14
1	D	239/247 (97%)	224 (94%)	13 (5%)	2 (1%)	19	43
All	All	956/988 (97%)	895 (94%)	44 (5%)	17 (2%)	8	21

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	603	GLY
1	C	601	GLU
1	C	571	SER
1	D	565	LEU
1	A	604	ALA
1	C	568	PRO
1	C	594	GLY
1	A	567	ASN
1	A	571	SER

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Mol	Chain	Res	Type
1	A	706	SER
1	B	551	ASP
1	B	601	GLU
1	C	567	ASN
1	C	706	SER
1	B	706	SER
1	D	706	SER
1	A	572	VAL

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	207/213 (97%)	192 (93%)	15 (7%)	14	34
1	B	207/213 (97%)	196 (95%)	11 (5%)	22	48
1	C	207/213 (97%)	194 (94%)	13 (6%)	18	40
1	D	207/213 (97%)	199 (96%)	8 (4%)	32	61
All	All	828/852 (97%)	781 (94%)	47 (6%)	20	44

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	517	ARG
1	A	525	GLN
1	A	552	ASN
1	A	553	VAL
1	A	556	ASN
1	A	561	ASP
1	A	586	ASP
1	A	606	LEU
1	A	623	ASN
1	A	629	PHE
1	A	636	LEU
1	A	664	LEU
1	A	672	ARG

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Mol	Chain	Res	Type
1	A	682	VAL
1	A	693	GLU
1	B	525	GLN
1	B	557	ARG
1	B	564	SER
1	B	565	LEU
1	B	587	PHE
1	B	621	VAL
1	B	629	PHE
1	B	636	LEU
1	B	664	LEU
1	B	672	ARG
1	B	705	GLN
1	C	517	ARG
1	C	525	GLN
1	C	556	ASN
1	C	586	ASP
1	C	602	GLN
1	C	606	LEU
1	C	613	ARG
1	C	618	ARG
1	C	629	PHE
1	C	664	LEU
1	C	672	ARG
1	C	682	VAL
1	C	693	GLU
1	D	525	GLN
1	D	564	SER
1	D	602	GLN
1	D	621	VAL
1	D	629	PHE
1	D	636	LEU
1	D	672	ARG
1	D	705	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	539	ASN
1	A	550	GLN
1	A	562	ASN
1	A	567	ASN

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Mol	Chain	Res	Type
1	A	612	GLN
1	A	705	GLN
1	B	539	ASN
1	B	556	ASN
1	B	562	ASN
1	B	567	ASN
1	B	612	GLN
1	B	623	ASN
1	B	642	HIS
1	B	705	GLN
1	C	539	ASN
1	C	562	ASN
1	C	612	GLN
1	C	623	ASN
1	C	705	GLN
1	D	539	ASN
1	D	552	ASN
1	D	556	ASN
1	D	562	ASN
1	D	567	ASN
1	D	602	GLN
1	D	612	GLN
1	D	623	ASN
1	D	642	HIS
1	D	705	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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	801	-	26,33,33	1.19	2 (7%)	31,52,52	1.53	4 (12%)
2	ATP	A	800	-	26,33,33	1.14	2 (7%)	31,52,52	1.53	4 (12%)
2	ATP	C	802	-	26,33,33	0.95	1 (3%)	31,52,52	1.62	4 (12%)
2	ATP	D	803	-	26,33,33	1.20	2 (7%)	31,52,52	1.51	5 (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	801	-	-	3/18/38/38	0/3/3/3
2	ATP	A	800	-	-	2/18/38/38	0/3/3/3
2	ATP	C	802	-	-	3/18/38/38	0/3/3/3
2	ATP	D	803	-	-	3/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ATP	PG-O1G	3.52	1.61	1.50
2	D	803	ATP	PG-O1G	3.34	1.61	1.50
2	A	800	ATP	PG-O1G	3.14	1.60	1.50
2	D	803	ATP	O4'-C1'	2.95	1.45	1.41
2	A	800	ATP	O4'-C1'	2.84	1.45	1.41
2	B	801	ATP	O4'-C1'	2.68	1.44	1.41
2	C	802	ATP	PG-O1G	2.26	1.57	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	802	ATP	N3-C2-N1	-4.55	121.57	128.68
2	A	800	ATP	N3-C2-N1	-4.33	121.91	128.68
2	D	803	ATP	N3-C2-N1	-4.19	122.13	128.68
2	B	801	ATP	N3-C2-N1	-4.15	122.20	128.68
2	A	800	ATP	O3G-PG-O3B	4.06	118.24	104.64
2	B	801	ATP	O3G-PG-O3B	3.67	116.95	104.64
2	C	802	ATP	O3G-PG-O3B	3.67	116.95	104.64
2	D	803	ATP	O3G-PG-O3B	3.51	116.40	104.64
2	B	801	ATP	PA-O3A-PB	-3.33	121.39	132.83
2	D	803	ATP	PA-O3A-PB	-3.11	122.16	132.83
2	D	803	ATP	O4'-C1'-C2'	-2.92	102.67	106.93
2	C	802	ATP	PB-O3B-PG	-2.86	123.02	132.83
2	C	802	ATP	PA-O3A-PB	-2.70	123.58	132.83
2	A	800	ATP	PA-O3A-PB	-2.52	124.18	132.83
2	B	801	ATP	O4'-C1'-C2'	-2.38	103.45	106.93
2	A	800	ATP	C4-C5-N7	-2.05	107.27	109.40
2	D	803	ATP	C4-C5-N7	-2.01	107.31	109.40

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	ATP	O4'-C4'-C5'-O5'
2	B	801	ATP	C3'-C4'-C5'-O5'
2	A	800	ATP	PA-O3A-PB-O1B
2	D	803	ATP	O4'-C4'-C5'-O5'
2	C	802	ATP	PA-O3A-PB-O1B
2	D	803	ATP	PA-O3A-PB-O2B
2	A	800	ATP	PA-O3A-PB-O2B
2	C	802	ATP	O4'-C4'-C5'-O5'
2	B	801	ATP	PA-O3A-PB-O2B
2	C	802	ATP	PA-O3A-PB-O2B
2	D	803	ATP	C3'-C4'-C5'-O5'

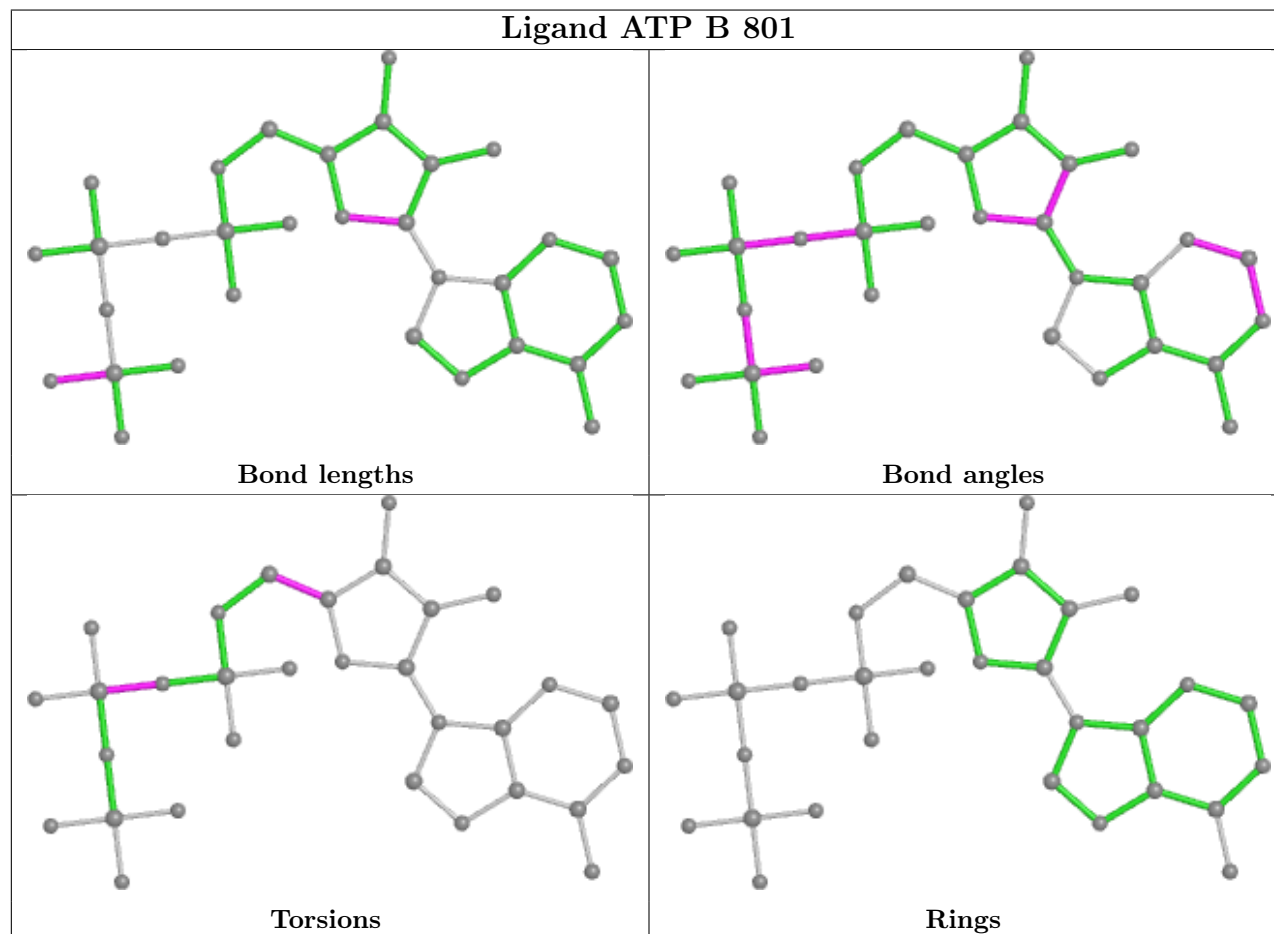
There are no ring outliers.

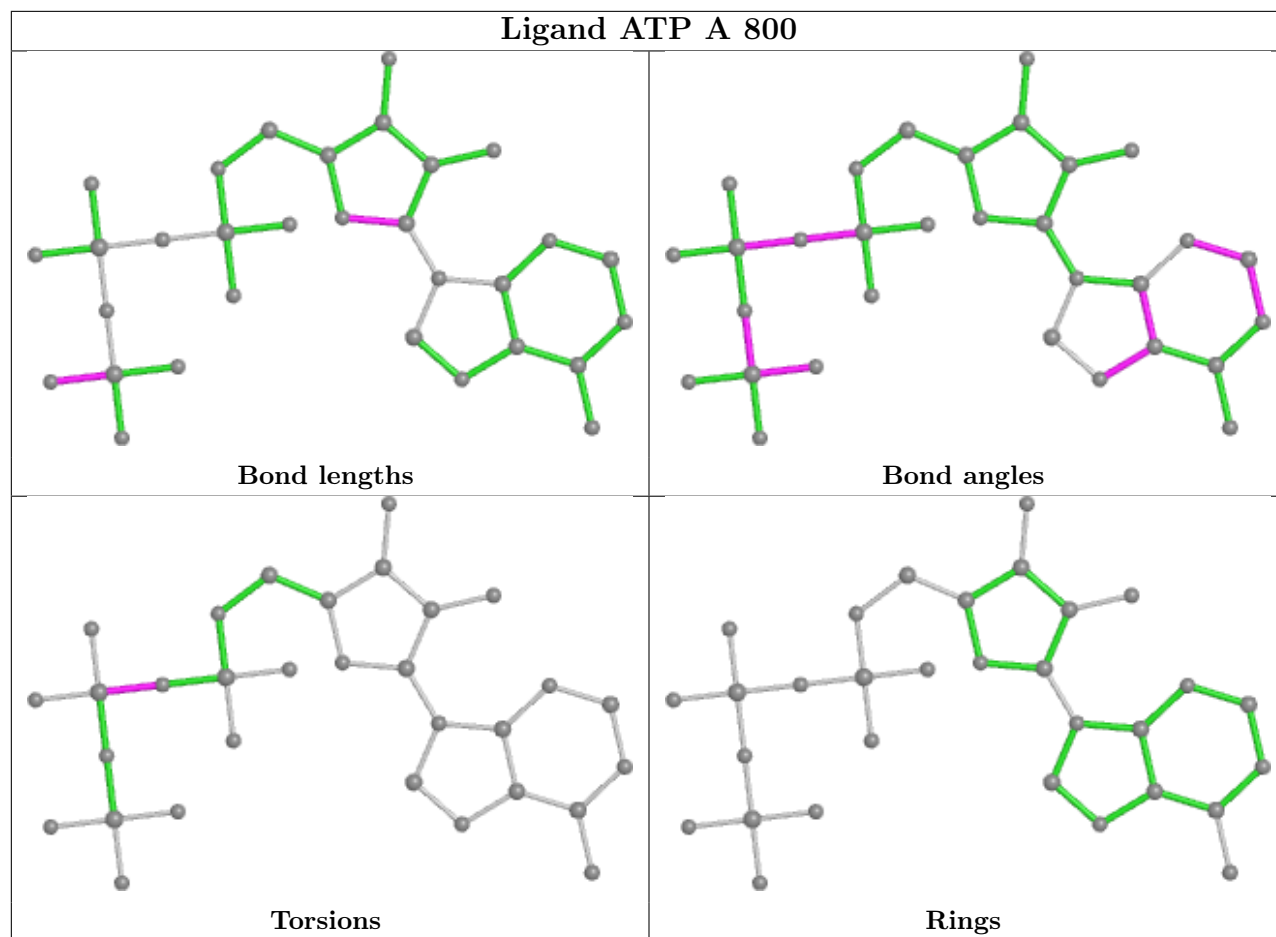
1 monomer is involved in 1 short contact:

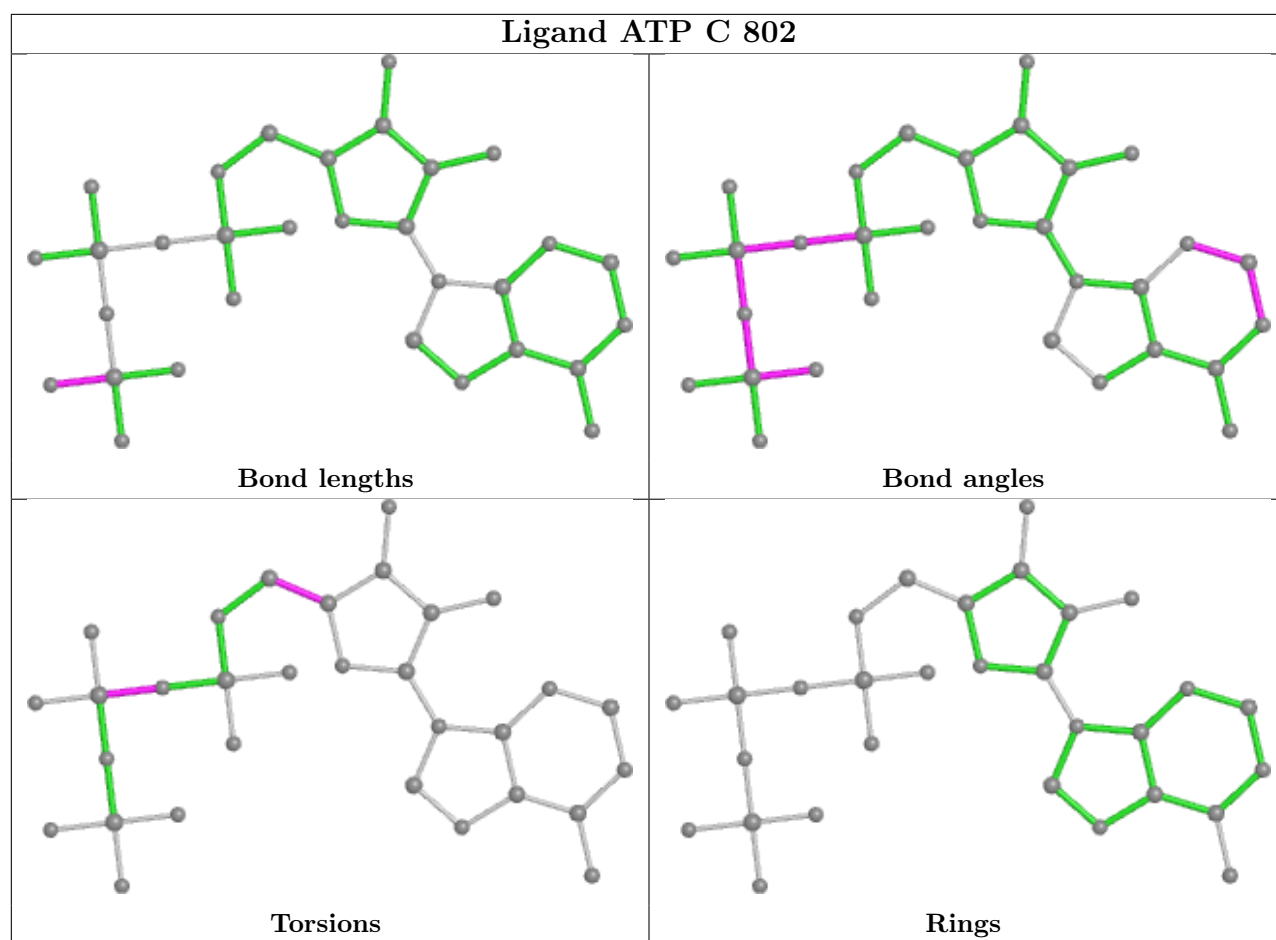
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	ATP	1	0

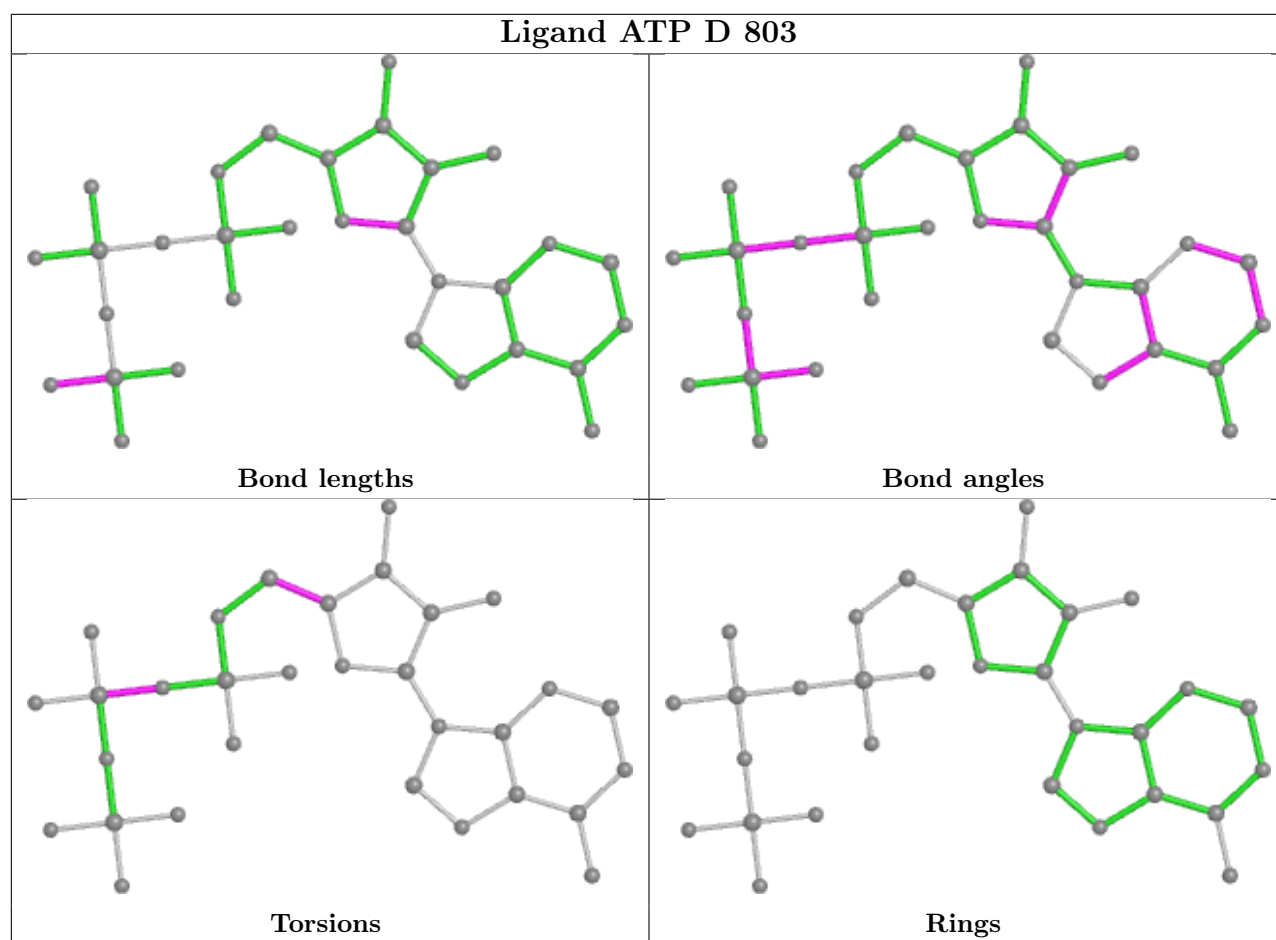
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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	241/247 (97%)	1.26	48 (19%) 1 0	39, 51, 62, 71	0
1	B	241/247 (97%)	1.10	40 (16%) 1 1	40, 51, 63, 70	0
1	C	241/247 (97%)	1.24	42 (17%) 1 1	37, 50, 61, 71	0
1	D	241/247 (97%)	1.14	43 (17%) 1 1	40, 51, 63, 71	0
All	All	964/988 (97%)	1.19	173 (17%) 1 1	37, 51, 63, 71	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	604	ALA	14.3
1	D	707	ASP	10.4
1	B	550	GLN	9.1
1	C	551	ASP	9.0
1	A	569	GLY	8.3
1	A	706	SER	7.9
1	B	553	VAL	7.7
1	D	566	ALA	7.5
1	C	601	GLU	7.3
1	A	603	GLY	7.2
1	D	694	PRO	7.1
1	D	480	ASP	6.5
1	A	596	ASN	6.3
1	D	564	SER	6.0
1	B	518	PHE	6.0
1	B	699	SER	5.9
1	A	604	ALA	5.6
1	C	577	TYR	5.5
1	C	553	VAL	5.4
1	C	569	GLY	5.4
1	C	581	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	519	TYR	5.2
1	C	561	ASP	5.1
1	A	573	GLU	5.1
1	B	687	HIS	5.0
1	C	550	GLN	4.9
1	B	602	GLN	4.9
1	C	537	ASP	4.7
1	C	552	ASN	4.7
1	A	560	ILE	4.7
1	D	486	ASP	4.6
1	D	652	CYS	4.6
1	D	706	SER	4.5
1	B	589	SER	4.3
1	A	592	ARG	4.2
1	A	494	GLN	4.2
1	A	593	GLU	4.2
1	A	555	LEU	4.1
1	C	562	ASN	4.1
1	C	598	ILE	4.0
1	A	565	LEU	3.9
1	D	545	VAL	3.9
1	A	597	THR	3.9
1	B	696	SER	3.9
1	C	592	ARG	3.9
1	C	555	LEU	3.8
1	A	567	ASN	3.8
1	C	637	ASP	3.8
1	C	475	PHE	3.7
1	D	592	ARG	3.7
1	B	691	LEU	3.7
1	B	688	LYS	3.7
1	B	549	LEU	3.7
1	D	565	LEU	3.6
1	C	507	GLY	3.6
1	B	701	LEU	3.6
1	B	521	PRO	3.6
1	A	602	GLN	3.6
1	B	601	GLU	3.5
1	A	576	ILE	3.5
1	C	563	ILE	3.5
1	C	511	LEU	3.4
1	B	470	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	562	ASN	3.3
1	D	597	THR	3.3
1	D	517	ARG	3.2
1	A	518	PHE	3.2
1	B	563	ILE	3.2
1	D	519	TYR	3.2
1	D	603	GLY	3.2
1	A	594	GLY	3.2
1	A	578	ALA	3.1
1	B	520	ILE	3.1
1	C	568	PRO	3.1
1	B	706	SER	3.1
1	D	703	GLN	3.1
1	C	556	ASN	3.1
1	C	572	VAL	3.0
1	A	480	ASP	3.0
1	B	603	GLY	3.0
1	A	697	LEU	3.0
1	B	624	PRO	3.0
1	A	705	GLN	3.0
1	C	554	LEU	2.9
1	C	582	ALA	2.9
1	A	622	ASN	2.9
1	A	554	LEU	2.9
1	A	535	LEU	2.9
1	A	492	ILE	2.9
1	B	478	LYS	2.9
1	D	571	SER	2.8
1	A	479	PRO	2.8
1	C	486	ASP	2.8
1	D	530	GLY	2.8
1	C	649	HIS	2.8
1	A	636	LEU	2.8
1	D	632	ALA	2.7
1	C	519	TYR	2.7
1	C	506	SER	2.7
1	D	520	ILE	2.7
1	A	670	ALA	2.6
1	D	605	GLY	2.6
1	B	645	MET	2.6
1	C	676	MET	2.6
1	D	494	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	683	GLU	2.6
1	C	595	TYR	2.6
1	A	687	HIS	2.6
1	B	604	ALA	2.6
1	B	540	TRP	2.6
1	B	536	ALA	2.5
1	C	470	PHE	2.5
1	D	578	ALA	2.5
1	D	495	GLY	2.5
1	A	537	ASP	2.5
1	D	669	ASN	2.5
1	C	536	ALA	2.5
1	D	531	HIS	2.5
1	A	652	CYS	2.5
1	C	493	LYS	2.5
1	A	688	LYS	2.4
1	A	707	ASP	2.4
1	D	654	GLY	2.4
1	A	568	PRO	2.4
1	C	523	ASN	2.4
1	A	553	VAL	2.4
1	D	523	ASN	2.4
1	B	551	ASP	2.4
1	C	560	ILE	2.4
1	D	679	GLY	2.4
1	D	633	THR	2.4
1	A	557	ARG	2.4
1	C	602	GLN	2.4
1	D	705	GLN	2.3
1	A	605	GLY	2.3
1	B	522	GLU	2.3
1	B	506	SER	2.3
1	D	510	THR	2.3
1	B	468	ILE	2.3
1	C	687	HIS	2.3
1	C	474	ARG	2.3
1	B	552	ASN	2.2
1	D	596	ASN	2.2
1	B	700	TYR	2.2
1	D	471	ARG	2.2
1	A	598	ILE	2.2
1	B	537	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	629	PHE	2.2
1	A	512	THR	2.2
1	C	498	ILE	2.2
1	D	560	ILE	2.2
1	D	549	LEU	2.2
1	B	635	ALA	2.2
1	B	637	ASP	2.2
1	A	519	TYR	2.2
1	A	471	ARG	2.2
1	D	677	GLU	2.2
1	B	543	ARG	2.2
1	A	559	ILE	2.1
1	A	583	GLY	2.1
1	B	554	LEU	2.1
1	C	658	ILE	2.1
1	D	661	ALA	2.1
1	C	707	ASP	2.1
1	A	570	MET	2.1
1	B	474	ARG	2.1
1	A	702	TYR	2.0
1	C	645	MET	2.0
1	B	668	LYS	2.0
1	A	648	MET	2.0
1	A	571	SER	2.0
1	D	546	GLY	2.0
1	D	653	LYS	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](#)

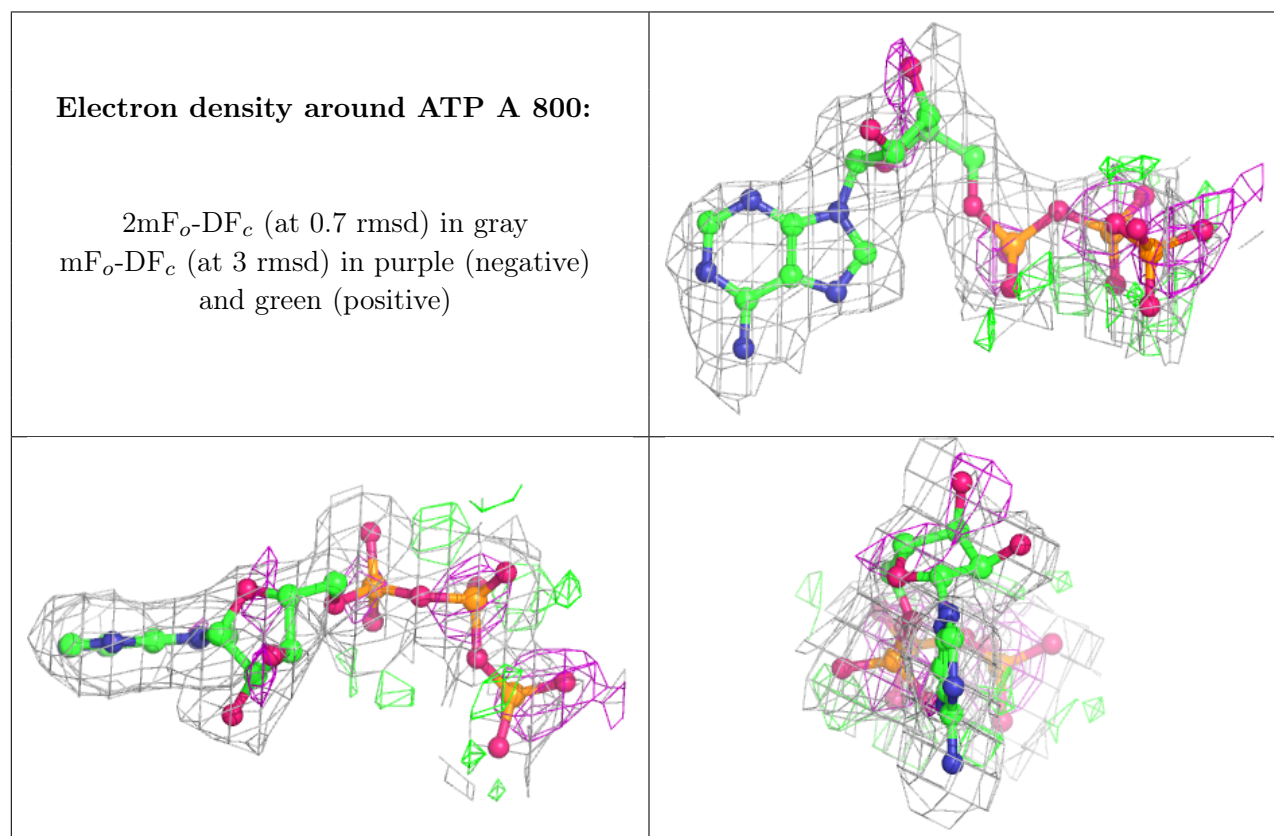
There are no monosaccharides in this entry.

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, 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.

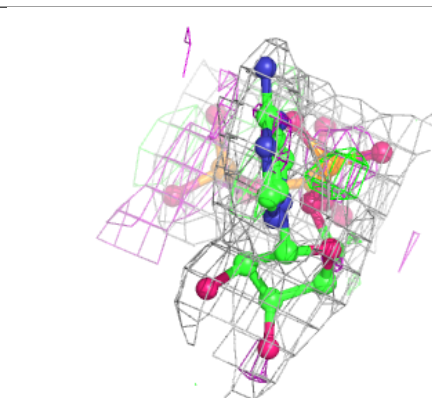
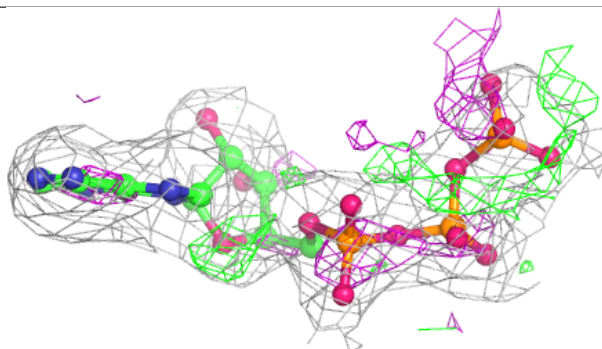
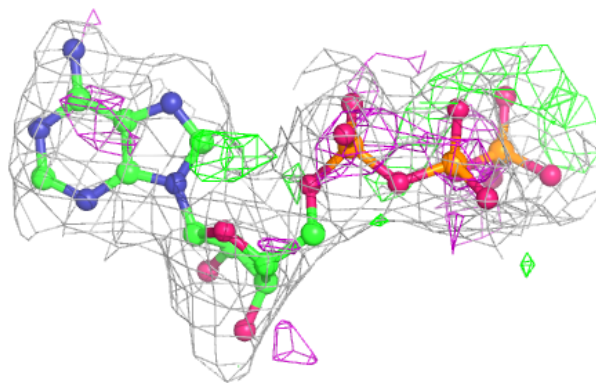
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ATP	A	800	31/31	0.91	0.19	32,41,44,44	0
2	ATP	C	802	31/31	0.92	0.17	28,40,43,44	0
2	ATP	D	803	31/31	0.92	0.24	38,46,47,50	0
2	ATP	B	801	31/31	0.93	0.16	37,42,44,45	0

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.

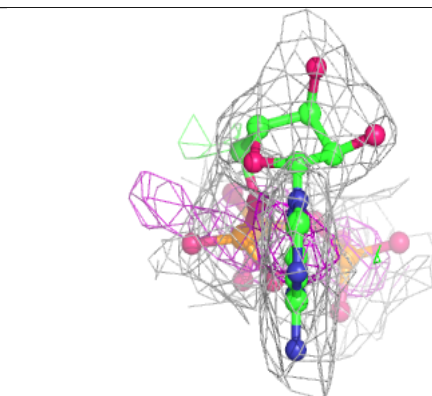
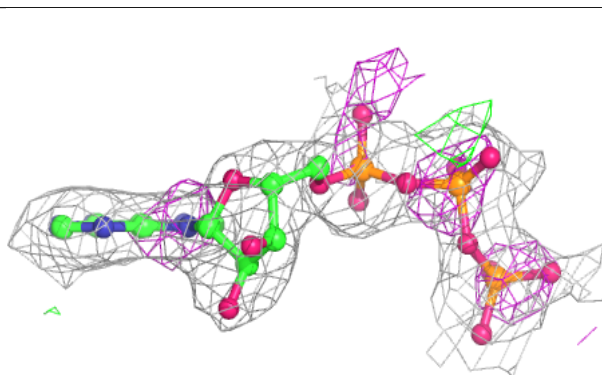
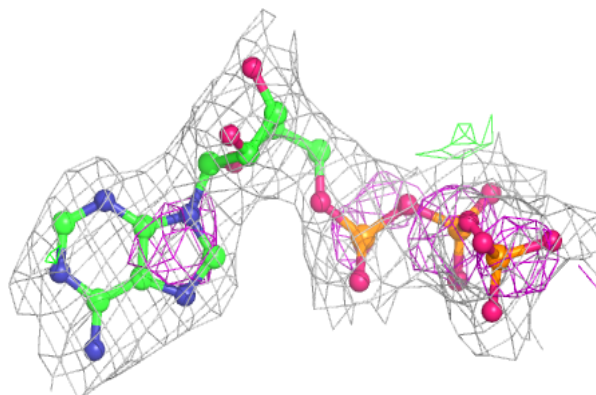


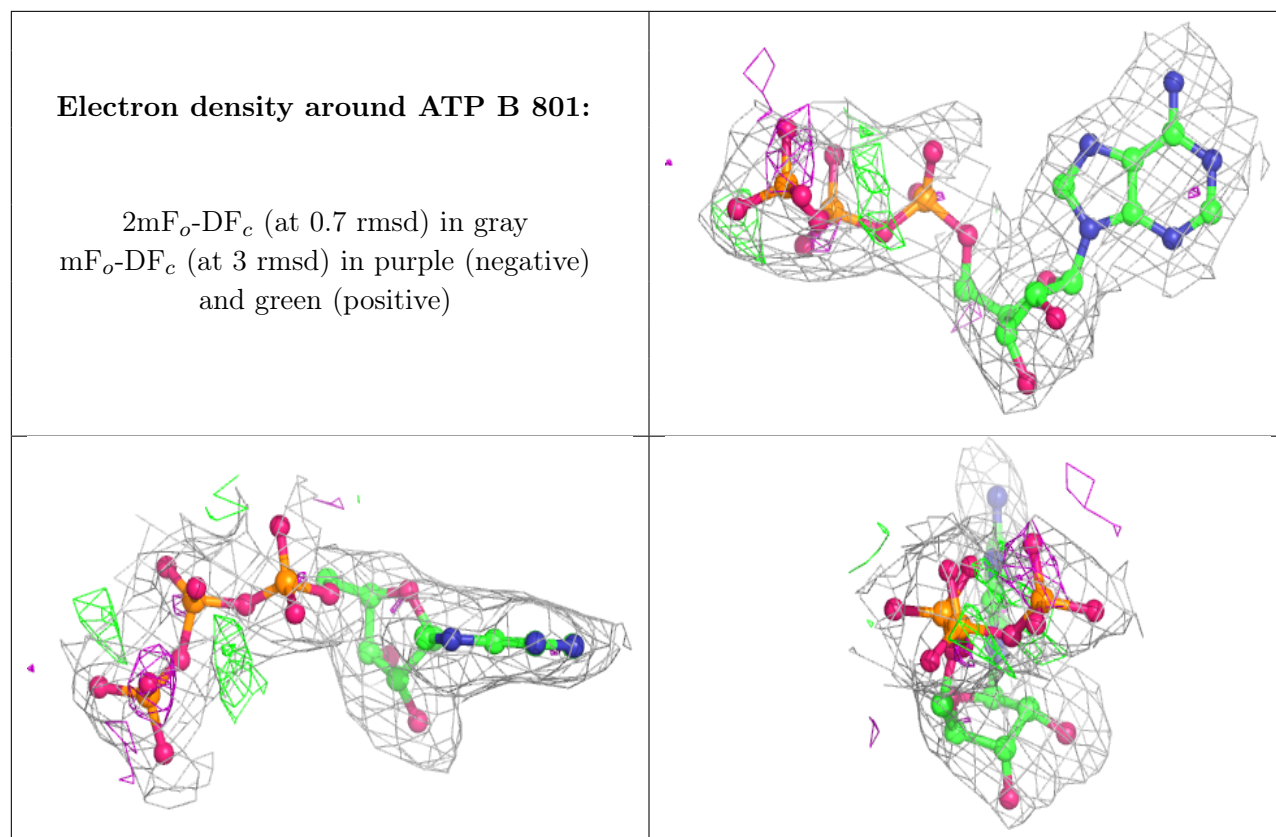
Electron density around ATP C 802:

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

**Electron density around ATP D 803:**

$2mF_o-DF_c$ (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.