Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 03:19 AM EST

PDB ID	:	1RYS
Title	:	REPLICATION OF A CIS-SYN THYMINE DIMER AT ATOMIC RESOLUTION
Authors	:	Ling, H.; Boudsocq, F.; Plosky, B.; Woodgate, R.; Yang, W.
Deposited on	:	2003-12-22
Resolution	:	2.03 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

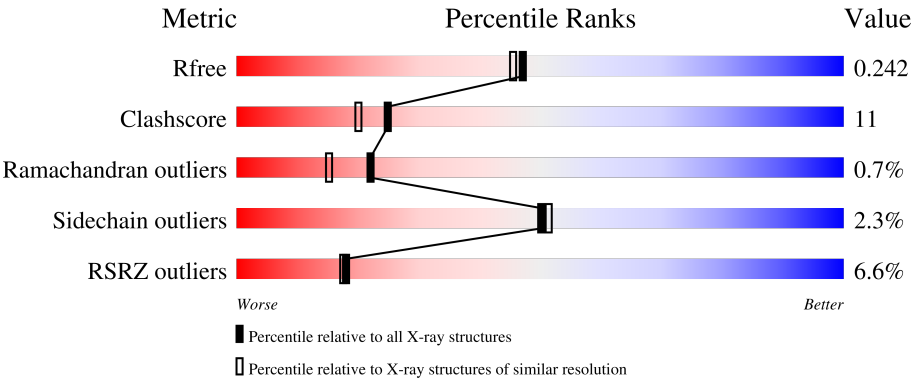
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 <=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	C	13	85% 15%
1	E	13	85% 15%
2	D	18	22% 44% 44% 11%
2	F	18	6% 56% 22% 11% 11%
3	A	352	7% 77% 18%

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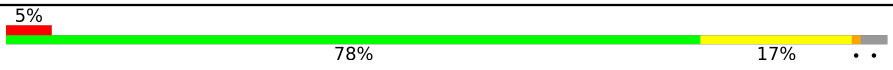
Mol	Chain	Length	Quality of chain
3	B	352	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7523 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 DNA chain called 5'-D(*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	13	Total	C	N	O	P	0	0	0
			272	129	57	74	12			
1	E	13	Total	C	N	O	P	0	0	0
			272	129	57	74	12			

- Molecule 2 is a DNA chain called 5'-D(*TP*CP*TP*TP*TP*GP*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	18	Total	C	N	O	P	0	0	1
			337	162	51	107	17			
2	F	18	Total	C	N	O	P	0	0	0
			353	172	53	111	17			

- Molecule 3 is a protein called DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	341	Total	C	N	O	S	0	0	0
			2743	1760	472	504	7			
3	B	341	Total	C	N	O	S	0	0	0
			2743	1760	472	504	7			

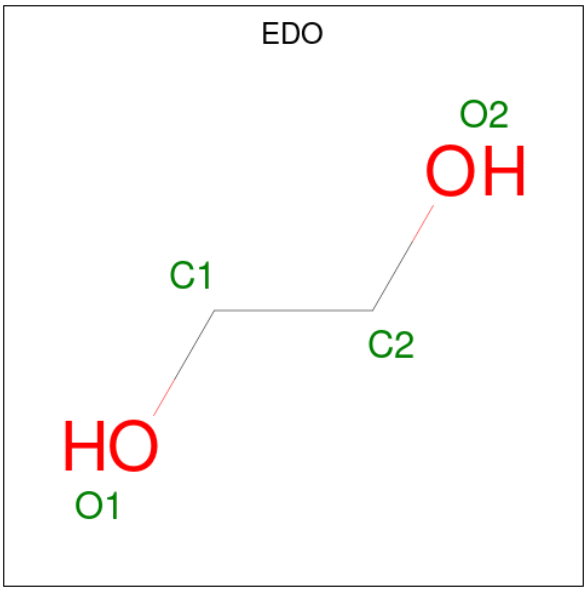
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

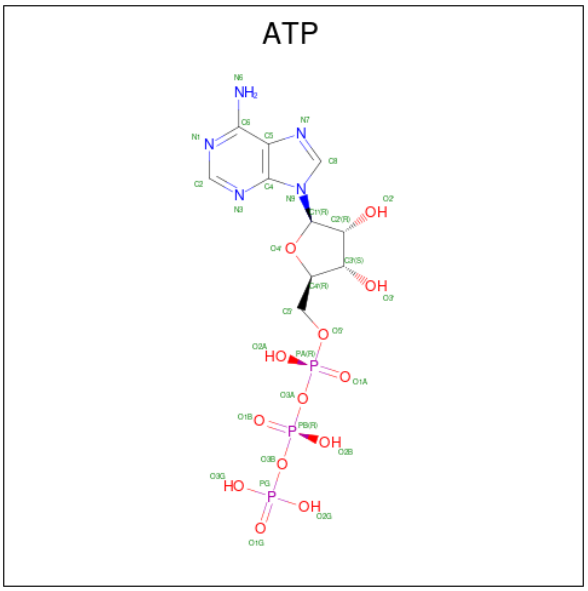
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total Na 1 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C O 4 2 2	0	0

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			29	10	5	11	3		
7	B	1	Total	C	N	O	P	0	0
			29	10	5	11	3		

- Molecule 8 is water.

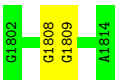
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	48	Total	O	0	0
			48	48		
8	D	42	Total	O	0	0
			42	42		
8	E	48	Total	O	0	0
			48	48		
8	F	75	Total	O	0	0
			75	75		
8	A	261	Total	O	0	0
			261	261		
8	B	261	Total	O	0	0
			261	261		

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: 5'-D(*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*CP*A)-3'

Chain C:



• Molecule 1: 5'-D(*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*CP*A)-3'

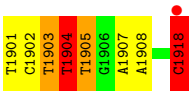
Chain E:

• Molecule 2: 5'-D(*TP*CP*TP*TP*TP*GP*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'

Chain D:

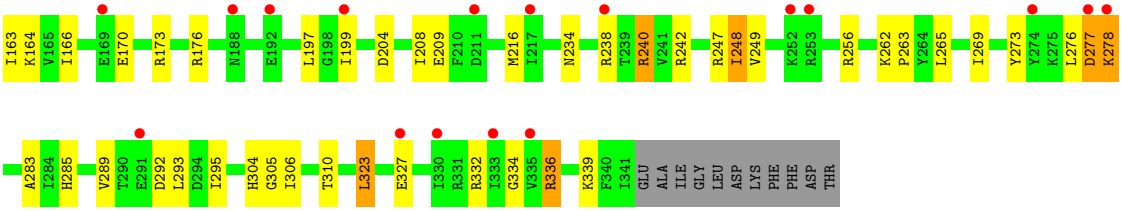
• Molecule 2: 5'-D(*TP*CP*TP*TP*TP*GP*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'

Chain F:



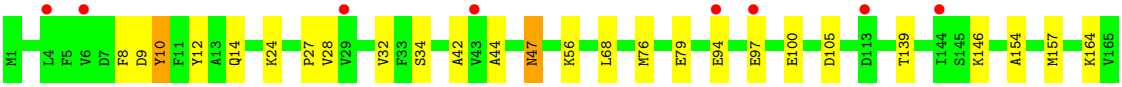
• Molecule 3: DNA polymerase IV

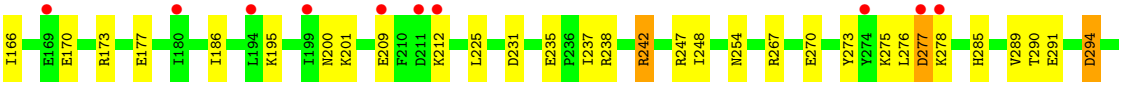
Chain A:

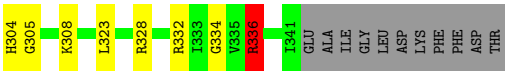


• Molecule 3: DNA polymerase IV

Chain B:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	98.73Å 102.29Å 106.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.03 19.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.90-2.03) 99.6 (19.85-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.256 0.213 , 0.242	Depositor DCC
R_{free} test set	1051 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7523	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 41.51 % 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 2.3348e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	C	0.59	0/307	0.87	0/474
1	E	0.62	0/307	0.90	0/474
2	D	2.04	5/373 (1.3%)	2.39	13/572 (2.3%)
2	F	1.80	5/391 (1.3%)	2.34	19/599 (3.2%)
3	A	0.46	0/2782	0.66	1/3736 (0.0%)
3	B	0.49	0/2782	0.68	1/3736 (0.0%)
All	All	0.79	10/6942 (0.1%)	1.05	34/9591 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
2	D	0	2
2	F	1	3
All	All	1	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1904	DT	C5-C6	24.61	1.51	1.34
2	D	1905	DT	C5-C6	21.86	1.49	1.34
2	F	1904	DT	C5-C6	21.83	1.49	1.34
2	F	1905	DT	C5-C6	19.33	1.47	1.34
2	D	1905	DT	N1-C6	14.76	1.48	1.38
2	F	1905	DT	N1-C6	11.82	1.46	1.38
2	F	1904	DT	N1-C6	6.22	1.42	1.38
2	F	1905	DT	C5-C7	5.87	1.53	1.50
2	D	1905	DT	C5-C7	5.67	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1904	DT	C5-C7	5.28	1.53	1.50

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1904	DT	C4-C5-C7	-37.03	96.78	119.00
2	F	1905	DT	C6-C5-C7	-25.36	107.68	122.90
2	F	1904	DT	C6-C5-C7	-24.23	108.36	122.90
2	F	1904	DT	C4-C5-C7	-17.11	108.74	119.00
2	D	1905	DT	C6-C5-C7	-15.68	113.50	122.90
2	D	1904	DT	C6-C5-C7	-14.95	113.93	122.90
2	F	1904	DT	O5'-P-OP1	-14.21	92.91	105.70
2	D	1905	DT	C5-C4-O4	-13.85	115.21	124.90
2	F	1904	DT	O5'-P-OP2	-13.43	93.62	105.70
2	D	1905	DT	C4-C5-C6	-12.00	110.80	118.00
2	D	1904	DT	C6-N1-C2	-11.83	115.39	121.30
2	F	1918	DC	C1'-O4'-C4'	-11.01	99.09	110.10
2	D	1905	DT	N3-C4-C5	9.76	121.05	115.20
2	F	1904	DT	C5-C4-O4	-8.30	119.09	124.90
2	F	1905	DT	C5-C4-O4	-7.99	119.31	124.90
2	D	1904	DT	C2-N1-C1'	7.92	130.87	118.20
2	F	1904	DT	C4-C5-C6	-7.73	113.36	118.00
2	D	1905	DT	C6-N1-C2	-7.17	117.72	121.30
2	F	1903	DT	OP1-P-O3'	6.92	120.42	105.20
2	D	1904	DT	N3-C4-O4	6.64	123.88	119.90
2	F	1904	DT	C6-N1-C2	-6.58	118.01	121.30
2	D	1905	DT	N3-C4-O4	6.39	123.73	119.90
2	F	1905	DT	C4-C5-C7	-6.26	115.25	119.00
2	F	1905	DT	N3-C4-O4	6.14	123.58	119.90
3	B	336	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	F	1905	DT	C6-N1-C2	-5.88	118.36	121.30
2	D	1904	DT	C6-N1-C1'	-5.81	111.69	120.40
3	A	336	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	F	1902	DC	P-O3'-C3'	5.50	126.30	119.70
2	F	1905	DT	N1-C1'-C2'	5.42	122.91	112.60
2	D	1904	DT	C5-C6-N1	-5.40	120.46	123.70
2	F	1905	DT	C5-C6-N1	-5.34	120.49	123.70
2	F	1904	DT	N3-C4-O4	5.16	122.99	119.90
2	F	1905	DT	O4'-C1'-N1	5.12	111.58	108.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1918	DC	C1'

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	1904	DT	Sidechain
2	D	1905	DT	Sidechain
1	E	1813	DC	Sidechain
2	F	1904	DT	Sidechain
2	F	1905	DT	Sidechain
2	F	1918	DC	Sidechain

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	C	272	0	147	5	0
1	E	272	0	147	1	0
2	D	337	0	194	17	0
2	F	353	0	207	12	1
3	A	2743	0	2889	63	1
3	B	2743	0	2889	59	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
5	F	1	0	0	0	0
6	F	4	0	6	2	0
7	A	29	0	8	4	0
7	B	29	0	8	3	0
8	A	261	0	0	11	0
8	B	261	0	0	10	1
8	C	48	0	0	1	1
8	D	42	0	0	1	0
8	E	48	0	0	0	0
8	F	75	0	0	2	0
All	All	7523	0	6495	143	2

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 11.

All (143) 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)
3:B:14:GLN:HE22	3:B:139:THR:H	1.15	0.95
3:A:14:GLN:HE22	3:A:139:THR:H	1.03	0.91
3:B:285:HIS:HD2	8:B:1857:HOH:O	1.56	0.88
2:D:1918:DC:H5'	3:B:200:ASN:ND2	1.90	0.85
3:A:51:ARG:HH22	7:A:1814:ATP:PG	2.04	0.81
3:A:242:ARG:HG3	3:A:242:ARG:HH11	1.50	0.77
7:A:1814:ATP:O2G	8:A:1945:HOH:O	2.03	0.77
3:A:157:MET:CE	3:A:166:ILE:HD11	2.15	0.76
3:B:68:LEU:HB3	8:B:2064:HOH:O	1.86	0.74
3:A:157:MET:HE2	3:A:166:ILE:HD11	1.69	0.73
3:A:51:ARG:NH2	7:A:1814:ATP:O3G	2.22	0.73
3:B:10:TYR:HA	7:B:1815:ATP:O2B	1.89	0.72
2:F:1918:DC:C2	2:F:1918:DC:H4'	2.23	0.71
3:B:304:HIS:HD2	3:B:305:GLY:O	1.75	0.70
3:B:14:GLN:NE2	3:B:139:THR:H	1.87	0.70
3:A:14:GLN:NE2	3:A:139:THR:H	1.86	0.69
3:A:285:HIS:HD2	8:A:1851:HOH:O	1.75	0.69
3:B:166:ILE:HG23	3:B:170:GLU:HG2	1.75	0.69
2:D:1904:DT:OP1	3:A:34:SER:CB	2.41	0.68
3:A:289:VAL:HG22	3:A:295:ILE:CD1	2.24	0.68
2:F:1907:DA:P	3:B:336:ARG:HH22	2.18	0.67
3:B:79:GLU:HG2	8:B:1998:HOH:O	1.94	0.66
2:D:1904:DT:OP1	3:A:34:SER:HB3	1.94	0.66
3:B:254:ASN:ND2	3:B:291:GLU:HG3	2.11	0.65
3:A:289:VAL:HG22	3:A:295:ILE:HD12	1.77	0.65
2:F:1904:DT:O2	6:F:1204:EDO:H22	1.99	0.63
3:A:283:ALA:HB2	3:A:339:LYS:HD2	1.79	0.63
3:B:157:MET:CE	3:B:166:ILE:HD11	2.29	0.63
2:F:1918:DC:C2	2:F:1918:DC:C4'	2.79	0.62
3:B:157:MET:HE2	3:B:166:ILE:HD11	1.81	0.62
3:B:247:ARG:NH1	8:B:1973:HOH:O	2.32	0.59
3:B:27:PRO:HA	3:B:47:ASN:HD21	1.68	0.59
3:A:262:LYS:HB2	3:A:263:PRO:HD3	1.86	0.58
8:C:632:HOH:O	3:A:339:LYS:HD3	2.04	0.57
2:F:1918:DC:H5"	8:F:669:HOH:O	2.04	0.57
3:B:157:MET:HE3	3:B:164:LYS:HD3	1.86	0.57
3:B:68:LEU:HD22	8:B:2064:HOH:O	2.03	0.57
3:B:177:GLU:O	3:B:201:LYS:NZ	2.35	0.57
3:A:97:GLU:OE1	3:A:97:GLU:N	2.32	0.56
3:A:277:ASP:O	8:A:2014:HOH:O	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1918:DC:C5'	3:B:200:ASN:ND2	2.66	0.56
3:B:154:ALA:HA	3:B:157:MET:HE2	1.87	0.55
3:A:289:VAL:CG2	3:A:332:ARG:HB2	2.37	0.55
3:A:157:MET:HE1	3:A:166:ILE:HD11	1.87	0.55
2:F:1907:DA:O5'	3:B:336:ARG:NH2	2.40	0.55
3:B:28:VAL:H	3:B:47:ASN:ND2	2.04	0.55
2:F:1918:DC:O2	2:F:1918:DC:O4'	2.24	0.55
2:F:1904:DT:OP1	3:B:34:SER:OG	2.17	0.54
1:C:1808:DG:H2"	1:C:1809:DG:C5'	2.37	0.53
3:A:79:GLU:O	3:A:83:GLN:HG3	2.08	0.53
3:A:248:ILE:HA	3:A:334:GLY:HA3	1.90	0.53
3:B:273:TYR:HA	3:B:276:LEU:HD12	1.90	0.53
3:B:12:TYR:HE2	3:B:76:MET:HE1	1.74	0.53
2:D:1902:DC:OP2	3:A:37:PHE:CE2	2.62	0.53
3:A:247:ARG:HE	3:A:249:VAL:CG1	2.21	0.53
3:A:31:CYS:HB3	3:A:61:ILE:HD11	1.91	0.52
3:A:157:MET:HE3	3:A:164:LYS:HD3	1.92	0.52
2:D:1906:DG:OP2	3:A:248:ILE:HG22	2.10	0.51
3:A:277:ASP:O	3:A:278:LYS:HB2	2.10	0.51
3:A:240:ARG:HA	8:A:1842:HOH:O	2.10	0.51
3:A:46:ALA:HB1	3:A:50:ALA:HB3	1.93	0.51
3:A:166:ILE:HG23	3:A:170:GLU:HG2	1.92	0.51
3:A:242:ARG:HH11	3:A:242:ARG:CG	2.23	0.50
3:B:294:ASP:CG	3:B:328:ARG:HH12	2.15	0.50
3:B:248:ILE:HA	3:B:334:GLY:HA3	1.92	0.50
3:A:242:ARG:HG3	3:A:242:ARG:NH1	2.23	0.49
3:A:240:ARG:O	3:A:240:ARG:HG3	2.13	0.49
6:F:1204:EDO:H21	3:B:76:MET:CE	2.42	0.49
3:A:199:ILE:HG23	3:A:204:ASP:HB2	1.95	0.49
3:B:209:GLU:HB3	3:B:212:LYS:HB2	1.94	0.49
3:A:9:ASP:O	3:A:10:TYR:C	2.52	0.49
3:A:32:VAL:HG23	3:A:44:ALA:HB2	1.93	0.48
1:C:1809:DG:H5'	8:A:1815:HOH:O	2.11	0.48
2:D:1917:DC:OP1	3:B:195:LYS:NZ	2.42	0.48
3:A:176:ARG:NH1	8:A:2047:HOH:O	2.46	0.48
7:B:1815:ATP:N6	8:B:1879:HOH:O	2.46	0.48
3:A:197:LEU:HD11	3:A:216:MET:HG2	1.94	0.48
3:A:208:ILE:HG12	3:A:209:GLU:N	2.29	0.48
3:A:248:ILE:CD1	3:A:332:ARG:HB3	2.44	0.47
3:B:56:LYS:HE3	8:B:1865:HOH:O	2.13	0.47
2:F:1904:DT:OP1	3:B:34:SER:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:8:PHE:HB2	3:B:105:ASP:HB2	1.97	0.47
2:D:1904:DT:C2	2:D:1905:DT:C2	3.03	0.46
3:A:327:GLU:HG2	8:A:1854:HOH:O	2.16	0.46
3:B:254:ASN:HD22	3:B:291:GLU:CG	2.28	0.46
3:B:97:GLU:OE1	3:B:97:GLU:N	2.35	0.46
3:A:277:ASP:O	3:A:278:LYS:CB	2.63	0.46
2:D:1903:DT:H2"	2:D:1904:DT:H5'	1.97	0.46
1:C:1808:DG:H2"	1:C:1809:DG:H5"	1.97	0.46
3:B:242:ARG:HD2	8:B:1918:HOH:O	2.15	0.46
3:A:289:VAL:HB	3:A:332:ARG:HB2	1.98	0.45
3:B:173:ARG:HG2	3:B:173:ARG:HH11	1.82	0.45
3:B:254:ASN:ND2	3:B:291:GLU:CG	2.79	0.45
3:B:267:ARG:HD2	8:B:1824:HOH:O	2.15	0.45
3:B:290:THR:OG1	3:B:294:ASP:HB2	2.17	0.45
3:A:8:PHE:CD2	3:A:105:ASP:HA	2.52	0.45
3:A:32:VAL:HA	8:A:1978:HOH:O	2.17	0.45
3:A:265:LEU:O	3:A:269:ILE:HG13	2.17	0.45
3:A:304:HIS:HD2	3:A:305:GLY:O	1.98	0.45
2:F:1903:DT:H1'	3:B:42:ALA:HB2	1.99	0.45
3:A:306:ILE:HG23	3:A:310:THR:HB	1.99	0.45
1:C:1808:DG:C2'	1:C:1809:DG:H5"	2.47	0.45
3:A:154:ALA:HA	3:A:157:MET:HE2	1.98	0.45
3:A:292:ASP:O	3:A:293:LEU:HB2	2.16	0.45
3:B:9:ASP:O	3:B:10:TYR:C	2.54	0.45
1:C:1808:DG:H2"	1:C:1809:DG:H5'	1.99	0.44
3:A:173:ARG:HG2	3:A:173:ARG:HH11	1.82	0.44
3:B:100:GLU:HB2	3:B:237:ILE:HG23	1.99	0.44
3:B:157:MET:HE1	3:B:166:ILE:HD11	2.00	0.44
2:D:1907:DA:P	3:A:336:ARG:HH22	2.41	0.44
3:A:248:ILE:HG23	3:A:332:ARG:NH2	2.31	0.44
3:B:247:ARG:NH2	3:B:275:LYS:HG3	2.33	0.44
2:F:1901:DT:H5'	8:F:572:HOH:O	2.17	0.43
3:A:247:ARG:CZ	8:A:2008:HOH:O	2.65	0.43
2:D:1904:DT:H6	2:D:1904:DT:H2'	1.55	0.43
2:D:1903:DT:H1'	3:A:42:ALA:HB2	2.01	0.43
2:D:1911:DC:H2"	2:D:1912:DT:C5'	2.49	0.43
3:A:173:ARG:HG2	3:A:173:ARG:NH1	2.34	0.42
3:A:289:VAL:HG21	3:A:332:ARG:HD3	2.01	0.42
3:B:289:VAL:HB	3:B:332:ARG:HB2	2.01	0.42
3:B:79:GLU:OE2	3:B:275:LYS:NZ	2.46	0.42
2:D:1918:DC:H5"	8:D:552:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1908:DA:OP1	3:B:242:ARG:NH1	2.52	0.42
2:D:1912:DT:H5'	2:D:1912:DT:H6	1.84	0.42
2:D:1918:DC:H4'	3:B:200:ASN:CB	2.50	0.42
3:A:142:VAL:O	3:A:163:ILE:HA	2.19	0.42
3:A:273:TYR:HA	3:A:276:LEU:HD12	2.02	0.42
1:E:1814:DA:H2"	7:B:1815:ATP:H4'	2.01	0.42
3:A:13:ALA:O	3:A:17:GLU:HG3	2.20	0.42
3:B:173:ARG:HG2	3:B:173:ARG:NH1	2.35	0.41
3:B:270:GLU:OE2	3:B:308:LYS:HD3	2.20	0.41
3:B:304:HIS:HE1	8:B:1820:HOH:O	2.02	0.41
3:B:186:ILE:HD11	3:B:225:LEU:HD21	2.03	0.41
2:D:1903:DT:H4'	8:A:1964:HOH:O	2.21	0.41
3:B:146:LYS:NZ	3:B:231:ASP:OD2	2.54	0.41
3:A:10:TYR:HA	7:A:1814:ATP:O1G	2.20	0.41
3:A:256:ARG:NH2	3:A:323:LEU:O	2.48	0.41
3:B:12:TYR:HE2	3:B:76:MET:CE	2.34	0.41
3:B:157:MET:HE3	3:B:164:LYS:CE	2.51	0.41
3:B:277:ASP:O	3:B:278:LYS:HB2	2.21	0.40
3:A:234:ASN:HA	8:A:1985:HOH:O	2.21	0.40
3:B:28:VAL:H	3:B:47:ASN:HD21	1.68	0.40
3:B:32:VAL:HG23	3:B:44:ALA:HB2	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1918:DC:N3	3:A:22:SER:OG[3_656]	2.03	0.17
8:C:337:HOH:O	8:B:1998:HOH:O[3_656]	2.18	0.02

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
3	A	339/352 (96%)	326 (96%)	10 (3%)	3 (1%)	17 10
3	B	339/352 (96%)	323 (95%)	14 (4%)	2 (1%)	25 18
All	All	678/704 (96%)	649 (96%)	24 (4%)	5 (1%)	22 15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	277	ASP
3	A	277	ASP
3	A	10	TYR
3	A	278	LYS
3	B	10	TYR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	300/309 (97%)	295 (98%)	5 (2%)	60 63
3	B	300/309 (97%)	291 (97%)	9 (3%)	41 40
All	All	600/618 (97%)	586 (98%)	14 (2%)	50 51

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	24	LYS
3	A	238	ARG
3	A	240	ARG
3	A	248	ILE
3	A	323	LEU
3	B	24	LYS
3	B	47	ASN
3	B	94	GLU
3	B	235	GLU
3	B	238	ARG
3	B	242	ARG

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Mol	Chain	Res	Type
3	B	294	ASP
3	B	323	LEU
3	B	336	ARG

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

Mol	Chain	Res	Type
3	A	14	GLN
3	A	188	ASN
3	A	285	HIS
3	A	304	HIS
3	B	14	GLN
3	B	47	ASN
3	B	188	ASN
3	B	234	ASN
3	B	304	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\#\|Z\|>2$
7	ATP	B	1815	4	25,31,33	1.60	6 (24%)	26,48,52	1.91	7 (26%)
6	EDO	F	1204	-	3,3,3	2.36	2 (66%)	2,2,2	0.53	0
7	ATP	A	1814	4	25,31,33	1.63	6 (24%)	26,48,52	2.00	4 (15%)

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
7	ATP	B	1815	4	-	2/18/31/38	0/3/3/3
6	EDO	F	1204	-	-	0/1/1/1	-
7	ATP	A	1814	4	-	1/18/31/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1814	ATP	PA-O5'	-3.91	1.43	1.59
7	B	1815	ATP	PG-O2G	-3.60	1.41	1.54
7	B	1815	ATP	C2-N3	3.33	1.37	1.32
7	A	1814	ATP	PG-O2G	-3.24	1.42	1.54
7	B	1815	ATP	PB-O2B	-3.19	1.40	1.55
7	A	1814	ATP	C2-N3	2.97	1.36	1.32
7	A	1814	ATP	PA-O2A	-2.87	1.41	1.55
6	F	1204	EDO	O1-C1	2.84	1.56	1.42
6	F	1204	EDO	O2-C2	2.73	1.56	1.42
7	B	1815	ATP	PA-O5'	-2.69	1.48	1.59
7	A	1814	ATP	C8-N7	-2.60	1.30	1.34
7	B	1815	ATP	PA-O2A	-2.18	1.45	1.55
7	A	1814	ATP	O4'-C1'	-2.17	1.37	1.42
7	B	1815	ATP	C2'-C3'	-2.02	1.48	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1814	ATP	O4'-C4'-C5'	-5.57	100.36	109.52
7	A	1814	ATP	PB-O3B-PG	4.84	149.44	132.83
7	A	1814	ATP	C4'-O4'-C1'	4.64	114.19	109.81
7	B	1815	ATP	O4'-C4'-C5'	-3.84	103.20	109.52
7	B	1815	ATP	PB-O3B-PG	3.78	145.79	132.83
7	B	1815	ATP	C4'-O4'-C1'	3.67	113.27	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1815	ATP	C3'-C2'-C1'	3.62	106.97	102.78
7	B	1815	ATP	O3G-PG-O3B	2.93	114.45	104.64
7	A	1814	ATP	C4-C5-N7	2.65	112.16	109.40
7	B	1815	ATP	C4-C5-N7	2.55	112.06	109.40
7	B	1815	ATP	C2'-C1'-N9	-2.31	108.13	112.48

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1814	ATP	PG-O3B-PB-O2B
7	B	1815	ATP	PG-O3B-PB-O2B
7	B	1815	ATP	PG-O3B-PB-O1B

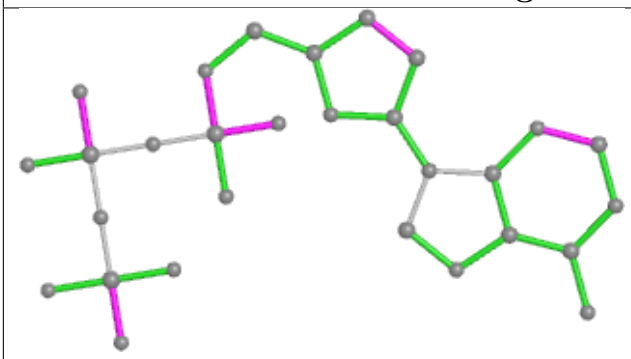
There are no ring outliers.

3 monomers are involved in 9 short contacts:

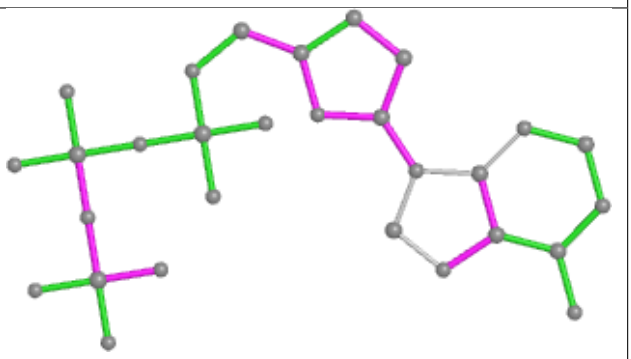
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1815	ATP	3	0
6	F	1204	EDO	2	0
7	A	1814	ATP	4	0

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

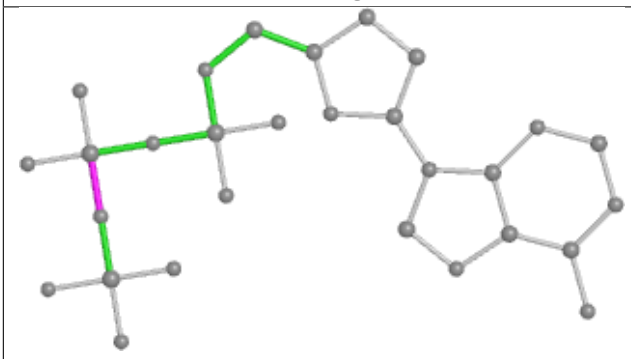
Ligand ATP B 1815



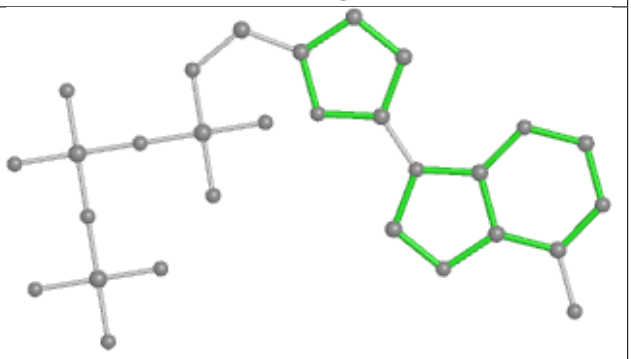
Bond lengths



Bond angles

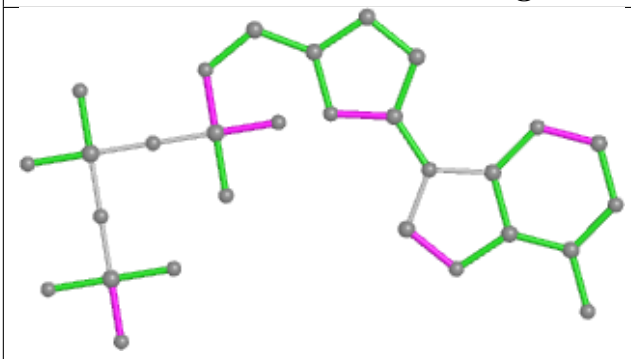


Torsions

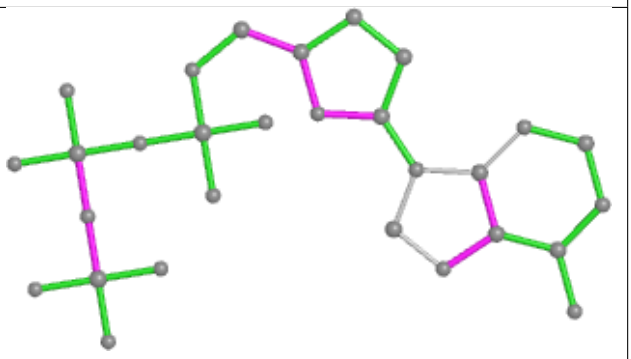


Rings

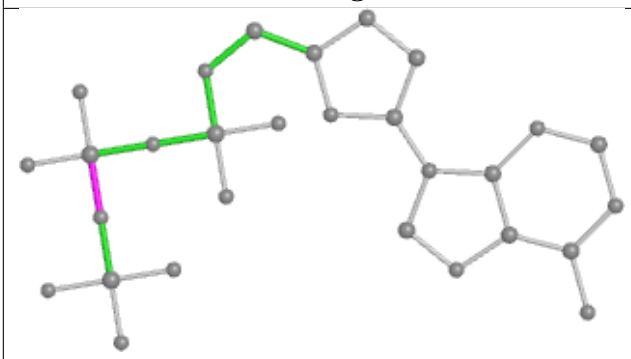
Ligand ATP A 1814



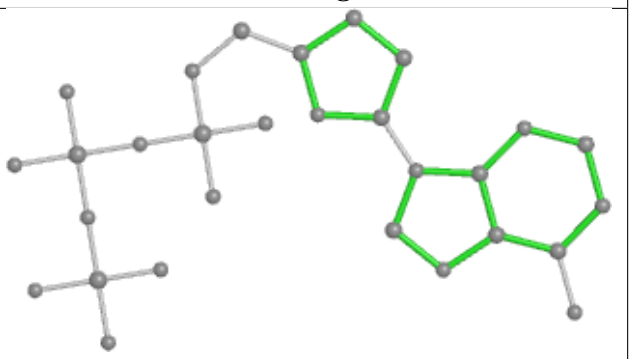
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	C	13/13 (100%)	-0.09	0 100 100	35, 44, 54, 58	0
1	E	13/13 (100%)	0.08	0 100 100	32, 42, 54, 55	0
2	D	18/18 (100%)	1.13	4 (22%) 0 0	39, 52, 110, 113	0
2	F	18/18 (100%)	0.11	1 (5%) 24 23	32, 44, 60, 88	0
3	A	341/352 (96%)	0.53	26 (7%) 13 13	28, 44, 67, 82	0
3	B	341/352 (96%)	0.43	18 (5%) 26 26	28, 40, 57, 73	0
All	All	744/766 (97%)	0.47	49 (6%) 18 17	28, 43, 65, 113	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1901	DT	13.4
3	A	252	LYS	7.0
3	B	169	GLU	4.5
3	A	274	TYR	4.1
3	A	38	GLU	3.9
2	D	1918	DC	3.7
3	A	36	ARG	3.6
3	A	253	ARG	3.5
3	A	116	ARG	3.5
2	D	1902	DC	3.4
3	A	333	ILE	3.4
3	B	209	GLU	3.4
3	A	94	GLU	3.2
3	B	194	LEU	3.1
2	F	1918	DC	3.0
2	D	1903	DT	2.9
3	A	169	GLU	2.8
3	A	238	ARG	2.8
3	B	211	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
3	A	278	LYS	2.7
3	A	277	ASP	2.6
3	B	97	GLU	2.6
3	A	35	GLY	2.5
3	A	211	ASP	2.5
3	B	43	VAL	2.5
3	B	199	ILE	2.5
3	A	43	VAL	2.4
3	B	113	ASP	2.4
3	B	180	ILE	2.4
3	B	6	VAL	2.3
3	B	278	LYS	2.3
3	B	212	LYS	2.3
3	B	277	ASP	2.3
3	B	4	LEU	2.2
3	A	144	ILE	2.2
3	A	113	ASP	2.2
3	B	144	ILE	2.2
3	B	29	VAL	2.2
3	A	291	GLU	2.2
3	B	94	GLU	2.1
3	A	330	ILE	2.1
3	A	327	GLU	2.1
3	A	30	VAL	2.1
3	A	217	ILE	2.0
3	A	188	ASN	2.0
3	A	335	VAL	2.0
3	B	274	TYR	2.0
3	A	192	GLU	2.0
3	A	199	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

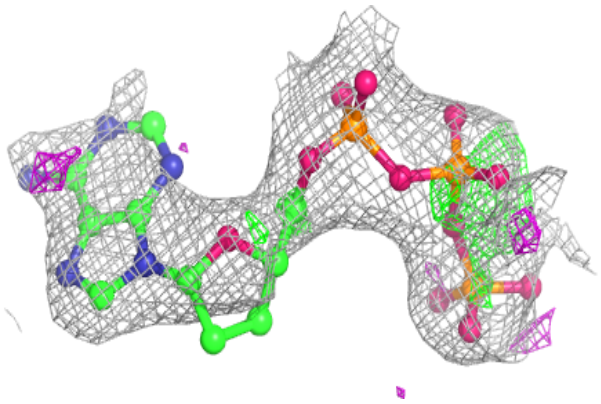
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

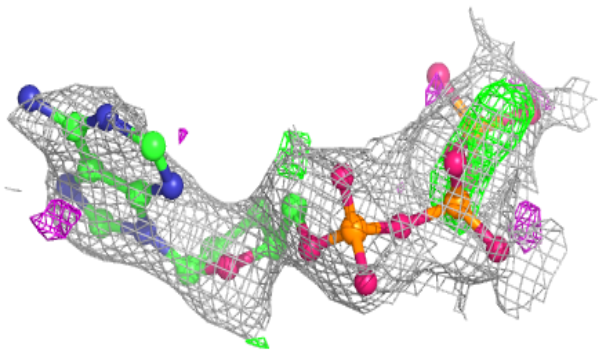
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	F	1204	4/4	0.65	0.39	53,54,55,58	0
7	ATP	A	1814	29/31	0.88	0.23	82,87,89,89	0
7	ATP	B	1815	29/31	0.92	0.15	41,46,55,59	0
5	NA	F	808	1/1	0.94	0.48	47,47,47,47	0
4	CA	A	801	1/1	0.97	0.07	36,36,36,36	0
4	CA	A	802	1/1	0.97	0.13	54,54,54,54	0
4	CA	B	803	1/1	0.99	0.08	38,38,38,38	0
4	CA	B	806	1/1	0.99	0.03	41,41,41,41	0
4	CA	C	805	1/1	0.99	0.15	50,50,50,50	0

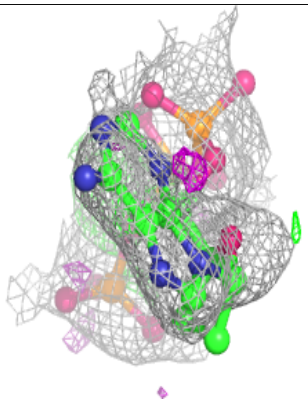
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 1814:

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

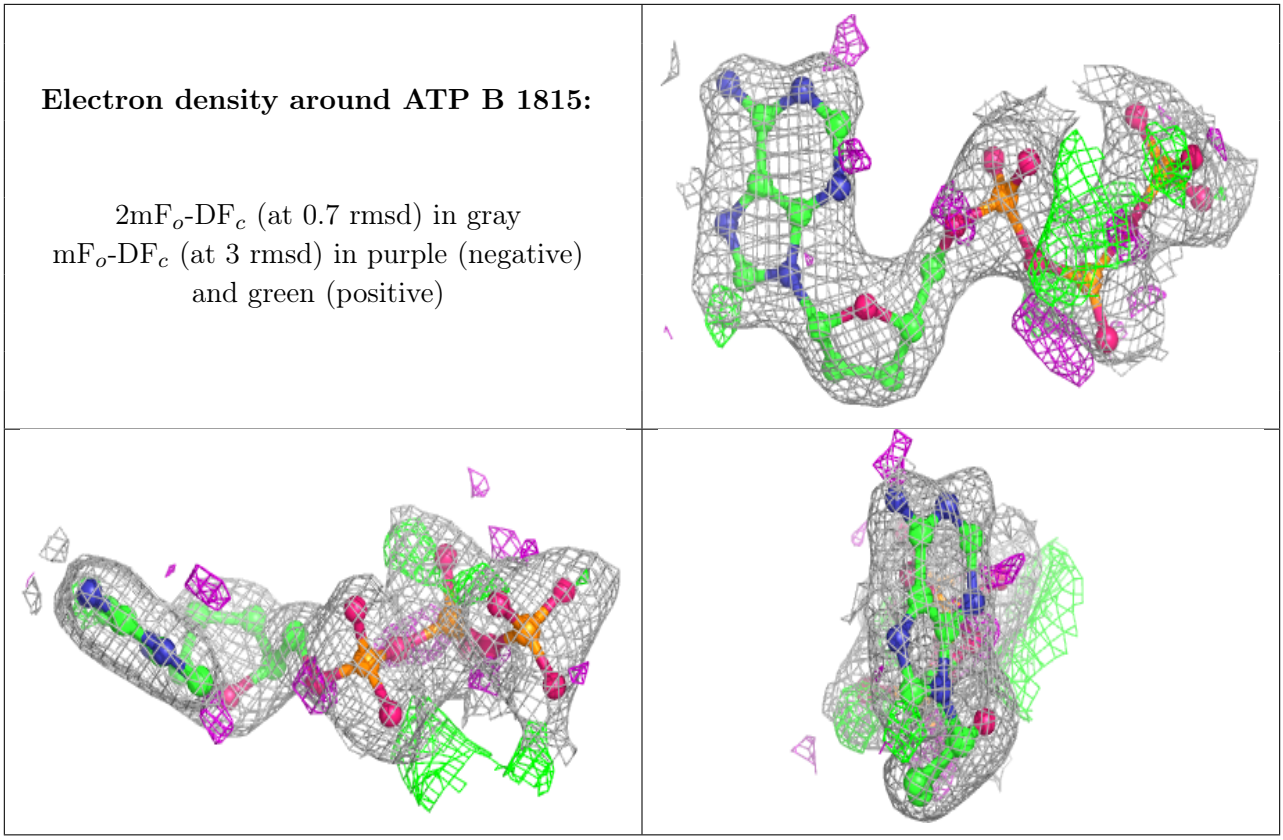






Electron density around ATP B 1815:

$2mF_o$-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.