Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:36 pm BST

PDB ID	:	1YXQ
Title	:	Crystal structure of actin in complex with swinholide A
Authors	:	Klenchin, V.A.; King, R.; Tanaka, J.; Marriott, G.; Rayment, I.
Deposited on	:	2005-02-22
Resolution	:	2.01 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:

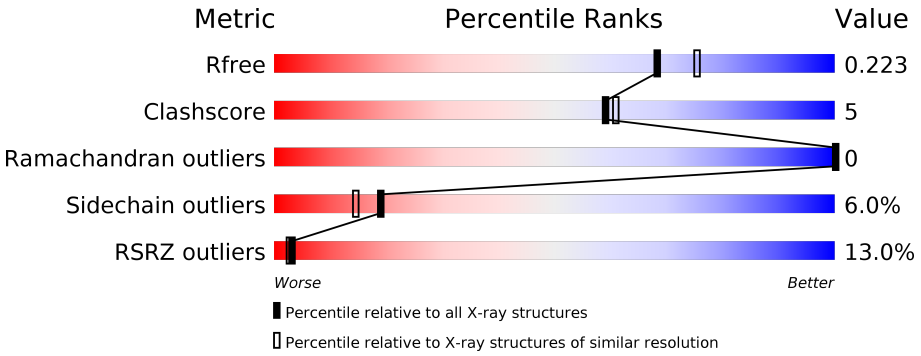
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	375	2% 84% 10% • 5%
1	B	375	23% 77% 17% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6057 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 actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	3	0
			2792	1769	470	535	18			
1	B	359	Total	C	N	O	S	0	0	0
			2812	1782	474	537	19			

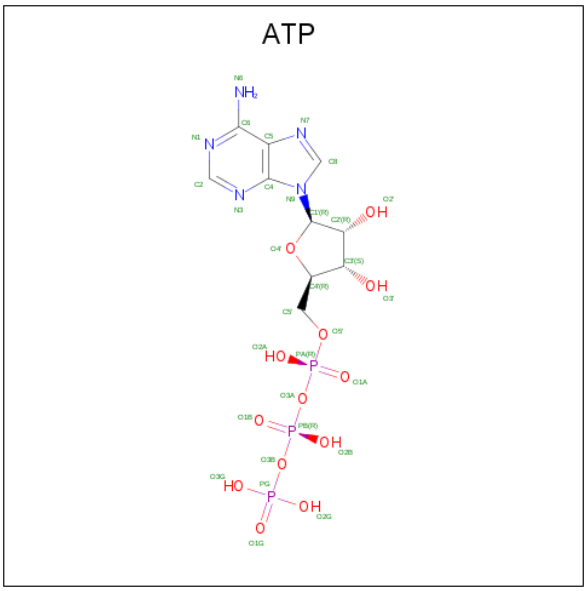
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	HIC	HIS	MODIFIED RESIDUE	UNP P68135
B	73	HIC	HIS	MODIFIED RESIDUE	UNP P68135

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

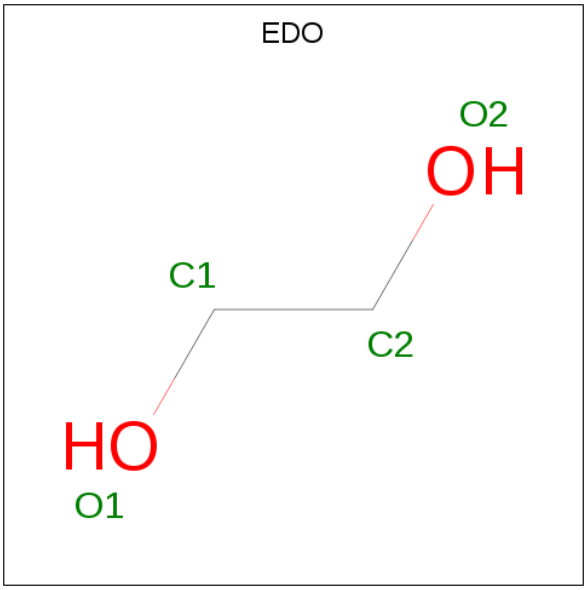
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



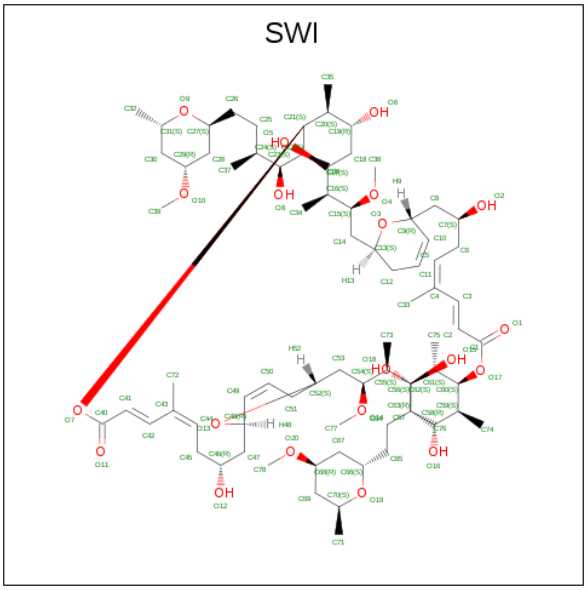
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is SWINHOLIDE A (three-letter code: SWI) (formula: $C_{78}H_{132}O_{20}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 98 78 20	0	0

- Molecule 6 is water.

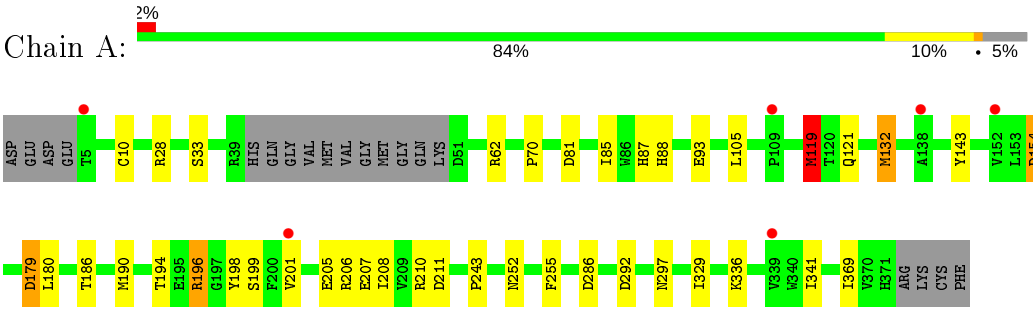
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	243	Total O 243 243	0	0
6	B	39	Total O 39 39	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

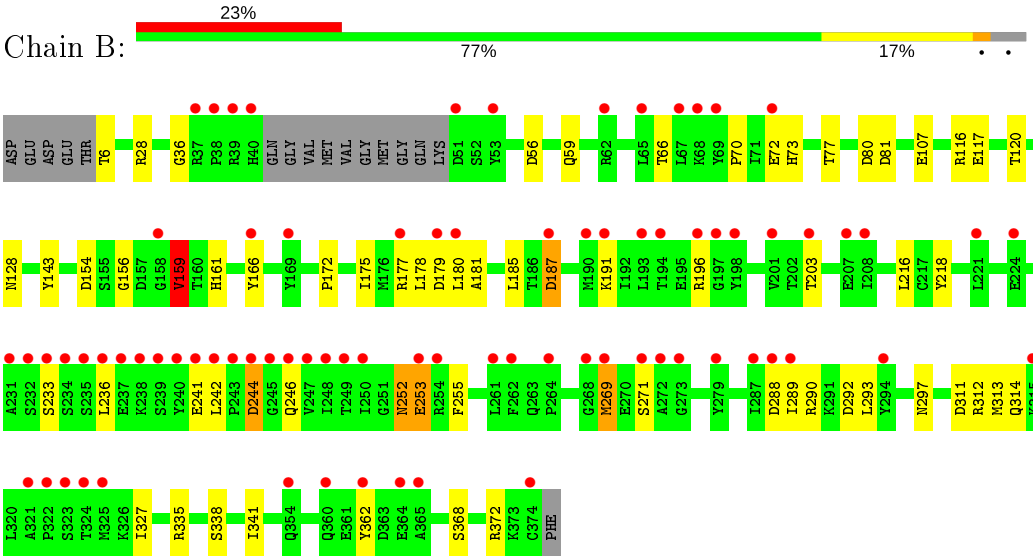
- Molecule 1: actin, alpha skeletal muscle

Chain A:



- Molecule 1: actin, alpha skeletal muscle

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.00Å 76.80Å 98.40Å 90.00° 101.20° 90.00°	Depositor
Resolution (Å)	50.00 – 2.01 33.60 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.01) 99.5 (33.60-2.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.184 , 0.219 0.197 , 0.223	Depositor DCC
R_{free} test set	3353 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6057	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SWI, MG, HIC, EDO, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.73	2/2853 (0.1%)	0.88	10/3867 (0.3%)
1	B	0.58	1/2860 (0.0%)	0.78	10/3875 (0.3%)
All	All	0.66	3/5713 (0.1%)	0.83	20/7742 (0.3%)

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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	269	MET	C-O	5.76	1.34	1.23
1	A	132	MET	SD-CE	-5.44	1.47	1.77
1	A	119	MET	SD-CE	5.04	2.06	1.77

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	196	ARG	NE-CZ-NH2	-13.94	113.33	120.30
1	A	196	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	A	154	ASP	CB-CG-OD2	6.89	124.50	118.30
1	B	311	ASP	CB-CG-OD2	6.67	124.30	118.30
1	A	196	ARG	CG-CD-NE	-6.49	98.17	111.80
1	A	179	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	154	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	179	ASP	CB-CG-OD2	6.38	124.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	286	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	187	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	80	ASP	CB-CG-OD2	5.76	123.48	118.30
1	B	244	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	292	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	159	VAL	CB-CA-C	-5.46	101.02	111.40
1	B	288	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	292	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	211	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	81	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	56	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	180	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	72	GLU	Peptide

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	2792	0	2756	23	0
1	B	2812	0	2781	24	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	B	98	0	131	11	0
6	A	243	0	0	7	0
6	B	39	0	0	2	0
All	All	6057	0	5704	54	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 5.

All (54) 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:119:MET:SD	1:A:119:MET:CE	2.06	1.43
5:B:600:SWI:H372	5:B:600:SWI:H361	1.10	1.07
5:B:600:SWI:C37	5:B:600:SWI:H361	1.88	1.01
5:B:600:SWI:H362	6:B:9013:HOH:O	1.72	0.89
5:B:600:SWI:C36	5:B:600:SWI:H372	2.03	0.79
1:A:207:GLU:OE1	1:A:210[A]:ARG:NH2	2.21	0.73
1:B:314:GLN:O	1:B:318:THR:HG23	1.89	0.73
1:A:207:GLU:OE1	1:A:210[A]:ARG:CZ	2.39	0.71
1:A:87:HIS:HD2	6:A:9085:HOH:O	1.74	0.71
1:B:191:LYS:NZ	6:B:9021:HOH:O	2.23	0.67
5:B:600:SWI:H363	5:B:600:SWI:O11	1.93	0.67
1:A:121:GLN:NE2	6:A:9163:HOH:O	2.31	0.64
1:B:313:MET:O	1:B:317:ILE:HG23	1.98	0.63
1:B:143:TYR:HB3	5:B:600:SWI:H763	1.81	0.62
1:A:297[A]:ASN:HD22	1:A:329:ILE:HD12	1.67	0.60
1:B:107:GLU:OE1	1:B:116:ARG:HG2	2.02	0.60
1:A:205:GLU:HA	1:A:208:ILE:HD12	1.84	0.58
1:B:318:THR:HG22	1:B:327:ILE:HD13	1.85	0.57
1:B:335:ARG:HA	1:B:338:SER:OG	2.04	0.57
1:B:73:HIC:HB2	1:B:159:VAL:HG13	1.88	0.55
1:A:341:ILE:HG23	5:B:600:SWI:H49	1.88	0.55
1:A:161:HIS:HD2	6:A:9138:HOH:O	1.91	0.54
1:A:88:HIS:HE1	1:A:93:GLU:OE2	1.92	0.51
1:B:218:TYR:O	1:B:255:PHE:HA	2.11	0.50
1:A:186:THR:O	1:A:190:MET:HG3	2.12	0.50
1:B:36:GLY:HA2	1:B:66:THR:O	2.11	0.50
1:A:179:ASP:HB3	6:A:9200:HOH:O	2.12	0.50
1:A:190:MET:SD	1:A:206:ARG:HG3	2.53	0.49
1:B:124:PHE:CD2	1:B:362:TYR:CG	3.01	0.49
1:B:172:PRO:HA	1:B:175:ILE:HD12	1.94	0.48
1:A:143:TYR:HB3	5:B:600:SWI:H373	1.96	0.48
1:A:201:VAL:HG13	6:A:9055:HOH:O	2.12	0.48
1:B:341:ILE:HG23	5:B:600:SWI:H10	1.96	0.47
5:B:600:SWI:C36	5:B:600:SWI:O11	2.61	0.47
1:A:70:PRO:HG2	1:A:85:ILE:HD12	1.98	0.46
1:B:117:GLU:HA	1:B:120:THR:HG22	1.96	0.46
1:B:161:HIS:NE2	1:B:177:ARG:HG3	2.31	0.46
1:B:73:HIC:HB2	1:B:159:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:THR:HA	1:A:198:TYR:O	2.16	0.45
5:B:600:SWI:C22	5:B:600:SWI:O11	2.59	0.45
1:A:154:ASP:CG	6:A:9140:HOH:O	2.54	0.45
1:A:119:MET:CB	1:A:119:MET:CE	2.95	0.45
1:B:117:GLU:O	1:B:120:THR:HG22	2.17	0.45
1:B:156:GLY:O	1:B:181:ALA:HB1	2.17	0.44
1:A:336:LYS:NZ	6:A:9098:HOH:O	2.50	0.44
1:A:10:CYS:HB3	1:A:105:LEU:HD23	1.99	0.44
1:B:178:LEU:CD1	1:B:271:SER:OG	2.67	0.42
1:A:252:ASN:HA	1:A:255:PHE:CE2	2.55	0.42
1:B:117:GLU:O	1:B:120:THR:CG2	2.67	0.42
1:B:124:PHE:O	1:B:128:ASN:HA	2.20	0.42
1:B:252:ASN:HD22	1:B:253:GLU:N	2.17	0.42
1:B:166:TYR:CE2	1:B:289:ILE:CG2	3.02	0.42
1:B:70:PRO:HG3	1:B:81:ASP:HB3	2.02	0.42
1:A:208:ILE:HD11	1:A:243:PRO:HG2	2.03	0.41

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	354/375 (94%)	348 (98%)	6 (2%)	0	100	100
1	B	354/375 (94%)	344 (97%)	10 (3%)	0	100	100
All	All	708/750 (94%)	692 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	303/317 (96%)	295 (97%)	8 (3%)	46 48
1	B	304/317 (96%)	276 (91%)	28 (9%)	9 5
All	All	607/634 (96%)	571 (94%)	36 (6%)	19 15

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	33	SER
1	A	62	ARG
1	A	119	MET
1	A	132	MET
1	A	196	ARG
1	A	199	SER
1	A	369	ILE
1	B	6	THR
1	B	28	ARG
1	B	59	GLN
1	B	77	THR
1	B	126	THR
1	B	159	VAL
1	B	180	LEU
1	B	185	LEU
1	B	187	ASP
1	B	196	ARG
1	B	203	THR
1	B	216	LEU
1	B	233	SER
1	B	236	LEU
1	B	241	GLU
1	B	242	LEU
1	B	244	ASP
1	B	246	GLN
1	B	252	ASN

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Mol	Chain	Res	Type
1	B	253	GLU
1	B	269	MET
1	B	290	ARG
1	B	293	LEU
1	B	297	ASN
1	B	312	ARG
1	B	317	ILE
1	B	368	SER
1	B	372	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	88	HIS
1	A	92	ASN
1	A	121	GLN
1	A	161	HIS
1	A	225	ASN
1	B	246	GLN
1	B	252	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	HIC	A	73	1	8,11,12	0.86	0	6,14,16	1.50	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	HIC	B	73	1	8,11,12	0.86	0	6,14,16	1.51	1 (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
1	HIC	A	73	1	-	1/5/6/8	0/1/1/1
1	HIC	B	73	1	-	2/5/6/8	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	73	HIC	CB-CA-C	-3.21	105.46	111.47
1	A	73	HIC	CB-CA-C	-3.16	105.54	111.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	O-C-CA-CB
1	B	73	HIC	N-CA-CB-CG
1	B	73	HIC	CA-CB-CG-ND1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	73	HIC	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
4	EDO	B	9002	-	3,3,3	0.65	0	2,2,2	0.27	0
5	SWI	B	600	-	102,102,102	2.21	40 (39%)	124,140,140	2.82	46 (37%)
3	ATP	B	2380	2	26,33,33	1.20	2 (7%)	31,52,52	1.53	3 (9%)
4	EDO	A	9001	-	3,3,3	0.49	0	2,2,2	0.22	0
3	ATP	A	1380	2	26,33,33	1.12	2 (7%)	31,52,52	1.44	2 (6%)

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
4	EDO	B	9002	-	-	1/1/1/1	-
5	SWI	B	600	-	-	30/126/170/170	0/4/5/5
3	ATP	B	2380	2	-	6/18/38/38	0/3/3/3
4	EDO	A	9001	-	-	0/1/1/1	-
3	ATP	A	1380	2	-	2/18/38/38	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	600	SWI	C63-C62	-5.77	1.43	1.53
5	B	600	SWI	O9-C27	-5.66	1.34	1.44
5	B	600	SWI	C26-C25	-5.51	1.37	1.53
5	B	600	SWI	C57-C56	-4.73	1.41	1.53
5	B	600	SWI	C6-C7	-4.68	1.46	1.53
5	B	600	SWI	C45-C44	-4.57	1.41	1.50
3	B	2380	ATP	C2-N3	4.34	1.39	1.32
5	B	600	SWI	O7-C21	4.19	1.51	1.44
3	A	1380	ATP	C2-N3	3.70	1.38	1.32
5	B	600	SWI	C69-C68	-3.61	1.43	1.52
5	B	600	SWI	C59-C58	-3.59	1.47	1.54
5	B	600	SWI	C22-C23	-3.57	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	600	SWI	C25-C24	-3.46	1.45	1.54
5	B	600	SWI	C28-C29	3.44	1.60	1.52
5	B	600	SWI	O20-C68	3.23	1.51	1.43
5	B	600	SWI	C20-C21	3.21	1.62	1.54
5	B	600	SWI	C42-C41	3.08	1.42	1.33
5	B	600	SWI	O17-C1	3.02	1.40	1.34
5	B	600	SWI	C69-C70	2.95	1.57	1.51
5	B	600	SWI	O2-C7	2.88	1.52	1.43
5	B	600	SWI	O13-C48	2.86	1.51	1.44
5	B	600	SWI	O13-C52	2.84	1.48	1.44
5	B	600	SWI	C55-C56	2.83	1.59	1.54
3	B	2380	ATP	C2-N1	2.78	1.39	1.33
5	B	600	SWI	O14-C77	2.67	1.51	1.42
5	B	600	SWI	C9-C10	2.64	1.54	1.50
3	A	1380	ATP	C2-N1	2.51	1.38	1.33
5	B	600	SWI	C8-C7	-2.51	1.46	1.52
5	B	600	SWI	O1-C1	-2.50	1.16	1.21
5	B	600	SWI	O9-C31	-2.37	1.40	1.44
5	B	600	SWI	C34-C16	2.36	1.58	1.53
5	B	600	SWI	C20-C19	2.32	1.58	1.54
5	B	600	SWI	C51-C50	-2.25	1.44	1.49
5	B	600	SWI	C72-C43	2.23	1.55	1.50
5	B	600	SWI	C10-C11	-2.23	1.26	1.32
5	B	600	SWI	O5-C17	-2.18	1.38	1.43
5	B	600	SWI	O10-C29	2.13	1.48	1.43
5	B	600	SWI	C57-C58	-2.13	1.47	1.53
5	B	600	SWI	C2-C1	2.12	1.53	1.48
5	B	600	SWI	O18-C62	-2.11	1.38	1.43
5	B	600	SWI	C42-C43	2.10	1.50	1.45
5	B	600	SWI	O3-C9	2.09	1.49	1.44
5	B	600	SWI	C2-C3	-2.03	1.26	1.33
5	B	600	SWI	O17-C60	2.00	1.47	1.44

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	600	SWI	C20-C21-C22	12.68	140.56	114.68
5	B	600	SWI	O8-C23-C24	9.28	127.27	109.83
5	B	600	SWI	C63-C62-C61	7.64	128.10	116.27
5	B	600	SWI	O17-C1-C2	7.03	127.35	111.38
5	B	600	SWI	C46-C45-C44	-6.90	101.69	113.15
5	B	600	SWI	C8-C9-C10	-5.97	102.59	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2380	ATP	N3-C2-N1	-5.68	119.80	128.68
5	B	600	SWI	C72-C43-C44	-5.62	112.58	123.59
3	A	1380	ATP	N3-C2-N1	-5.16	120.61	128.68
5	B	600	SWI	C33-C4-C3	-5.02	110.17	118.08
5	B	600	SWI	C8-C7-C6	5.01	122.78	113.18
5	B	600	SWI	O7-C21-C22	-5.01	95.84	107.50
5	B	600	SWI	C37-C24-C23	4.74	120.32	111.54
5	B	600	SWI	C72-C43-C42	-4.70	110.68	118.08
5	B	600	SWI	C13-C12-C11	-4.54	100.12	109.52
5	B	600	SWI	O7-C40-O11	-4.50	116.03	123.35
5	B	600	SWI	C7-C6-C5	4.10	119.95	113.15
5	B	600	SWI	C41-C42-C43	-4.00	120.19	126.23
3	B	2380	ATP	PA-O3A-PB	-3.96	119.25	132.83
5	B	600	SWI	C78-O20-C68	3.86	123.27	113.87
5	B	600	SWI	O1-C1-C2	-3.81	110.26	123.58
5	B	600	SWI	O9-C27-C26	3.63	117.53	107.89
5	B	600	SWI	C47-C48-C49	-3.62	106.67	112.94
5	B	600	SWI	C36-C22-C21	3.60	117.87	111.40
5	B	600	SWI	C64-C63-C62	3.42	116.95	111.39
5	B	600	SWI	O2-C7-C6	-3.39	100.41	109.47
5	B	600	SWI	C21-O7-C40	-3.29	112.15	117.47
5	B	600	SWI	C48-C49-C50	-3.25	114.33	122.88
5	B	600	SWI	O9-C31-C32	3.21	113.70	106.88
5	B	600	SWI	O7-C21-C20	-3.09	100.32	107.50
5	B	600	SWI	C13-O3-C9	2.94	117.89	112.84
5	B	600	SWI	C39-O10-C29	2.88	120.89	113.87
5	B	600	SWI	C28-C29-C30	-2.83	106.63	112.07
3	B	2380	ATP	O3G-PG-O3B	2.82	114.09	104.64
5	B	600	SWI	O18-C62-C63	-2.75	104.65	109.83
5	B	600	SWI	O17-C60-C61	2.68	113.75	107.50
5	B	600	SWI	O9-C27-C28	-2.65	105.81	110.04
5	B	600	SWI	O10-C29-C28	2.56	117.39	109.42
5	B	600	SWI	C32-C31-C30	-2.54	109.41	113.40
5	B	600	SWI	C31-O9-C27	2.41	118.94	114.00
5	B	600	SWI	C47-C46-C45	2.40	117.78	113.18
5	B	600	SWI	O13-C52-C53	-2.38	102.06	107.70
5	B	600	SWI	O4-C15-C14	2.37	115.02	109.29
3	A	1380	ATP	O3G-PG-O3B	2.33	112.45	104.64
5	B	600	SWI	O16-C58-C57	-2.32	104.45	109.11
5	B	600	SWI	O6-C19-C20	-2.32	104.69	109.98
5	B	600	SWI	O3-C9-C10	-2.31	105.30	110.91
5	B	600	SWI	O18-C62-C61	2.23	114.44	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	600	SWI	C24-C23-C22	-2.20	112.87	116.27
5	B	600	SWI	C52-C51-C50	2.15	113.97	109.52
5	B	600	SWI	O11-C40-C41	2.10	130.95	123.58

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2380	ATP	PB-O3B-PG-O3G
3	A	1380	ATP	PB-O3B-PG-O3G
5	B	600	SWI	O7-C21-C22-C36
5	B	600	SWI	C20-C21-C22-C23
5	B	600	SWI	C20-C21-C22-C36
5	B	600	SWI	C22-C23-C24-C25
5	B	600	SWI	C22-C23-C24-C37
5	B	600	SWI	O8-C23-C24-C37
5	B	600	SWI	C28-C29-O10-C39
5	B	600	SWI	C41-C42-C43-C44
5	B	600	SWI	C42-C43-C44-C45
5	B	600	SWI	C45-C46-C47-C48
5	B	600	SWI	O12-C46-C47-C48
5	B	600	SWI	C61-C62-C63-C76
5	B	600	SWI	C61-C62-C63-C64
5	B	600	SWI	O18-C62-C63-C76
5	B	600	SWI	O18-C62-C63-C64
5	B	600	SWI	C67-C68-O20-C78
5	B	600	SWI	C63-C64-C65-C66
5	B	600	SWI	C2-C3-C4-C33
5	B	600	SWI	O7-C21-C22-C23
5	B	600	SWI	O8-C23-C24-C25
5	B	600	SWI	C30-C29-O10-C39
5	B	600	SWI	C2-C3-C4-C5
5	B	600	SWI	C22-C21-O7-C40
5	B	600	SWI	C44-C45-C46-O12
4	B	9002	EDO	O1-C1-C2-O2
5	B	600	SWI	C46-C47-C48-O13
3	B	2380	ATP	PG-O3B-PB-O1B
5	B	600	SWI	C69-C68-O20-C78
5	B	600	SWI	C60-C61-C62-O18
5	B	600	SWI	C46-C47-C48-C49
5	B	600	SWI	C36-C22-C23-C24
5	B	600	SWI	C13-C14-C15-O4

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Mol	Chain	Res	Type	Atoms
3	A	1380	ATP	PB-O3B-PG-O1G
3	B	2380	ATP	PB-O3B-PG-O2G
3	B	2380	ATP	C3'-C4'-C5'-O5'
3	B	2380	ATP	PG-O3B-PB-O2B
3	B	2380	ATP	PB-O3B-PG-O1G

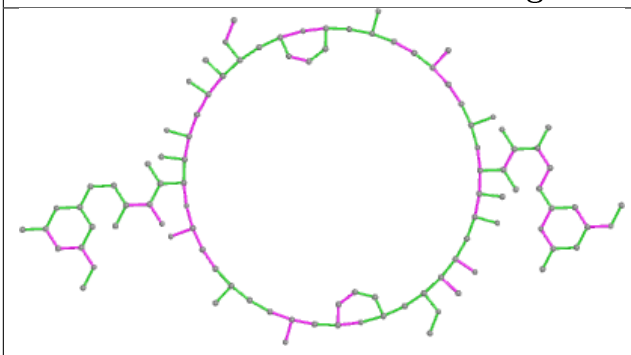
There are no ring outliers.

1 monomer is involved in 11 short contacts:

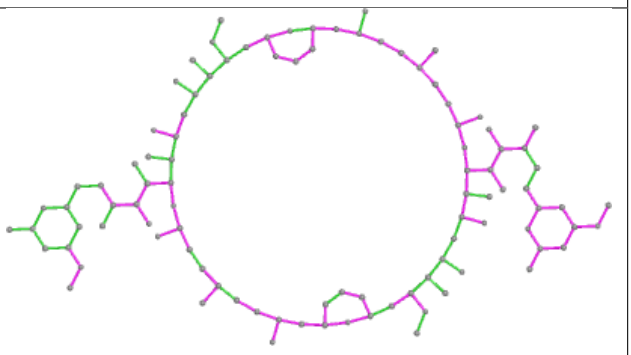
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	600	SWI	11	0

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.

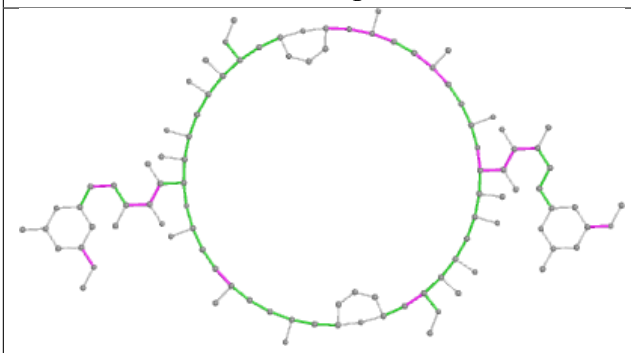
Ligand SWI B 600



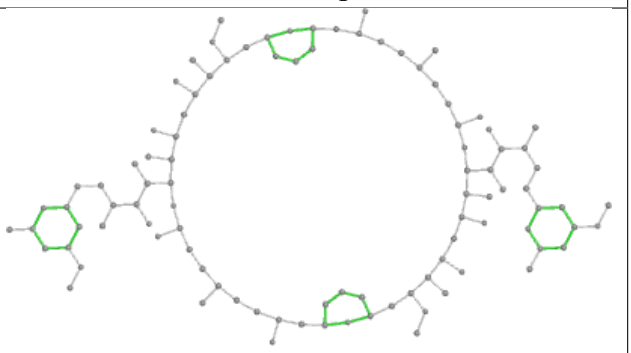
Bond lengths



Bond angles

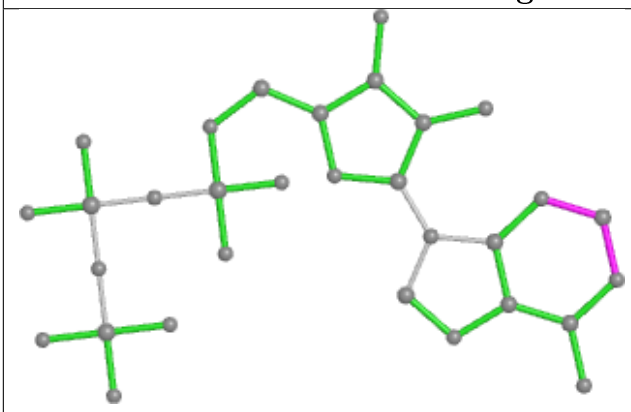


Torsions

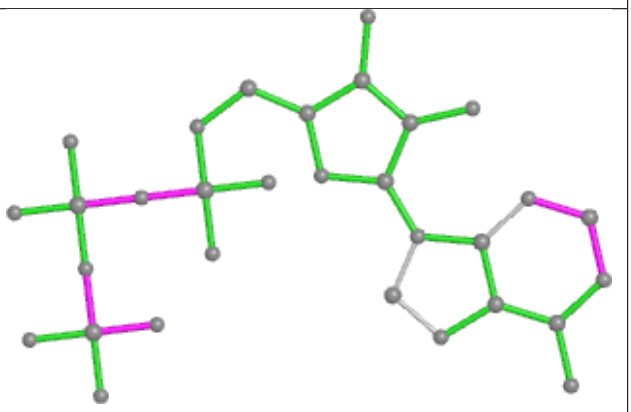


Rings

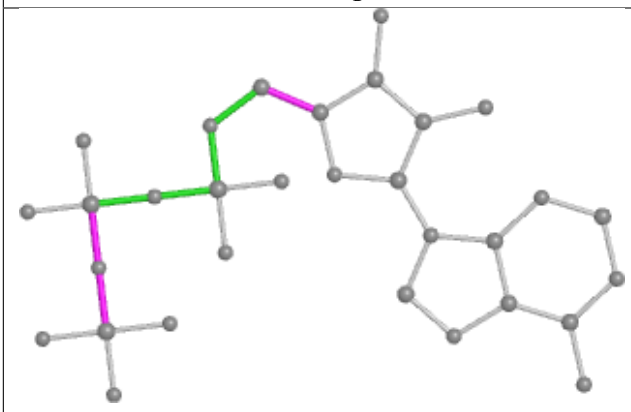
Ligand ATP B 2380



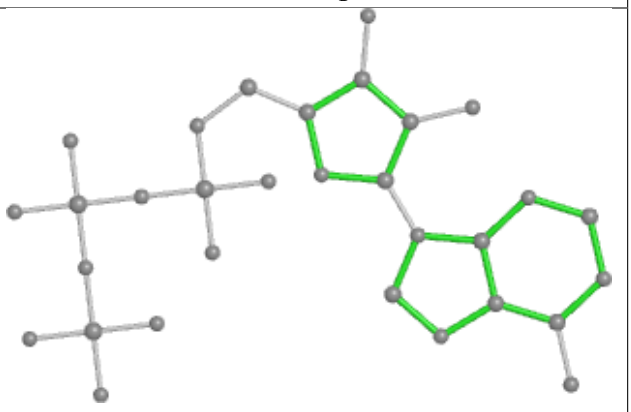
Bond lengths



Bond angles

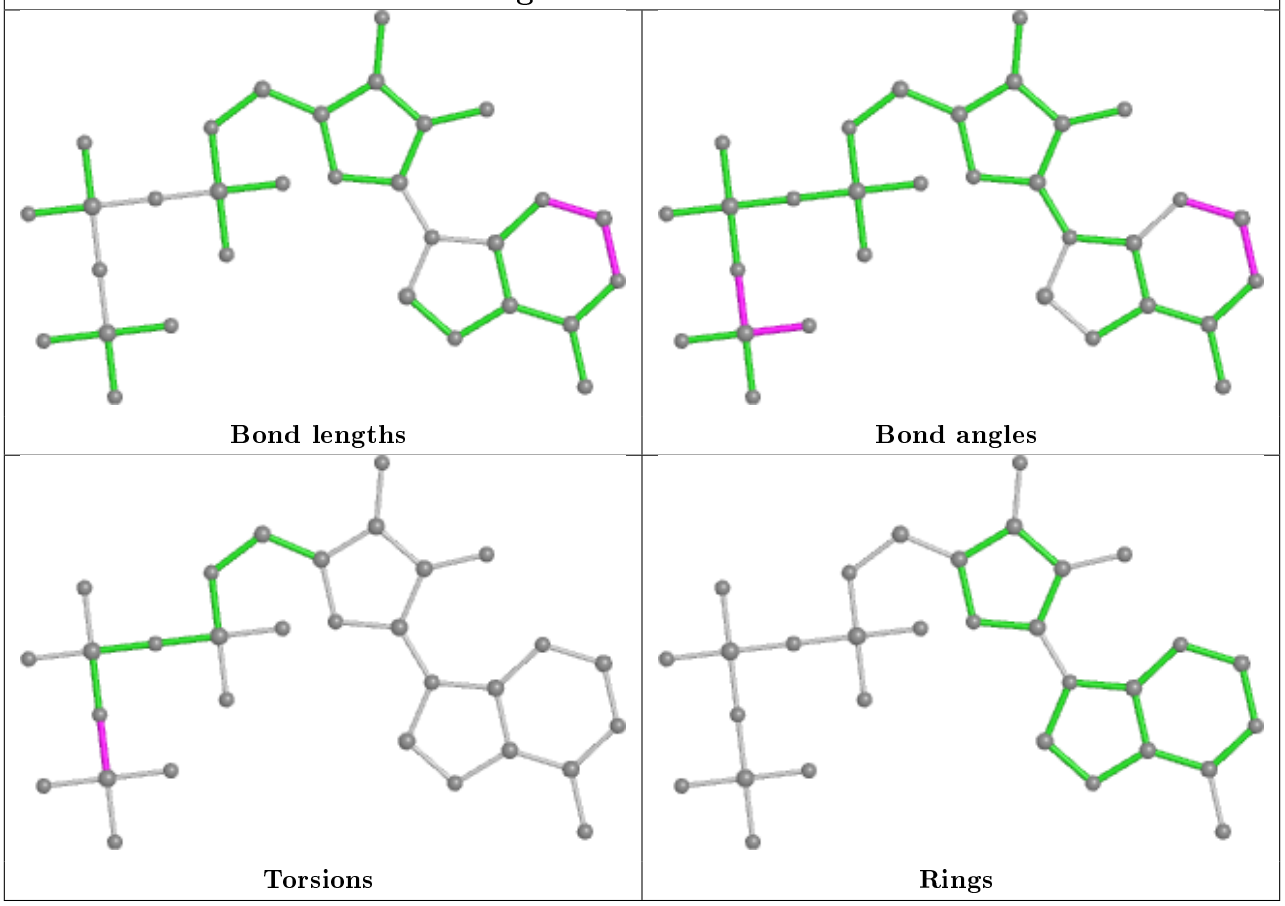


Torsions



Rings

Ligand ATP A 1380



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	355/375 (94%)	-0.03	7 (1%) 65 63	13, 22, 34, 47	0
1	B	358/375 (95%)	1.28	86 (24%) 0 0	14, 27, 40, 51	0
All	All	713/750 (95%)	0.63	93 (13%) 3 3	13, 23, 38, 51	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	231	ALA	10.6
1	B	243	PRO	9.4
1	B	245	GLY	8.4
1	B	193	LEU	8.3
1	B	232	SER	8.3
1	B	198	TYR	7.7
1	B	235	SER	7.1
1	B	250	ILE	7.0
1	B	248	ILE	6.3
1	B	279	TYR	6.2
1	B	242	LEU	6.2
1	B	203	THR	6.1
1	B	239	SER	6.0
1	B	324	THR	5.7
1	B	323	SER	5.6
1	B	236	LEU	5.5
1	B	194	THR	5.4
1	B	247	VAL	5.2
1	B	197	GLY	5.1
1	B	230	ALA	5.0
1	B	233	SER	4.9
1	B	271	SER	4.8
1	B	227	MET	4.6
1	B	272	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	325	MET	4.5
1	B	65	LEU	4.4
1	B	318	THR	4.3
1	B	287	ILE	4.3
1	B	241	GLU	4.2
1	B	246	GLN	4.2
1	A	201	VAL	4.1
1	B	234	SER	4.0
1	B	228	ALA	3.9
1	B	207	GLU	3.8
1	B	40	HIS	3.8
1	B	244	ASP	3.7
1	B	179	ASP	3.7
1	B	237	GLU	3.7
1	B	39	ARG	3.6
1	B	190	MET	3.5
1	B	67	LEU	3.5
1	B	319	ALA	3.5
1	B	249	THR	3.4
1	B	254	ARG	3.4
1	B	273	GLY	3.4
1	B	240	TYR	3.4
1	B	374	CYS	3.4
1	B	196	ARG	3.3
1	B	289	ILE	3.3
1	B	229	THR	3.2
1	B	69	TYR	3.2
1	B	53	TYR	3.2
1	B	321	ALA	3.2
1	B	224	GLU	3.0
1	B	208	ILE	2.9
1	B	269	MET	2.9
1	B	221	LEU	2.7
1	B	261	LEU	2.7
1	B	362	TYR	2.7
1	B	62	ARG	2.7
1	B	51	ASP	2.7
1	B	354	GLN	2.7
1	B	166	TYR	2.6
1	B	322	PRO	2.6
1	B	187	ASP	2.6
1	B	127	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	364	GLU	2.6
1	B	238	LYS	2.5
1	B	360	GLN	2.5
1	B	68	LYS	2.5
1	B	201	VAL	2.5
1	B	169	TYR	2.5
1	B	315	LYS	2.4
1	B	365	ALA	2.4
1	A	5	THR	2.4
1	A	339	VAL	2.4
1	B	191	LYS	2.4
1	B	38	PRO	2.4
1	B	294	TYR	2.4
1	B	37	ARG	2.3
1	A	175	ILE	2.3
1	B	253	GLU	2.3
1	B	158	GLY	2.2
1	B	288	ASP	2.2
1	A	109	PRO	2.2
1	B	180	LEU	2.2
1	B	264	PRO	2.2
1	A	138	ALA	2.1
1	A	152	VAL	2.1
1	B	72	GLU	2.1
1	B	177	ARG	2.0
1	B	262	PHE	2.0
1	B	268	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	HIC	B	73	11/12	0.83	0.27	32,33,37,39	0
1	HIC	A	73	11/12	0.97	0.12	22,25,39,44	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

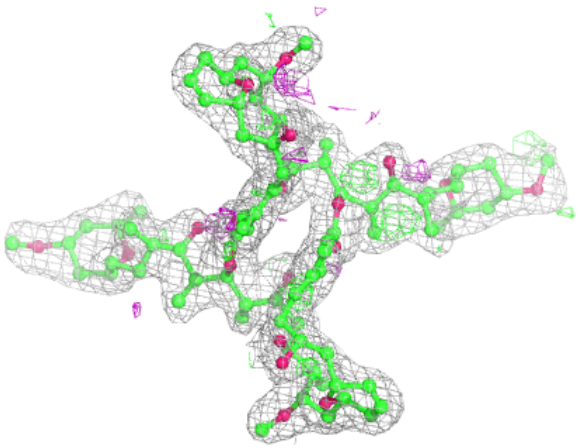
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

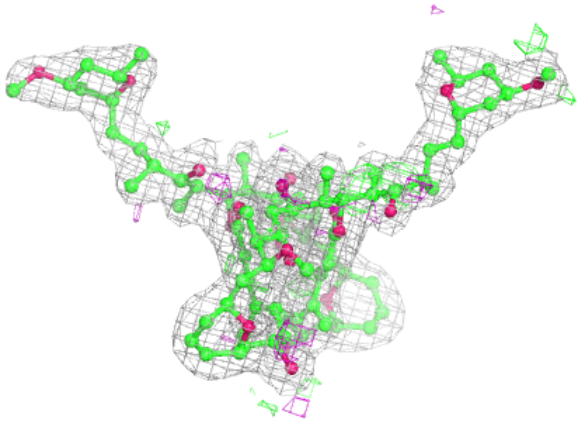
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	9002	4/4	0.79	0.22	38,42,49,52	0
2	MG	B	2390	1/1	0.84	0.11	47,47,47,47	0
2	MG	A	5001	1/1	0.92	0.07	56,56,56,56	0
5	SWI	B	600	98/98	0.93	0.13	26,36,50,59	0
4	EDO	A	9001	4/4	0.93	0.16	35,42,42,44	0
3	ATP	B	2380	31/31	0.93	0.20	20,25,29,32	0
2	MG	A	1390	1/1	0.97	0.18	26,26,26,26	0
3	ATP	A	1380	31/31	0.98	0.09	17,21,25,27	0

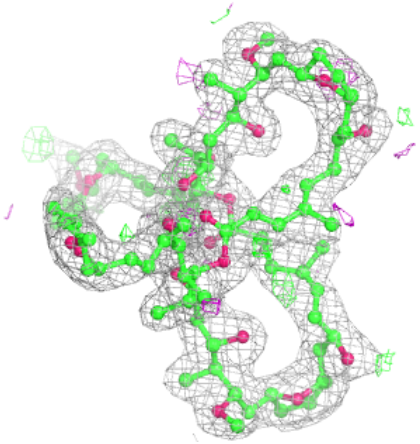
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SWI B 600:

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

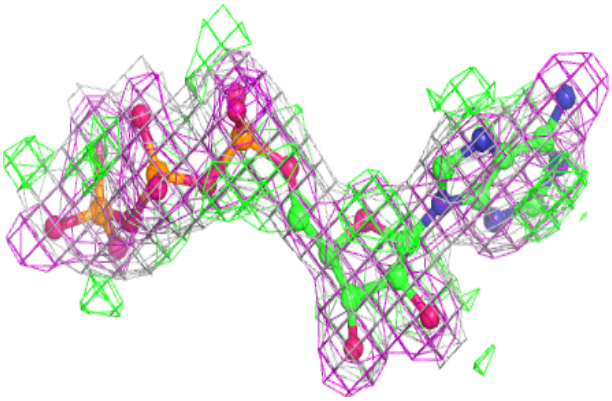


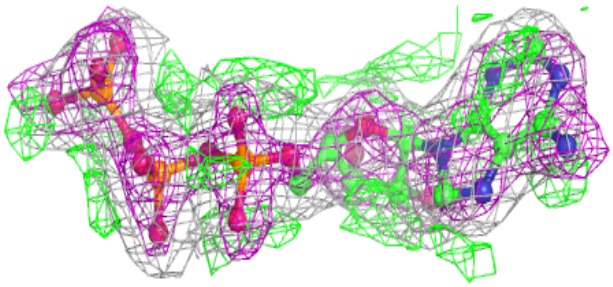


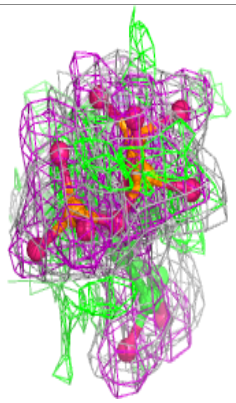


Electron density around ATP B 2380:

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

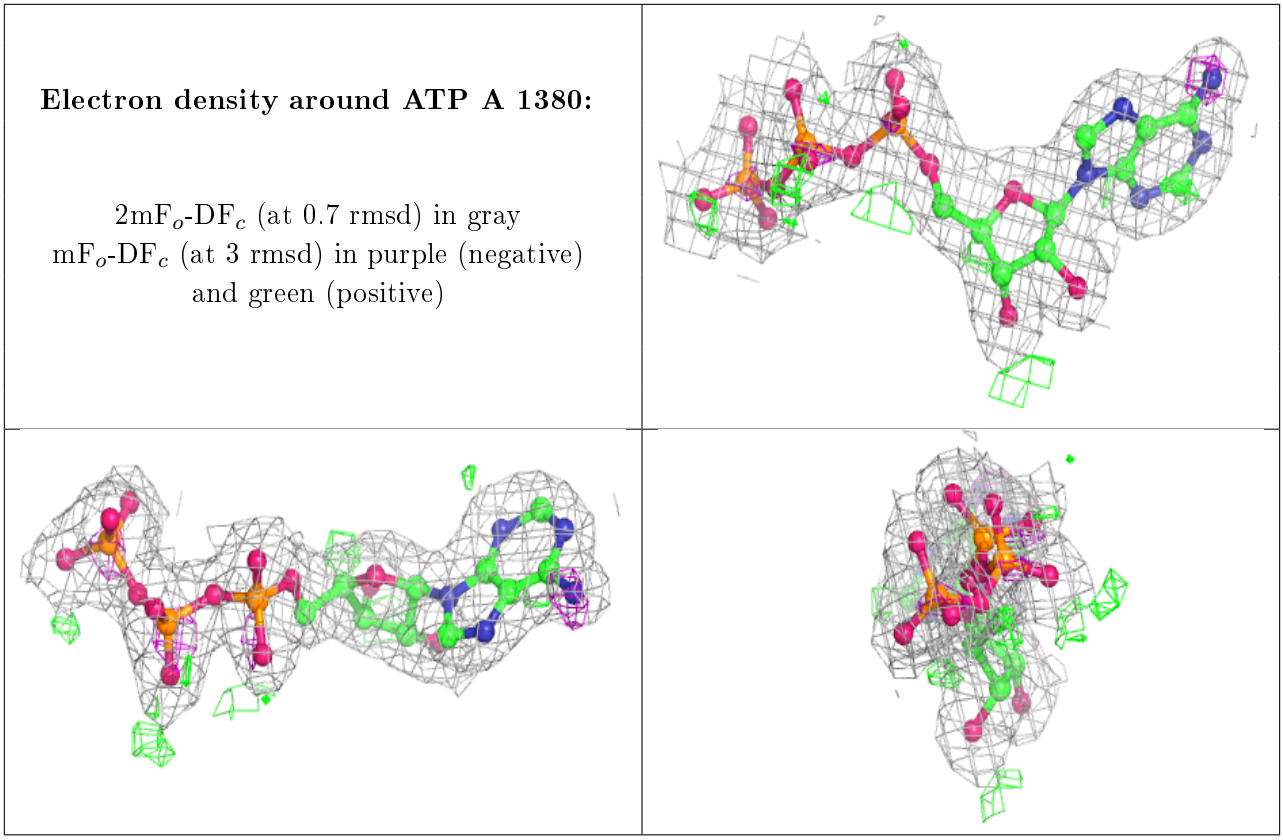






Electron density around ATP A 1380:

$2mF_o$-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.