Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 09:35 am GMT

PDB ID	:	2V7Q
Title	:	The structure of F1-ATPase inhibited by I1-60HIS, a monomeric form of the inhibitor protein, IF1.
Authors	:	Gledhill, J.R.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on	:	2007-07-31
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

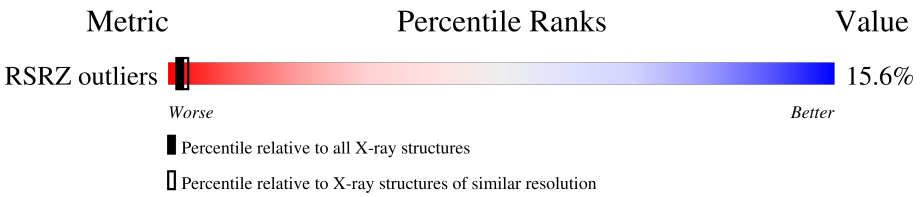
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.10 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))
RSRZ outliers	127900	5083 (2.10-2.10)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 27418 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 ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3715	2341	656	706	12	0	0	0
1	B	479	3656	2303	647	694	12	0	0	0
1	C	473	3607	2279	637	679	12	0	0	0

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	469	3558	2254	605	688	11	0	0	0
2	E	465	3523	2234	599	679	11	0	0	0
2	F	466	3530	2238	600	681	11	0	0	0

- Molecule 3 is a protein called ATP SYNTHASE GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	263	2054	1293	357	396	8	0	0	0

- Molecule 4 is a protein called ATP SYNTHASE DELTA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	131	970	609	164	195	2	0	0	0

- Molecule 5 is a protein called ATP SYNTHASE EPSILON CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	I	47	369	237	66	64	2	0	0	0

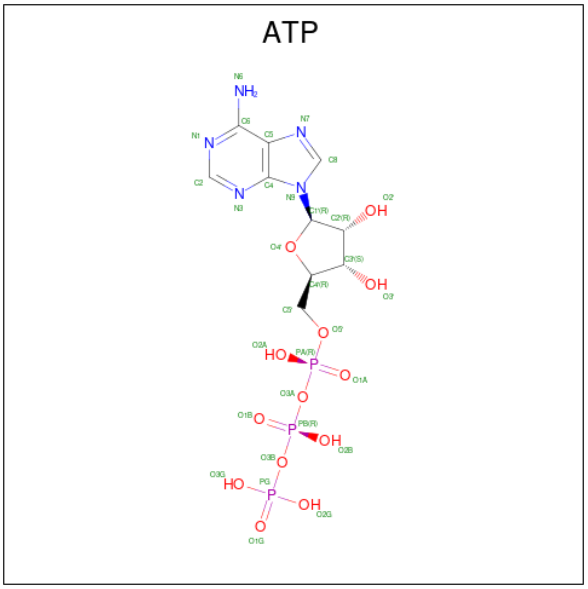
- Molecule 6 is a protein called ATPASE INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	J	43	339	206	71	62	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	61	HIS	-	expression tag	UNP P01096
J	62	HIS	-	expression tag	UNP P01096
J	63	HIS	-	expression tag	UNP P01096
J	64	HIS	-	expression tag	UNP P01096
J	65	HIS	-	expression tag	UNP P01096
J	66	HIS	-	expression tag	UNP P01096

- 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
			Total	C	N	O	P		
7	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
7	B	1	31	10	5	13	3	0	0

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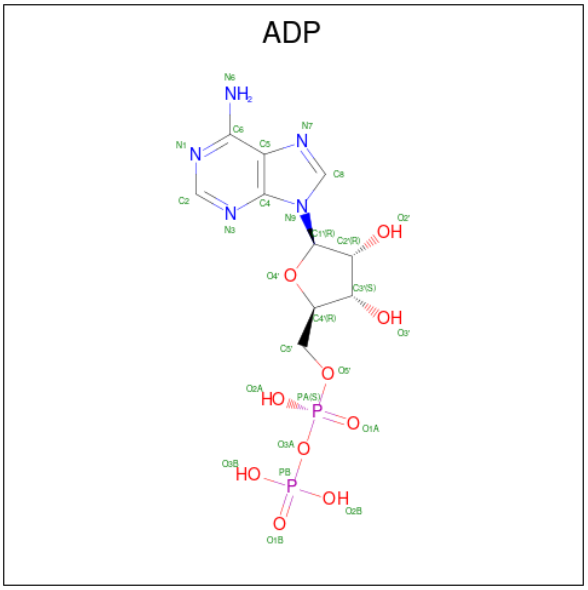
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	C	1	31	10	5	13	3	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

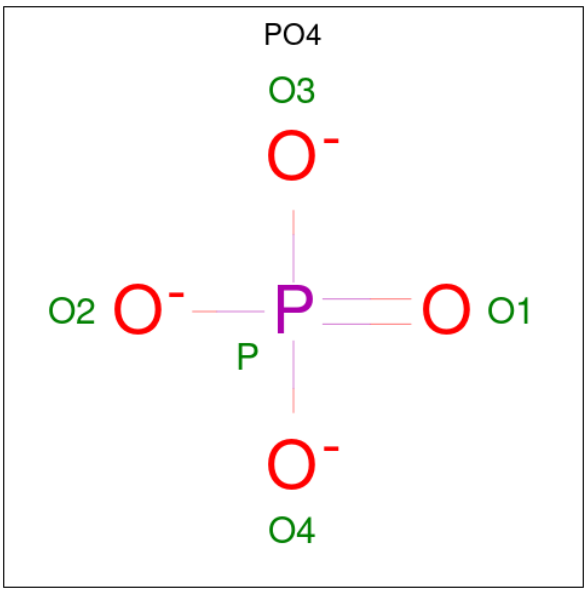
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
8	A	1	1	1	0	0
8	B	1	1	1	0	0
8	C	1	1	1	0	0
8	D	1	1	1	0	0
8	F	1	1	1	0	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	D	1	27	10	5	10	2	0	0
9	F	1	27	10	5	10	2	0	0

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	E	1	Total O P 5 4 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	286	Total O 286 286	0	0
11	B	294	Total O 294 294	0	0
11	C	296	Total O 296 296	0	0
11	D	367	Total O 367 367	0	0
11	E	216	Total O 216 216	0	0
11	F	316	Total O 316 316	0	0
11	G	112	Total O 112 112	0	0
11	H	27	Total O 27 27	0	0
11	I	6	Total O 6 6	0	0
11	J	20	Total O 20 20	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	262.53Å 103.27Å 135.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.19 – 2.10 35.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.19-2.10) 99.0 (35.01-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.245 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	27418	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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.

4 Model quality (i)

4.1 Standard geometry (i)

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4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
9	ADP	F	1475	8	24,29,29	0.99	1 (4%)	29,45,45	1.28	3 (10%)
9	ADP	D	1478	8	24,29,29	1.10	2 (8%)	29,45,45	1.35	2 (6%)
10	PO4	E	1475	-	4,4,4	0.90	0	6,6,6	0.45	0
7	ATP	B	1511	8	26,33,33	0.99	1 (3%)	31,52,52	1.31	2 (6%)
7	ATP	C	1511	8	26,33,33	0.92	1 (3%)	31,52,52	1.30	2 (6%)
7	ATP	A	1511	8	26,33,33	0.96	1 (3%)	31,52,52	1.34	4 (12%)

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
9	ADP	F	1475	8	-	2/12/32/32	0/3/3/3
9	ADP	D	1478	8	-	2/12/32/32	0/3/3/3
7	ATP	B	1511	8	-	0/18/38/38	0/3/3/3
7	ATP	C	1511	8	-	3/18/38/38	0/3/3/3
7	ATP	A	1511	8	-	4/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1511	ATP	C5-C4	2.64	1.47	1.40
9	D	1478	ADP	C5-C4	2.64	1.47	1.40
7	A	1511	ATP	C5-C4	2.60	1.47	1.40
9	F	1475	ADP	C5-C4	2.48	1.47	1.40
7	C	1511	ATP	C5-C4	2.41	1.47	1.40
9	D	1478	ADP	C2-N3	2.14	1.35	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	1475	ADP	N3-C2-N1	-3.81	122.72	128.68
7	A	1511	ATP	N3-C2-N1	-3.62	123.02	128.68
7	B	1511	ATP	N3-C2-N1	-3.54	123.15	128.68
7	C	1511	ATP	N3-C2-N1	-3.32	123.49	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	1478	ADP	C4-C5-N7	-3.22	106.05	109.40
9	D	1478	ADP	N3-C2-N1	-3.10	123.83	128.68
7	C	1511	ATP	C4-C5-N7	-3.06	106.21	109.40
7	A	1511	ATP	C4-C5-N7	-2.81	106.47	109.40
9	F	1475	ADP	C4-C5-N7	-2.63	106.66	109.40
7	A	1511	ATP	O4'-C1'-C2'	-2.52	103.25	106.93
7	B	1511	ATP	C4-C5-N7	-2.20	107.11	109.40
7	A	1511	ATP	O2A-PA-O1A	2.08	122.53	112.24
9	F	1475	ADP	C2-N1-C6	2.07	122.30	118.75

There are no chirality outliers.

All (11) torsion outliers are listed below:

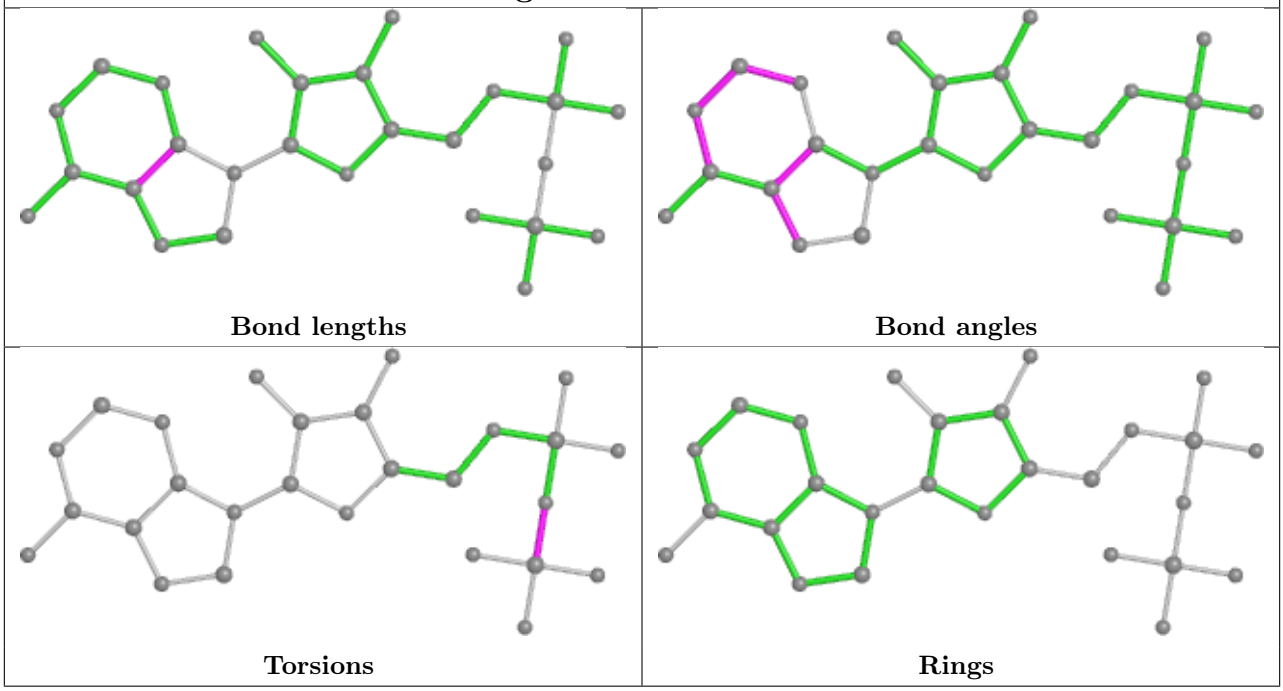
Mol	Chain	Res	Type	Atoms
7	A	1511	ATP	PB-O3B-PG-O2G
7	C	1511	ATP	PB-O3B-PG-O2G
9	D	1478	ADP	PA-O3A-PB-O2B
9	F	1475	ADP	PA-O3A-PB-O2B
9	F	1475	ADP	PA-O3A-PB-O1B
7	A	1511	ATP	PB-O3B-PG-O1G
7	A	1511	ATP	PB-O3B-PG-O3G
7	C	1511	ATP	PB-O3B-PG-O3G
9	D	1478	ADP	PA-O3A-PB-O3B
7	A	1511	ATP	PG-O3B-PB-O1B
7	C	1511	ATP	PG-O3B-PB-O1B

There are no ring outliers.

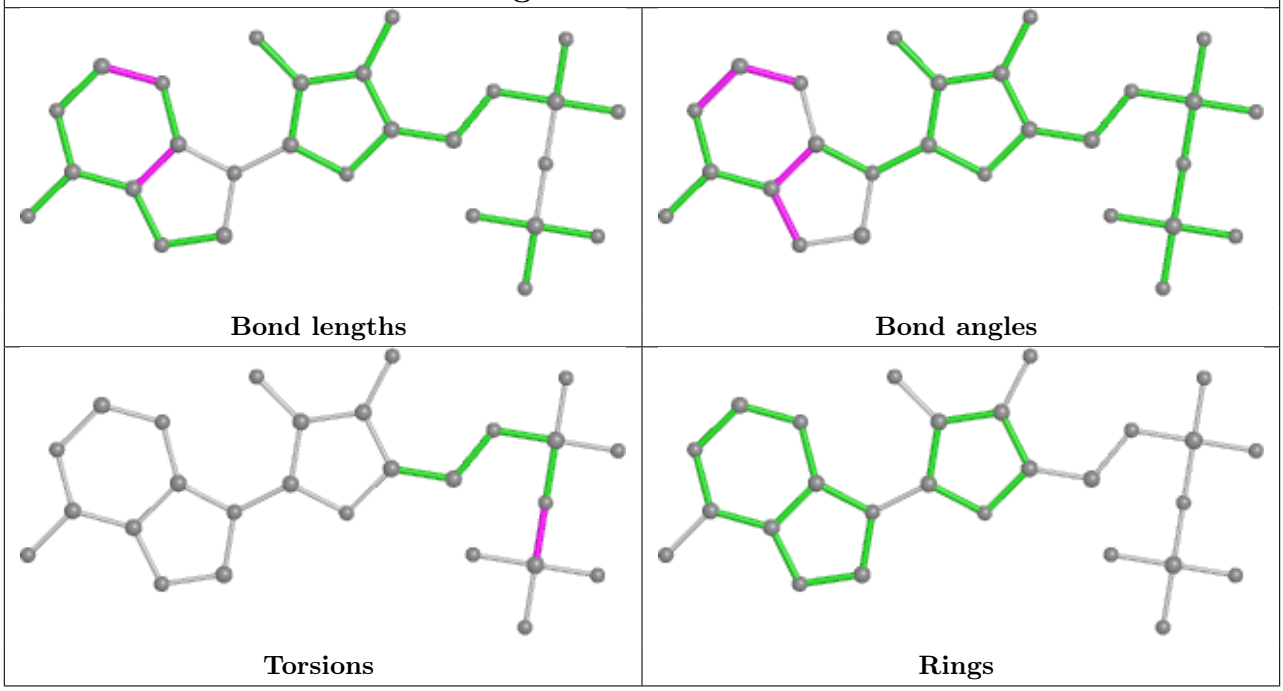
No monomer is involved in short contacts.

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.

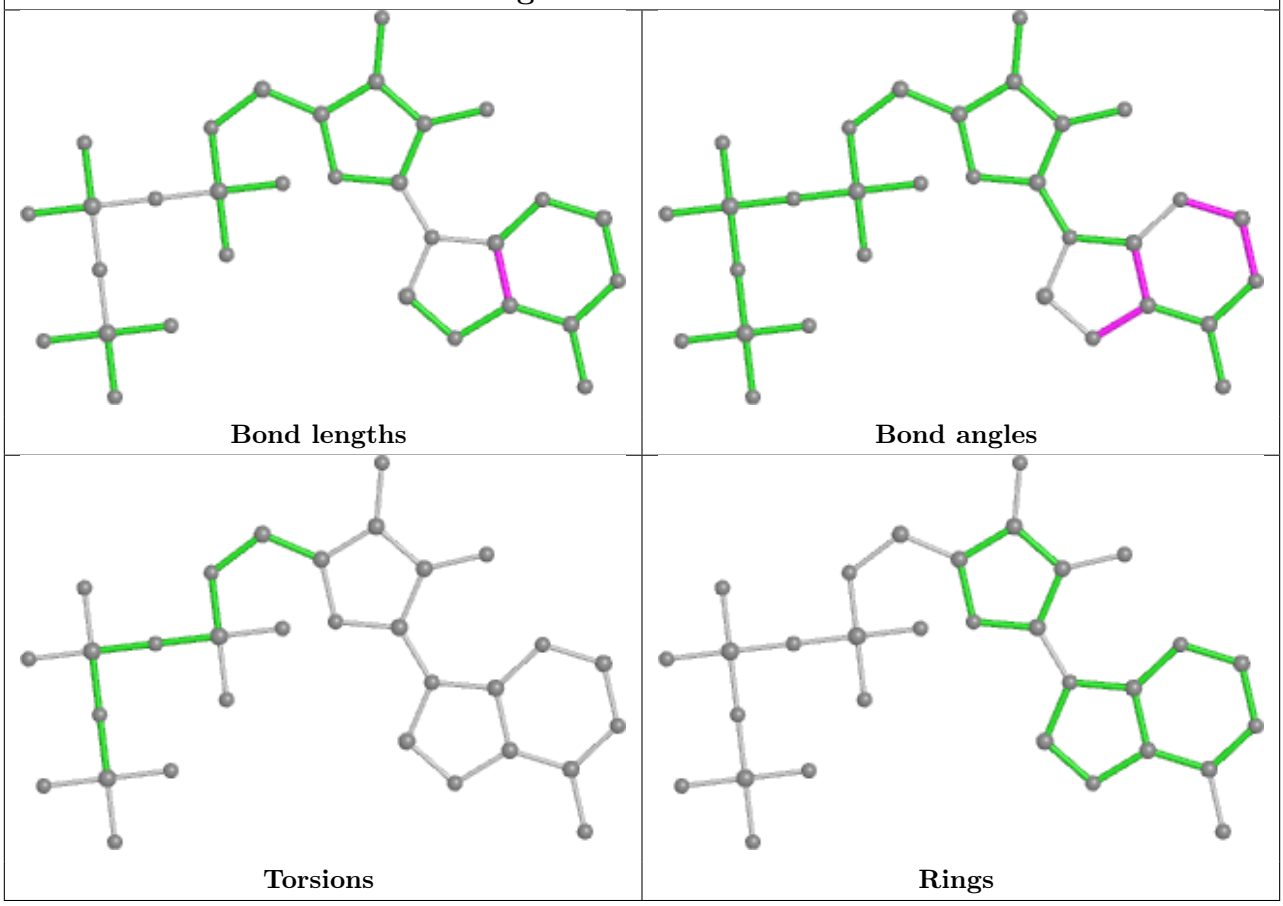
Ligand ADP F 1475



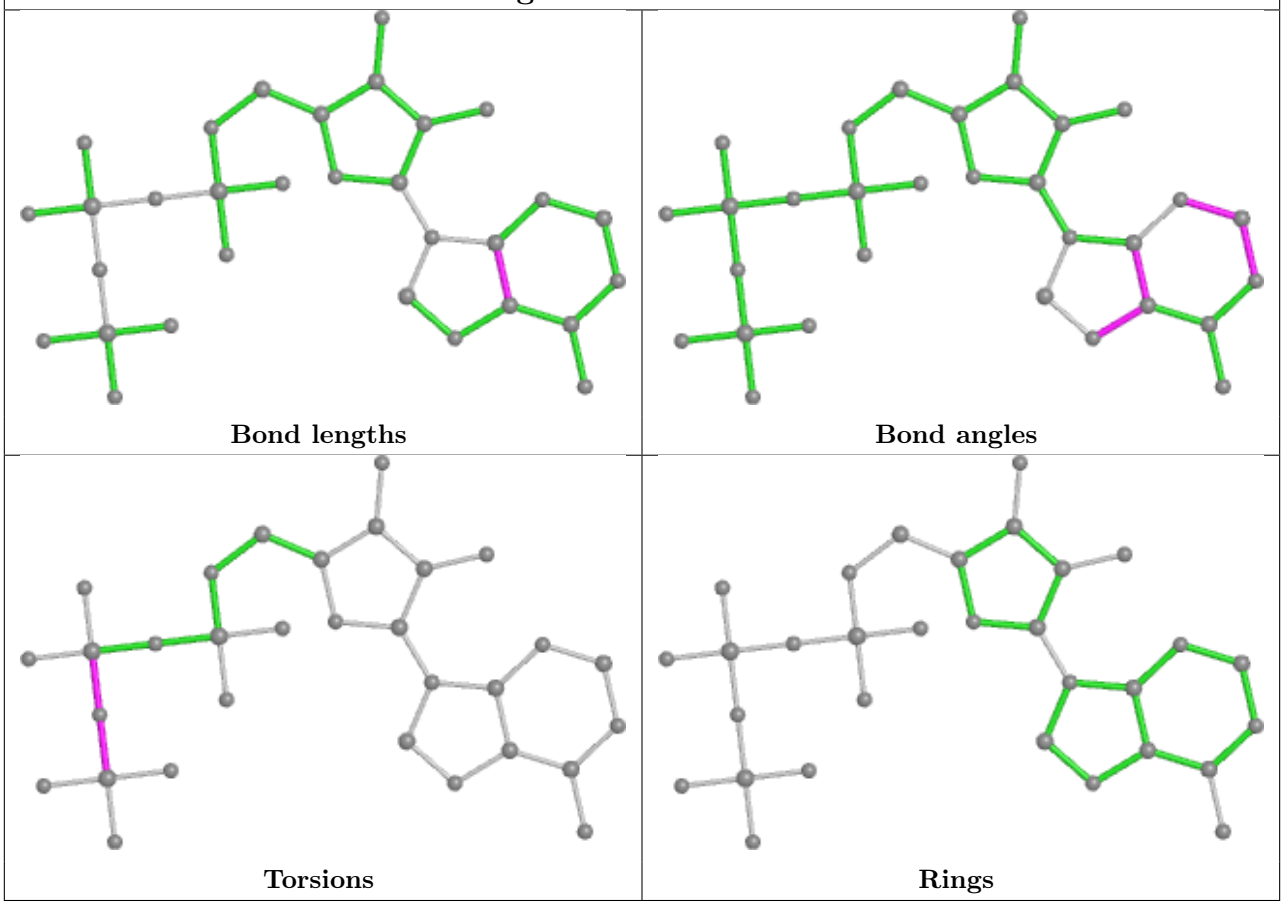
Ligand ADP D 1478



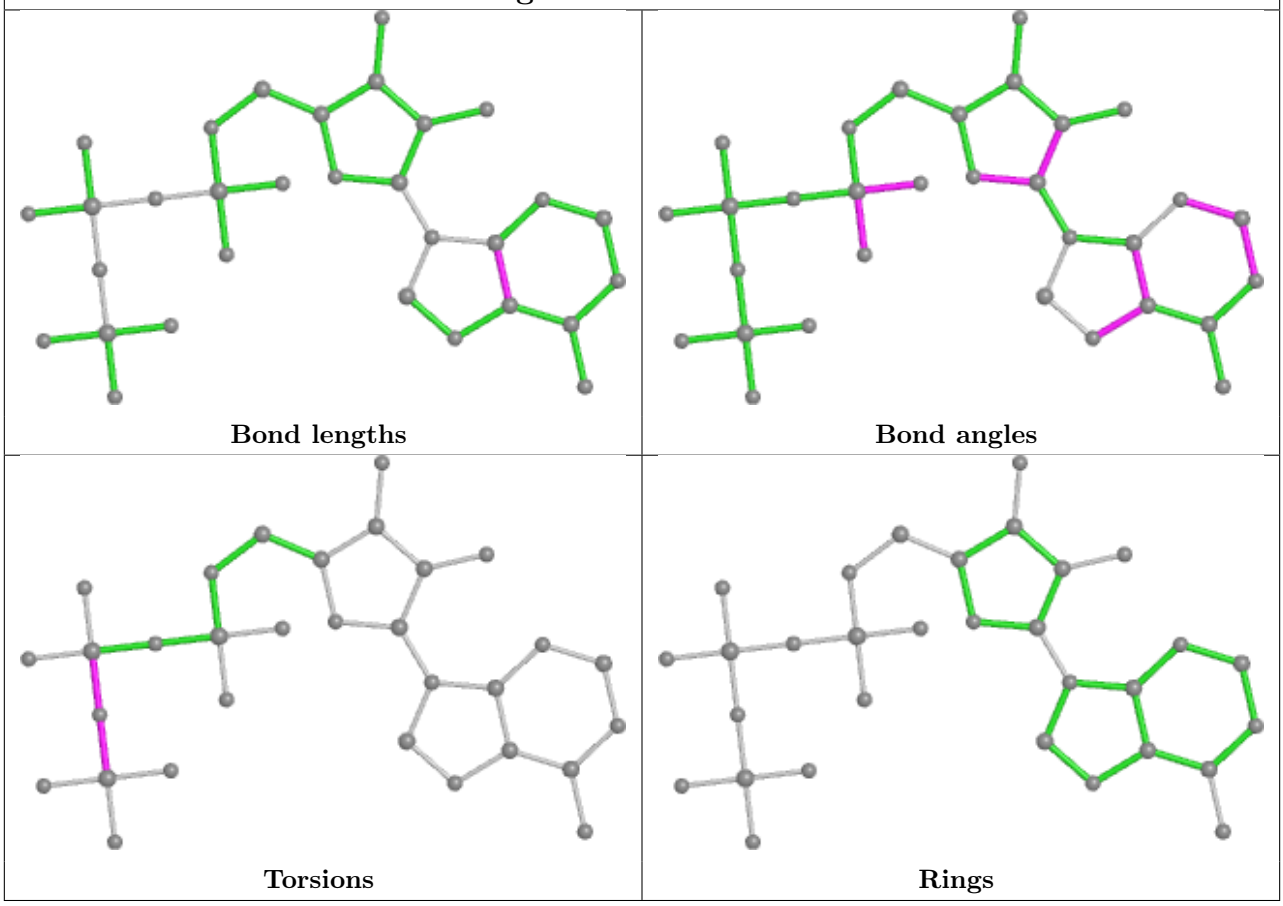
Ligand ATP B 1511



Ligand ATP C 1511



Ligand ATP A 1511



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

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	487/510 (95%)	0.79	60 (12%)	4	5	22, 34, 60, 86	0
1	B	479/510 (93%)	0.93	75 (15%)	2	2	21, 33, 70, 82	0
1	C	473/510 (92%)	0.79	61 (12%)	3	4	22, 32, 65, 87	0
2	D	469/482 (97%)	0.56	28 (5%)	21	27	21, 30, 47, 65	0
2	E	465/482 (96%)	1.21	93 (20%)	1	1	23, 40, 84, 89	0
2	F	466/482 (96%)	0.61	33 (7%)	16	20	22, 32, 58, 77	0
3	G	263/272 (96%)	1.70	91 (34%)	0	0	26, 53, 83, 93	0
4	H	131/146 (89%)	1.75	44 (33%)	0	0	36, 54, 75, 76	0
5	I	47/50 (94%)	2.89	29 (61%)	0	0	46, 60, 105, 108	0
6	J	43/66 (65%)	0.88	6 (13%)	2	3	12, 24, 56, 65	0
All	All	3323/3510 (94%)	0.95	520 (15%)	2	2	12, 35, 74, 108	0

All (520) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	510	ALA	13.1
1	C	377	ALA	11.1
1	B	410	LEU	10.8
2	E	387	ILE	9.2
4	H	123	ALA	9.1
2	E	384	LEU	8.7
2	E	394	ASP	8.1
2	E	474	ALA	8.0
3	G	191	SER	8.0
4	H	120	LEU	7.8
5	I	47	VAL	7.8
2	E	396	LEU	7.7
4	H	121	GLY	7.5

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Mol	Chain	Res	Type	RSRZ
5	I	1	VAL	7.4
3	G	183	THR	7.4
1	C	414	THR	7.3
1	A	406	PHE	7.2
3	G	184	ILE	7.2
1	B	414	THR	7.1
5	I	36	LYS	7.1
4	H	122	ALA	7.1
5	I	35	MET	7.0
2	E	390	ILE	6.9
5	I	40	SER	6.8
2	E	389	ALA	6.7
3	G	94	ALA	6.7
5	I	42	ILE	6.6
2	E	457	PHE	6.5
1	B	509	GLU	6.5
1	B	418	LEU	6.4
1	A	412	ALA	6.4
3	G	56	ASP	6.4
2	E	425	THR	6.3
3	G	181	LEU	6.3
1	C	376	SER	6.3
4	H	128	ARG	6.2
3	G	95	ASN	6.2
2	E	395	GLU	6.1
5	I	30	PHE	6.1
3	G	196	ILE	6.0
2	E	470	ALA	6.0
3	G	185	SER	6.0
2	E	427	HIS	5.9
3	G	122	ASP	5.9
2	E	405	SER	5.8
1	A	411	ASP	5.8
1	B	411	ASP	5.8
1	A	409	ASP	5.7
2	E	402	LEU	5.7
1	B	412	ALA	5.7
3	G	153	TYR	5.6
5	I	39	GLY	5.6
1	A	403	PHE	5.6
3	G	188	GLU	5.5
4	H	119	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
2	E	473	LEU	5.4
3	G	96	LEU	5.4
4	H	124	ASP	5.4
3	G	189	SER	5.3
2	E	403	THR	5.3
4	H	42	THR	5.3
1	A	418	LEU	5.3
1	C	451	GLY	5.2
3	G	212	ILE	5.2
1	A	392	LEU	5.2
1	B	401	ALA	5.2
1	A	410	LEU	5.2
2	E	428	LEU	5.1
5	I	44	ILE	5.1
1	C	206	ILE	5.0
1	B	388	GLY	5.0
2	E	399	GLU	5.0
4	H	68	GLU	5.0
3	G	156	ASP	5.0
1	B	413	ALA	5.0
3	G	195	ASP	5.0
3	G	187	ALA	4.9
6	J	48	HIS	4.9
1	B	508	PHE	4.9
2	E	398	GLU	4.9
1	C	378	ALA	4.9
4	H	126	ALA	4.9
2	E	388	ILE	4.9
2	E	393	MET	4.9
3	G	180	SER	4.8
1	C	483	ILE	4.8
1	B	507	GLY	4.8
3	G	121	SER	4.8
3	G	118	ARG	4.8
3	G	124	PHE	4.7
4	H	135	ILE	4.7
1	A	408	SER	4.7
2	E	472	LYS	4.6
1	A	479	LEU	4.6
2	F	176	ALA	4.6
2	E	409	LYS	4.6
3	G	108	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
2	E	429	GLY	4.6
2	E	455	GLN	4.6
2	E	424	PHE	4.6
1	B	376	SER	4.6
2	E	380	ASP	4.6
3	G	194	ASP	4.6
2	E	456	ALA	4.6
1	A	405	GLN	4.5
2	E	392	GLY	4.5
1	C	404	ALA	4.5
3	G	71	VAL	4.5
3	G	182	ASP	4.5
2	F	474	ALA	4.5
1	C	193	THR	4.5
2	E	458	TYR	4.4
3	G	57	ILE	4.4
1	A	510	ALA	4.4
5	I	28	THR	4.4
4	H	130	GLU	4.4
1	C	267	ILE	4.4
1	A	407	GLY	4.4
1	B	456	LEU	4.4
4	H	131	ILE	4.4
4	H	117	SER	4.4
1	B	416	GLN	4.3
4	H	125	GLU	4.3
2	E	447	GLY	4.3
4	H	86	ALA	4.3
4	H	71	THR	4.3
4	H	107	ALA	4.3
5	I	4	TRP	4.3
5	I	7	ALA	4.3
1	C	411	ASP	4.3
3	G	179	PHE	4.2
2	E	385	GLN	4.2
2	E	386	ASP	4.2
3	G	213	ILE	4.2
3	G	141	ALA	4.2
1	B	396	GLN	4.2
1	A	491	GLU	4.2
3	G	210	ALA	4.2
4	H	45	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	381	ARG	4.2
1	A	490	SER	4.2
3	G	66	HIS	4.1
3	G	59	THR	4.1
2	E	464	GLU	4.1
2	E	365	SER	4.1
5	I	29	GLU	4.1
1	C	375	GLY	4.1
1	A	505	LEU	4.1
1	B	487	GLY	4.1
2	E	361	ASN	4.0
4	H	110	ALA	4.0
4	H	44	ALA	4.0
1	B	271	LEU	4.0
2	E	410	ILE	4.0
1	A	478	ALA	4.0
2	E	426	GLY	4.0
1	A	414	THR	4.0
1	A	413	ALA	4.0
2	F	28	GLY	4.0
2	E	422	GLU	4.0
2	E	210	ASP	3.9
2	E	406	ARG	3.9
2	E	401	LYS	3.9
1	A	486	ASP	3.9
1	B	389	THR	3.9
3	G	151	SER	3.8
2	F	473	LEU	3.8
4	H	113	GLU	3.8
5	I	6	GLN	3.8
6	J	49	HIS	3.8
3	G	209	LEU	3.8
3	G	186	SER	3.8
3	G	55	ALA	3.8
3	G	207	TYR	3.8
2	F	424	PHE	3.8
1	B	446	TYR	3.7
1	A	416	GLN	3.7
1	A	385	GLN	3.7
4	H	41	GLN	3.7
2	F	471	ASP	3.7
2	D	475	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	360	PRO	3.7
2	E	369	ASP	3.7
1	A	415	GLN	3.6
5	I	43	LYS	3.6
4	H	88	SER	3.6
5	I	37	THR	3.6
2	E	373	GLY	3.6
4	H	93	LEU	3.6
1	C	460	LYS	3.6
3	G	138	PHE	3.6
2	F	402	LEU	3.6
1	A	404	ALA	3.6
4	H	118	GLU	3.6
3	G	214	TYR	3.6
2	F	175	LYS	3.6
3	G	65	LYS	3.6
2	D	473	LEU	3.5
3	G	125	LEU	3.5
1	B	419	SER	3.5
1	C	382	ALA	3.5
2	F	398	GLU	3.5
3	G	149	LEU	3.5
3	G	117	HIS	3.5
1	B	342	VAL	3.5
1	C	374	VAL	3.5
2	E	418	PHE	3.5
1	B	495	ALA	3.5
1	B	451	GLY	3.5
3	G	199	ASP	3.5
1	C	475	GLN	3.5
2	E	460	VAL	3.5
3	G	93	ALA	3.4
5	I	24	ASP	3.4
1	C	504	PHE	3.4
3	G	197	ASP	3.4
1	C	271	LEU	3.4
2	E	397	SER	3.4
2	F	247	GLU	3.4
3	G	272	LEU	3.4
4	H	142	VAL	3.4
1	B	415	GLN	3.3
3	G	148	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	207	ASN	3.3
6	J	10	SER	3.3
6	J	47	LYS	3.3
1	B	399	GLU	3.3
1	B	345	ILE	3.3
1	B	305	LEU	3.3
1	B	454	ASP	3.3
2	E	471	ASP	3.3
2	E	404	VAL	3.3
2	F	470	ALA	3.3
1	C	476	HIS	3.3
2	D	477	HIS	3.3
1	B	298	VAL	3.3
2	E	423	VAL	3.3
3	G	102	GLU	3.3
2	E	364	GLY	3.3
3	G	119	THR	3.2
1	B	24	ASP	3.2
3	G	215	TYR	3.2
2	E	439	LYS	3.2
1	C	121	ILE	3.2
1	C	495	ALA	3.2
2	F	329	LEU	3.2
1	C	499	GLU	3.1
1	B	358	TYR	3.1
3	G	154	GLU	3.1
1	B	324	LEU	3.1
3	G	217	LEU	3.1
2	D	339	ILE	3.1
3	G	144	ILE	3.1
1	A	401	ALA	3.1
1	C	266	ILE	3.1
1	C	205	ALA	3.1
2	E	379	GLN	3.1
2	D	334	VAL	3.1
1	C	122	GLY	3.1
2	E	466	ALA	3.1
5	I	41	THR	3.0
2	E	28	GLY	3.0
6	J	45	LEU	3.0
3	G	103	VAL	3.0
5	I	45	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
3	G	90	LYS	3.0
2	D	425	THR	3.0
2	E	382	LYS	3.0
1	C	500	ILE	3.0
1	A	509	GLU	3.0
1	C	474	SER	3.0
1	C	413	ALA	3.0
1	A	206	ILE	2.9
3	G	92	GLU	2.9
4	H	114	LYS	2.9
2	E	381	TYR	2.9
1	A	271	LEU	2.9
2	E	391	LEU	2.9
3	G	160	ILE	2.9
5	I	38	SER	2.9
2	F	27	GLU	2.9
3	G	170	SER	2.9
3	G	152	GLY	2.8
4	H	111	ASN	2.8
3	G	72	SER	2.8
4	H	15	GLN	2.8
1	A	449	VAL	2.8
2	D	111	LYS	2.8
2	F	399	GLU	2.8
1	C	203	TYR	2.8
1	A	497	LEU	2.8
2	E	445	LEU	2.8
5	I	27	LYS	2.8
5	I	31	LYS	2.8
4	H	49	ALA	2.8
3	G	91	SER	2.8
1	B	306	LEU	2.8
1	C	224	ASP	2.8
2	D	154	LEU	2.8
3	G	131	VAL	2.8
5	I	46	LYS	2.8
3	G	150	ASN	2.8
2	E	446	ALA	2.8
1	A	193	THR	2.8
2	D	310	ILE	2.8
3	G	123	GLN	2.8
1	C	410	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	194	ASP	2.7
1	C	204	VAL	2.7
2	D	61	ILE	2.7
3	G	192	ILE	2.7
1	C	497	LEU	2.7
1	B	506	ALA	2.7
1	B	392	LEU	2.7
1	B	299	PHE	2.7
3	G	134	ARG	2.7
1	A	487	GLY	2.7
1	C	323	ALA	2.7
3	G	139	GLY	2.7
2	E	463	ILE	2.7
5	I	33	ASN	2.7
2	F	391	LEU	2.7
4	H	132	GLN	2.7
1	C	326	VAL	2.7
4	H	101	ASP	2.7
3	G	202	ARG	2.7
1	B	204	VAL	2.6
1	B	276	VAL	2.6
3	G	220	SER	2.6
1	A	489	ILE	2.6
3	G	2	THR	2.6
1	B	301	LEU	2.6
2	D	428	LEU	2.6
2	E	452	LEU	2.6
1	C	380	THR	2.6
2	E	363	VAL	2.6
1	A	56	SER	2.6
1	B	167	ILE	2.6
2	E	255	ILE	2.6
4	H	69	ASP	2.6
1	C	417	LEU	2.6
1	B	326	VAL	2.6
1	C	268	TYR	2.6
3	G	193	TYR	2.6
1	A	246	ALA	2.6
2	D	474	ALA	2.6
3	G	41	ALA	2.6
3	G	271	ALA	2.6
2	D	424	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	457	GLU	2.6
1	A	417	LEU	2.6
1	B	166	LEU	2.6
1	C	452	TYR	2.5
2	D	285	LEU	2.5
6	J	8	VAL	2.5
1	A	399	GLU	2.5
1	C	501	VAL	2.5
2	E	368	TYR	2.5
2	F	177	HIS	2.5
1	A	122	GLY	2.5
2	E	252	LEU	2.5
2	E	359	ASP	2.5
1	B	193	THR	2.5
2	F	472	LYS	2.5
1	A	419	SER	2.5
4	H	32	ASN	2.5
2	D	378	LEU	2.5
1	C	496	LYS	2.5
3	G	54	LYS	2.5
2	E	128	VAL	2.5
1	A	143	ARG	2.5
4	H	134	ARG	2.5
1	A	508	PHE	2.5
2	E	417	PRO	2.4
1	C	213	VAL	2.4
2	E	467	VAL	2.4
2	F	310	ILE	2.4
1	A	485	THR	2.4
1	C	176	THR	2.4
4	H	102	MET	2.4
1	C	242	LEU	2.4
2	D	351	LEU	2.4
3	G	216	SER	2.4
1	A	457	GLU	2.4
1	B	500	ILE	2.4
2	D	258	ILE	2.4
1	A	506	ALA	2.4
4	H	115	ALA	2.4
1	B	384	LYS	2.4
1	C	235	THR	2.4
2	E	435	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	G	120	HIS	2.4
5	I	8	GLY	2.4
2	E	307	VAL	2.4
2	E	108	ILE	2.4
2	F	451	HIS	2.4
1	C	455	LYS	2.4
1	C	510	ALA	2.4
1	B	268	TYR	2.4
3	G	33	ARG	2.4
1	A	301	LEU	2.4
2	F	396	LEU	2.4
1	B	374	VAL	2.4
1	C	506	ALA	2.4
1	B	303	SER	2.4
1	B	381	ARG	2.4
1	C	419	SER	2.4
2	E	408	ARG	2.4
3	G	190	MET	2.4
4	H	104	ASP	2.4
2	D	307	VAL	2.3
4	H	43	GLY	2.3
1	B	338	ILE	2.3
2	F	296	ILE	2.3
1	B	300	TYR	2.3
2	E	400	ASP	2.3
2	F	222	MET	2.3
4	H	50	ALA	2.3
1	B	327	ILE	2.3
2	F	311	TYR	2.3
2	E	462	PRO	2.3
1	B	494	ASP	2.3
2	E	337	ARG	2.3
1	A	267	ILE	2.3
1	B	457	GLU	2.3
3	G	69	ILE	2.3
1	C	305	LEU	2.3
2	E	461	GLY	2.3
2	D	155	PHE	2.3
1	B	450	ARG	2.3
2	F	286	ALA	2.3
1	A	461	ILE	2.3
2	D	335	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	491	GLU	2.3
1	C	178	ILE	2.3
1	A	240	ALA	2.2
1	B	482	LYS	2.2
2	E	449	TYR	2.2
4	H	112	LEU	2.2
2	E	430	LYS	2.2
1	A	305	LEU	2.2
1	C	265	LEU	2.2
2	D	414	LEU	2.2
1	B	244	TYR	2.2
1	B	256	TYR	2.2
1	B	488	LYS	2.2
2	E	202	GLU	2.2
3	G	178	ILE	2.2
2	F	174	ALA	2.2
1	A	394	LEU	2.2
2	F	428	LEU	2.2
1	A	482	LYS	2.2
1	B	196	LYS	2.2
2	D	255	ILE	2.2
4	H	127	THR	2.2
1	C	472	VAL	2.2
2	E	246	GLN	2.2
2	D	427	HIS	2.2
1	B	206	ILE	2.2
2	E	343	GLY	2.2
2	D	350	PRO	2.2
2	E	352	ASP	2.2
3	G	140	ASP	2.2
3	G	58	LYS	2.2
1	A	276	VAL	2.2
2	D	20	VAL	2.2
5	I	3	TYR	2.2
1	A	354	THR	2.2
2	D	466	ALA	2.2
1	C	120	PRO	2.2
1	A	265	LEU	2.1
2	F	186	VAL	2.1
2	E	459	MET	2.1
1	A	388	GLY	2.1
1	B	423	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	442	GLN	2.1
1	B	417	LEU	2.1
2	F	285	LEU	2.1
1	B	485	THR	2.1
2	F	9	THR	2.1
1	C	167	ILE	2.1
1	C	183	ILE	2.1
2	E	296	ILE	2.1
1	C	216	LEU	2.1
2	F	143	LEU	2.1
2	D	353	SER	2.1
4	H	129	ALA	2.1
5	I	2	ALA	2.1
1	A	194	ASP	2.1
2	F	327	ALA	2.1
1	B	343	ILE	2.1
2	E	377	ILE	2.1
3	G	116	LEU	2.1
3	G	201	LEU	2.1
1	A	484	ARG	2.1
1	B	499	GLU	2.1
3	G	221	THR	2.1
3	G	112	ILE	2.0
5	I	26	LEU	2.0
1	B	462	THR	2.0
1	C	298	VAL	2.0
2	D	348	VAL	2.0
3	G	44	TYR	2.0
1	B	455	LYS	2.0
1	B	240	ALA	2.0
3	G	198	ALA	2.0
5	I	32	ALA	2.0
1	A	144	GLU	2.0
1	B	371	VAL	2.0
2	E	420	VAL	2.0
1	B	219	ARG	2.0
3	G	45	GLY	2.0
1	B	397	TYR	2.0
1	C	177	SER	2.0
1	C	415	GLN	2.0
2	E	350	PRO	2.0
2	E	354	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	425	THR	2.0
1	A	400	VAL	2.0
2	F	248	GLY	2.0

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

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

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 Ligands (i)

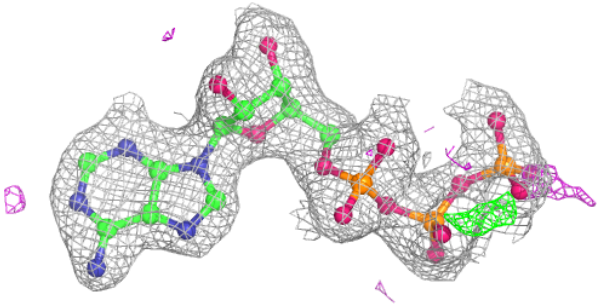
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

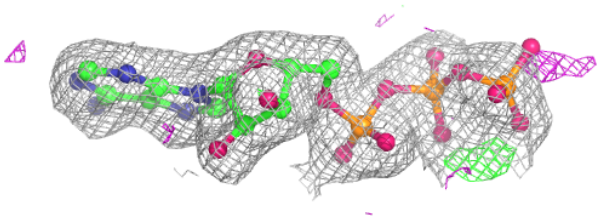
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MG	A	1512	1/1	0.82	0.18	27,27,27,27	0
8	MG	B	1512	1/1	0.83	0.18	27,27,27,27	0
8	MG	F	1476	1/1	0.83	0.16	27,27,27,27	0
8	MG	C	1512	1/1	0.85	0.13	29,29,29,29	0
8	MG	D	1479	1/1	0.90	0.15	24,24,24,24	0
10	PO4	E	1475	5/5	0.91	0.28	88,90,90,90	0
7	ATP	A	1511	31/31	0.95	0.14	23,28,38,40	4
7	ATP	B	1511	31/31	0.96	0.11	23,34,37,44	0
9	ADP	D	1478	27/27	0.97	0.11	22,29,33,36	0
9	ADP	F	1475	27/27	0.97	0.13	27,32,37,41	0
7	ATP	C	1511	31/31	0.97	0.14	25,30,37,39	4

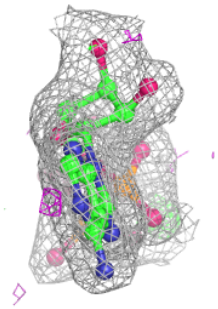
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 1511:

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

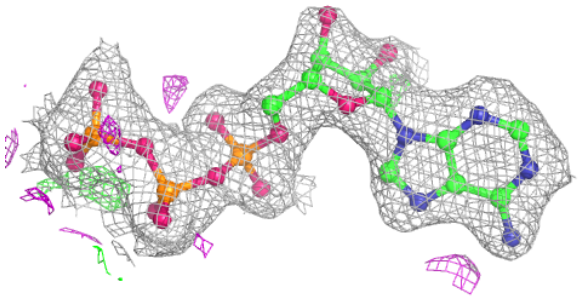


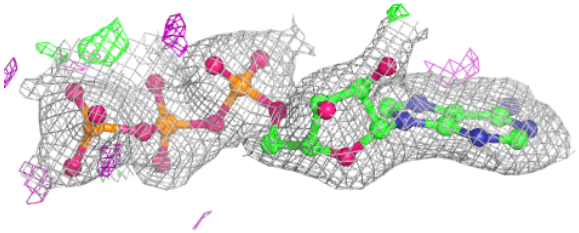


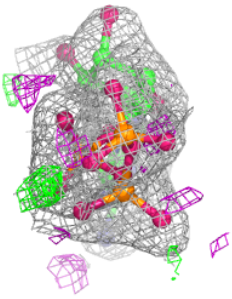


Electron density around ATP B 1511:

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

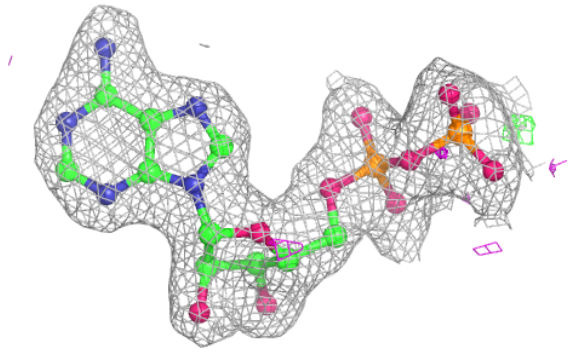


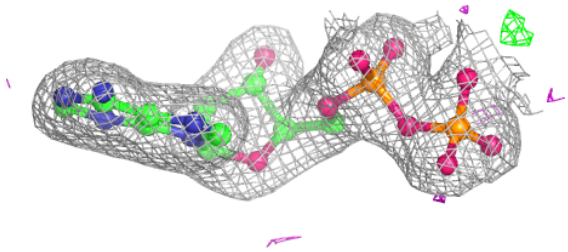


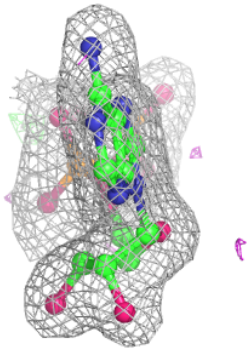


Electron density around ADP D 1478:

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

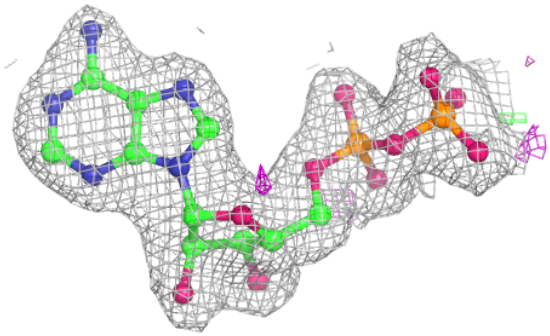


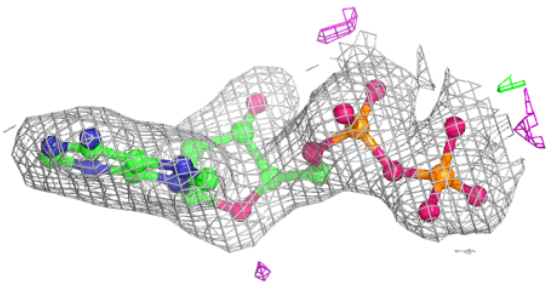


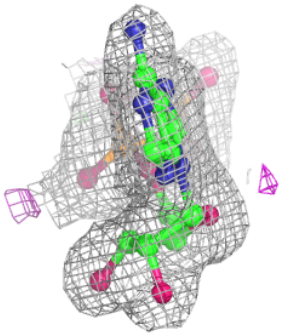


Electron density around ADP F 1475:

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

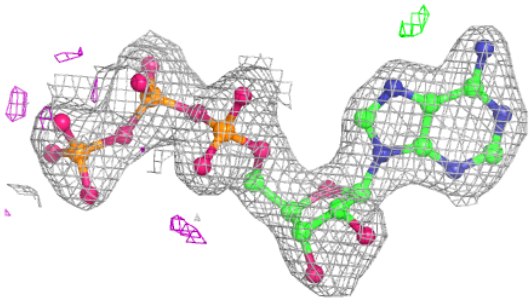


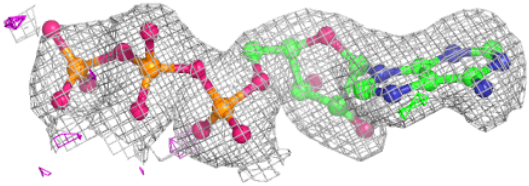


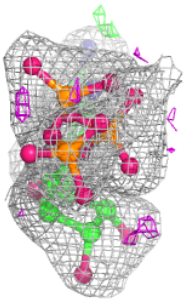


Electron density around ATP C 1511:

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







5.5 Other polymers (i)

There are no such residues in this entry.