wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary 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:

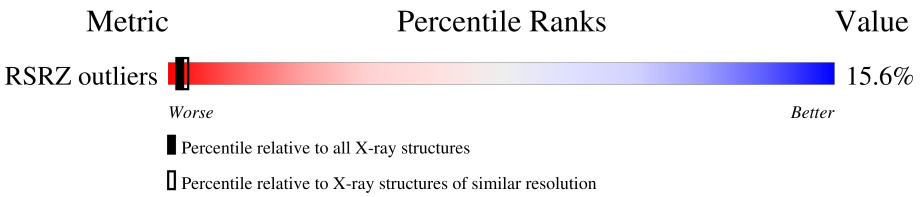
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

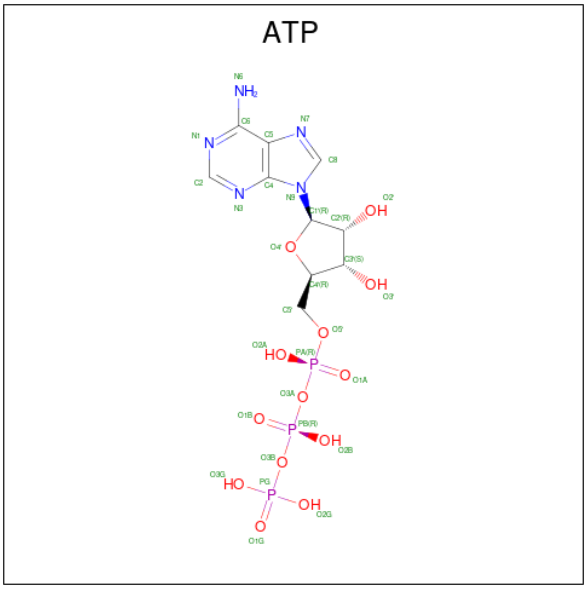
- Molecule 6 is a protein called ATPASE INHIBITOR.

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
7	B	1	31	10	5	13	3	0	0

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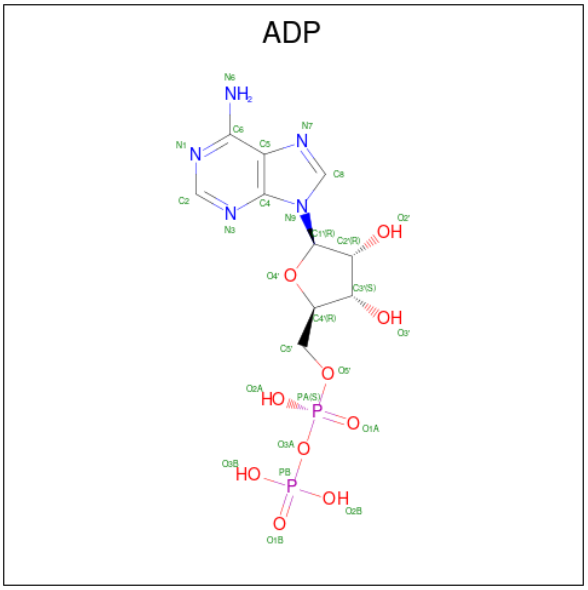
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	C	1	31	10	5	13	3	0	0

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

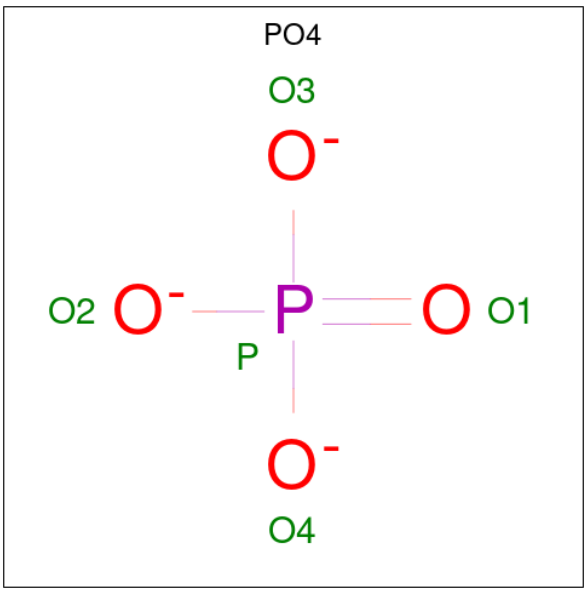
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
8	A	1	1	1	0	0
8	B	1	1	1	0	0
8	C	1	1	1	0	0
8	D	1	1	1	0	0
8	F	1	1	1	0	0

- 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)

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

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

The worst 5 of 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

The worst 5 of 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
9	D	1478	ADP	C4-C5-N7	-3.22	106.05	109.40

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

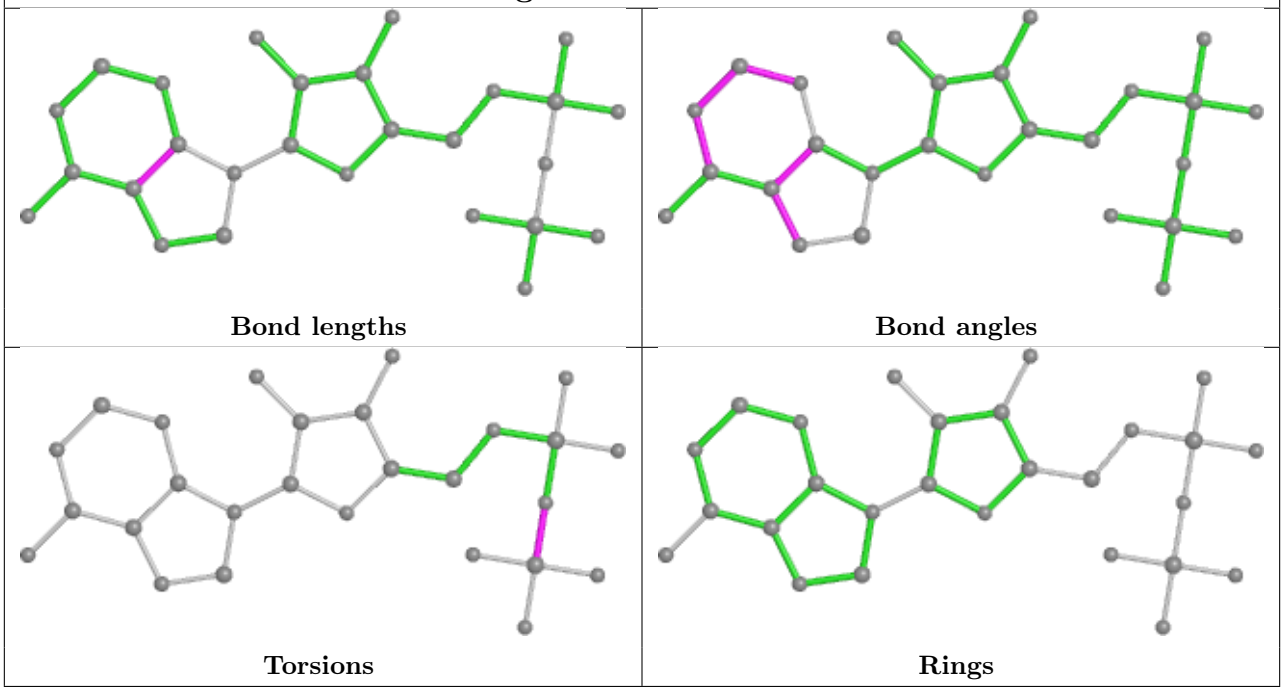
Mol	Chain	Res	Type	Atoms
7	A	1511	ATP	PB-O3B-PG-O2G
7	C	1511	ATP	PB-O3B-PG-O2G
9	D	1478	ADP	PA-O3A-PB-O2B
9	F	1475	ADP	PA-O3A-PB-O2B
9	F	1475	ADP	PA-O3A-PB-O1B

There are no ring outliers.

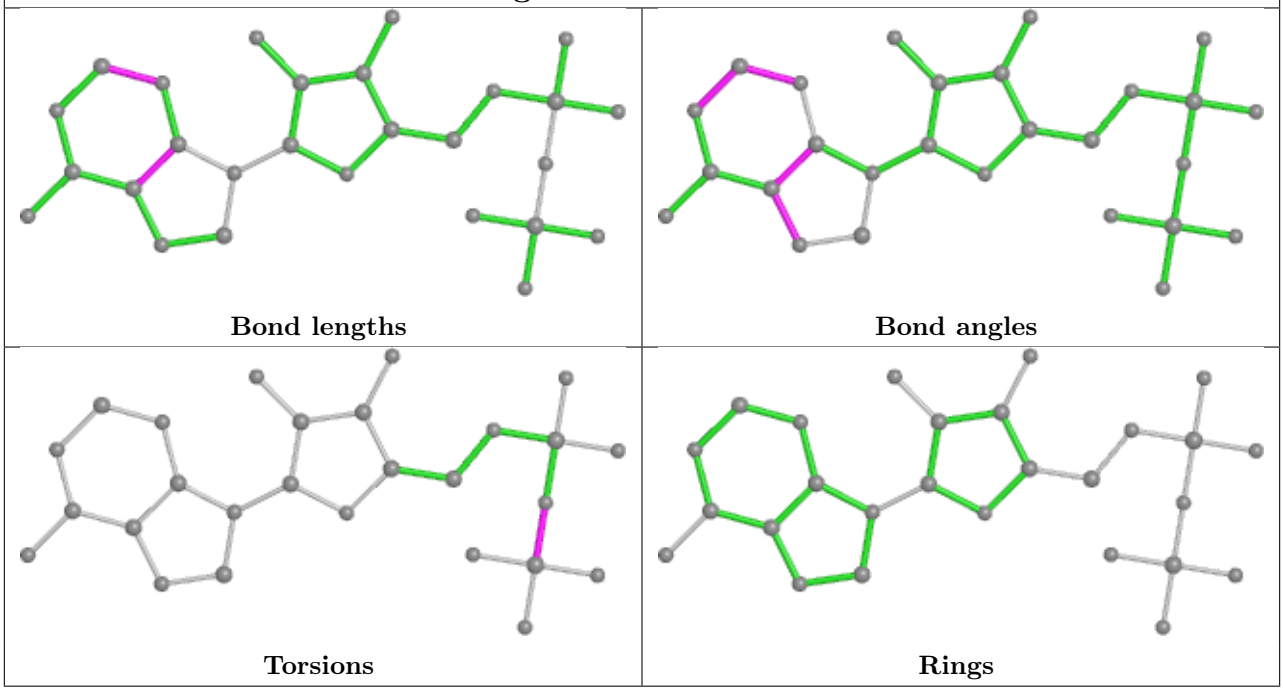
No monomer is involved in short contacts.

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.

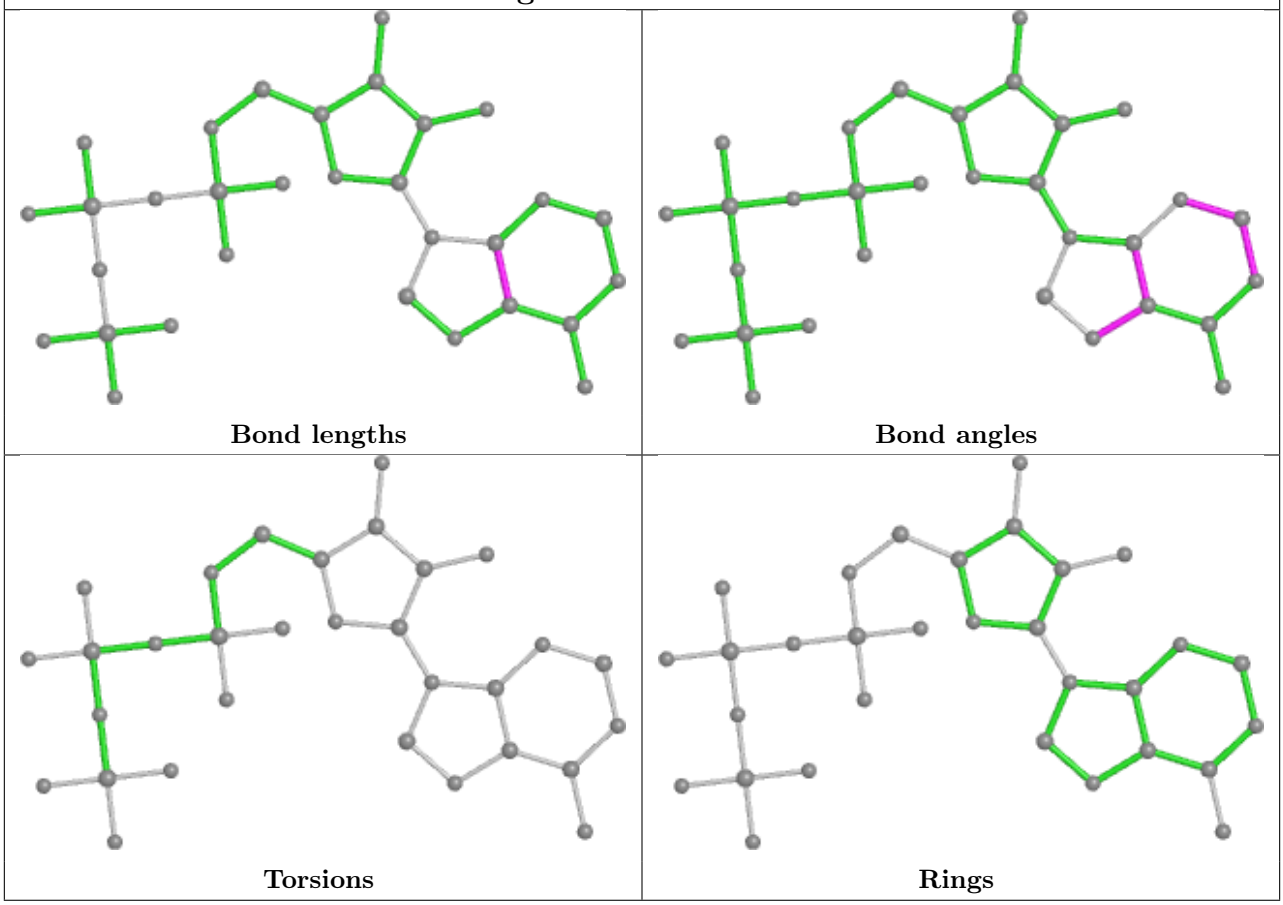
Ligand ADP F 1475



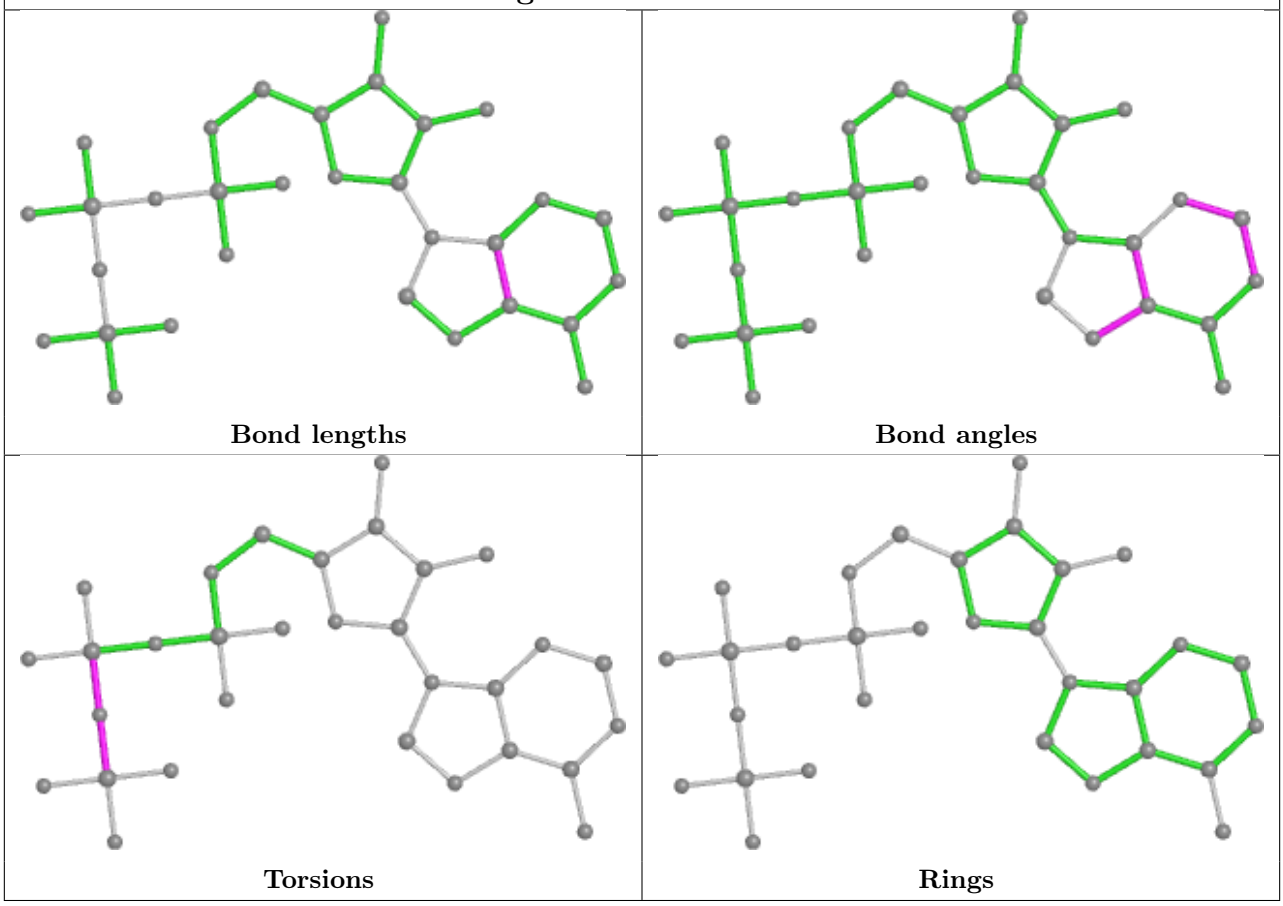
Ligand ADP D 1478



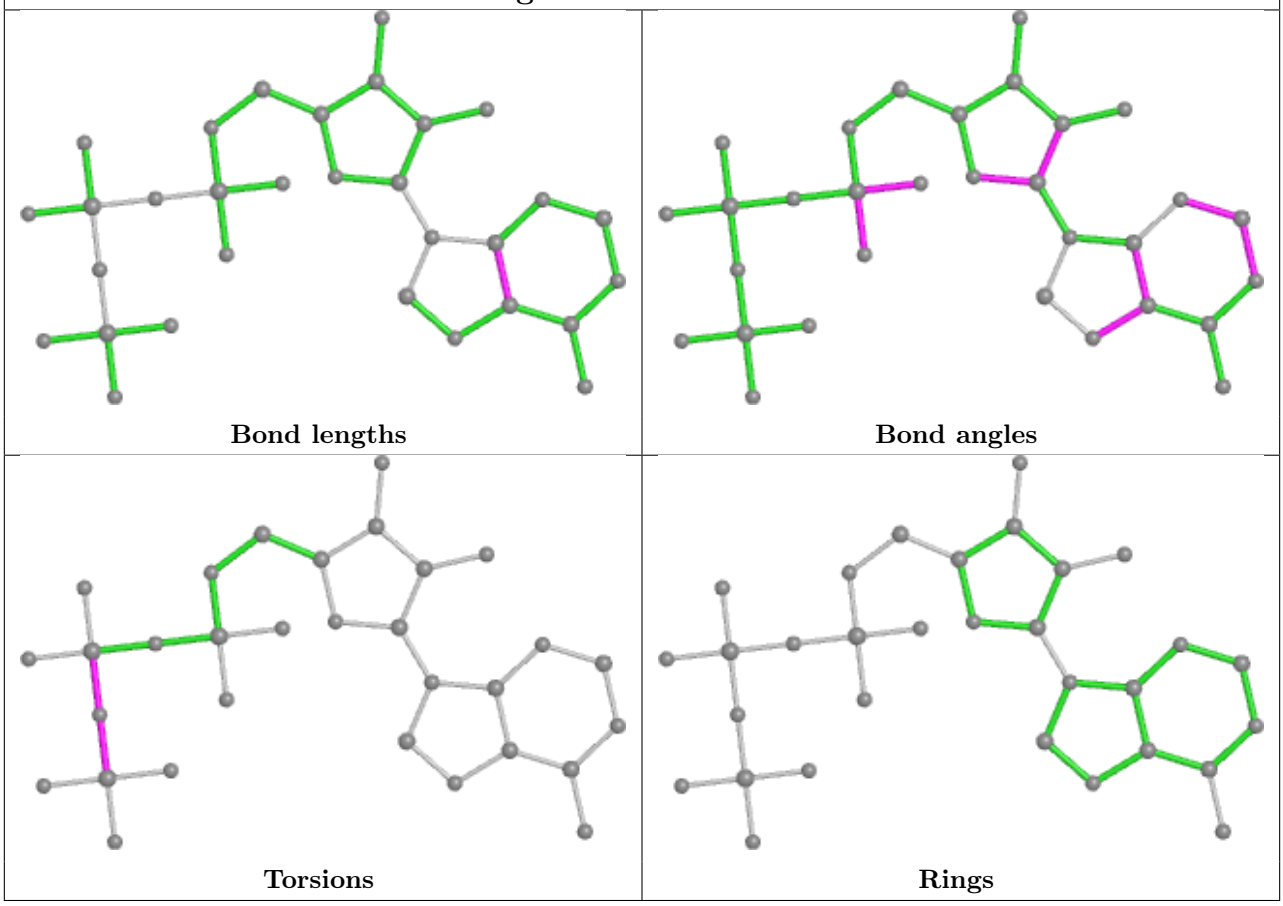
Ligand ATP B 1511



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

The worst 5 of 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

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)

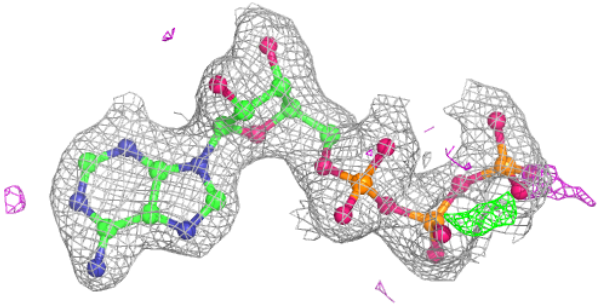
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

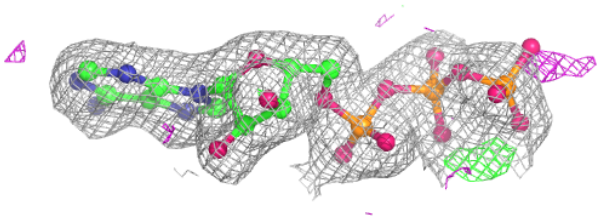
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MG	A	1512	1/1	0.82	0.18	27,27,27,27	0
8	MG	B	1512	1/1	0.83	0.18	27,27,27,27	0
8	MG	F	1476	1/1	0.83	0.16	27,27,27,27	0
8	MG	C	1512	1/1	0.85	0.13	29,29,29,29	0
8	MG	D	1479	1/1	0.90	0.15	24,24,24,24	0
10	PO4	E	1475	5/5	0.91	0.28	88,90,90,90	0
7	ATP	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

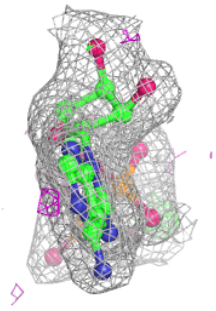
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

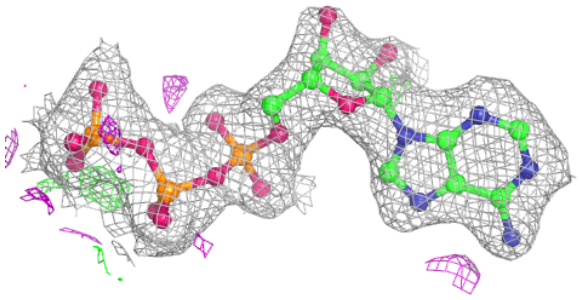


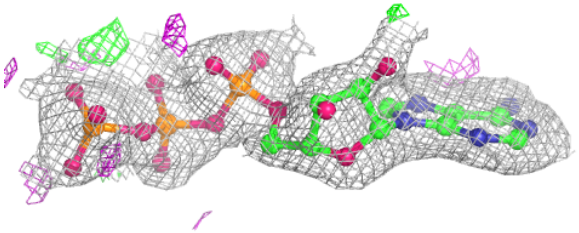


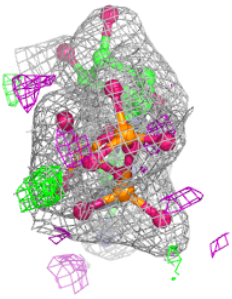


Electron density around ATP B 1511:

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

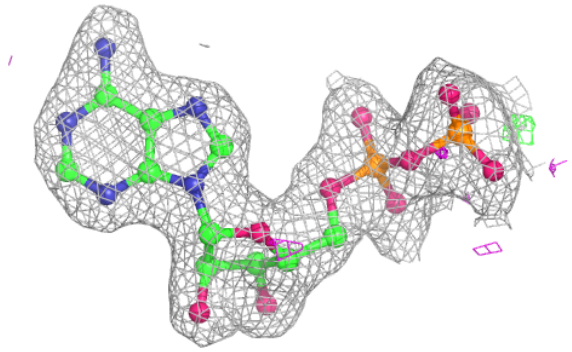


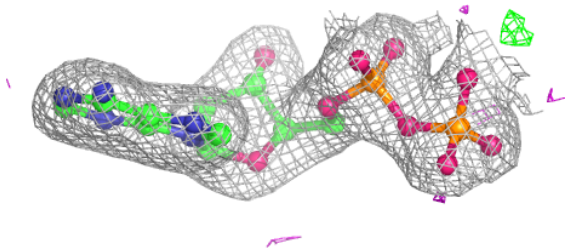


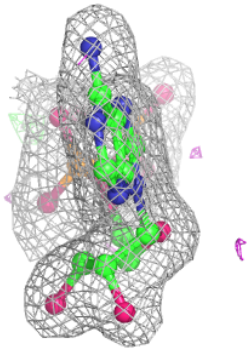


Electron density around ADP D 1478:

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

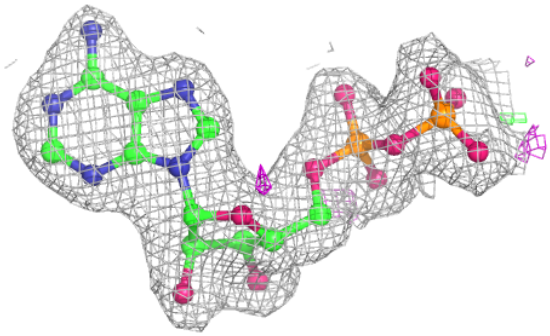


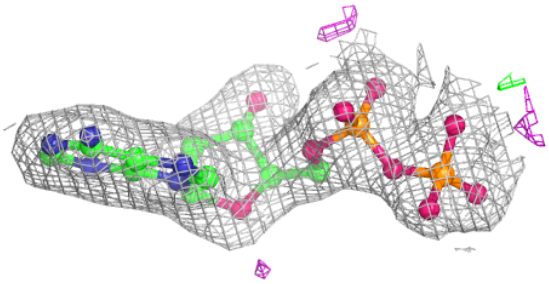


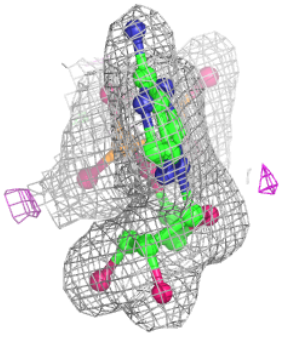


Electron density around ADP F 1475:

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

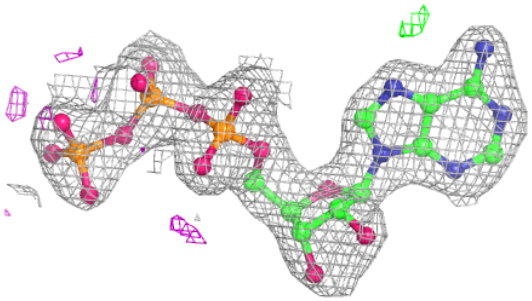


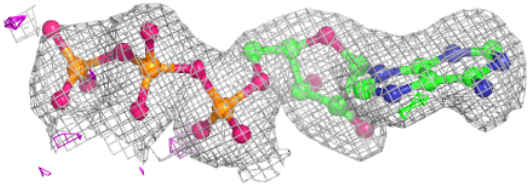


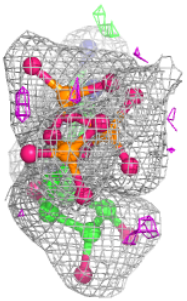


Electron density around ATP C 1511:

$2mF_o$-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.