



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:52 PM UTC

PDB ID : 2V7Q / pdb_00002v7q
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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

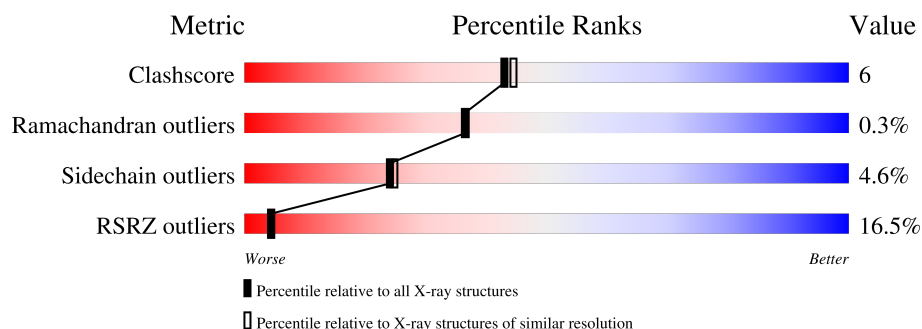
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
2	D	482	
2	E	482	
2	F	482	
3	G	272	

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Mol	Chain	Length	Quality of chain
4	H	146	26% 75% 13% 10%
5	I	50	64% 78% 14% 6%
6	J	66	5% 52% 12% 35%

2 Entry composition

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
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	C	473	Total	C	N	O	S	0	0	0
			3607	2279	637	679	12			

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

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

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

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

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

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

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

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

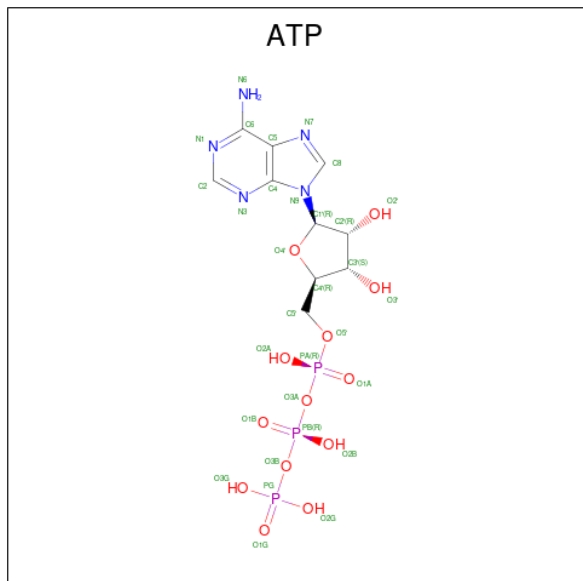
- Molecule 6 is a protein called ATPASE INHIBITOR.

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

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 (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



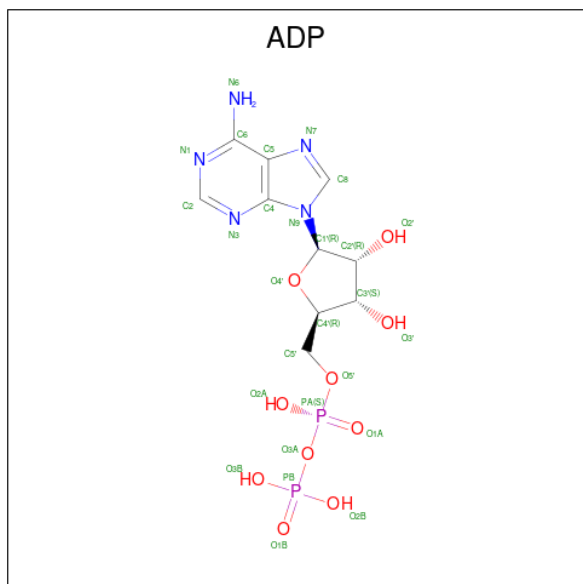
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

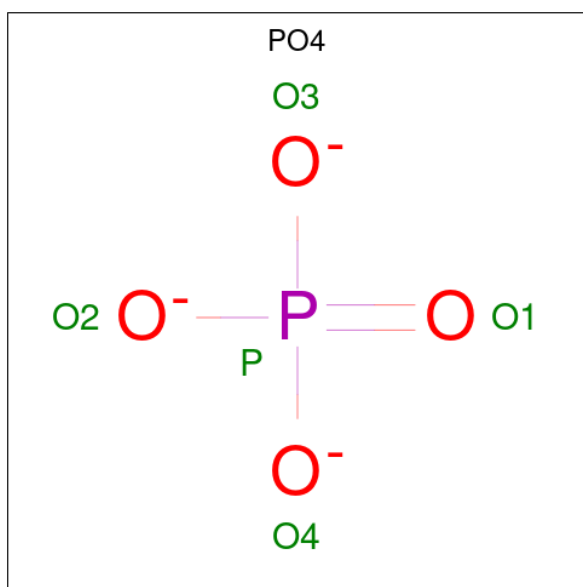
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

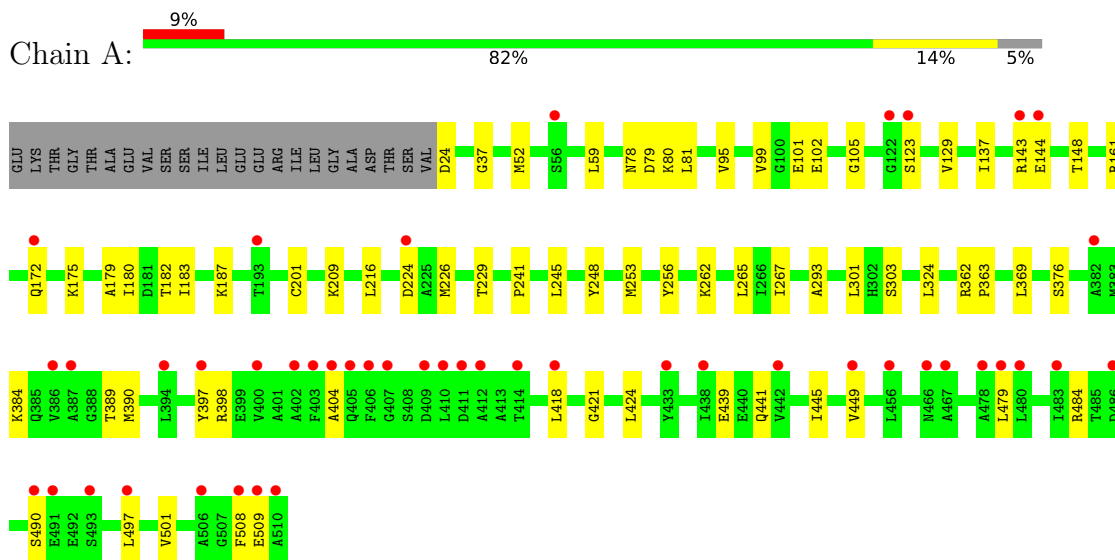
- Molecule 11 is water.

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

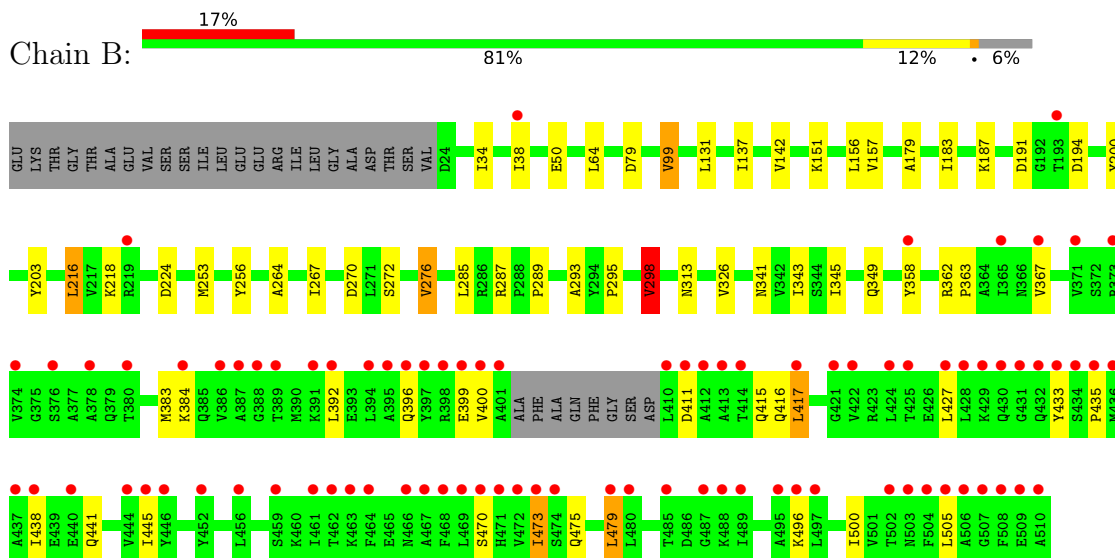
3 Residue-property plots [i](#)

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.

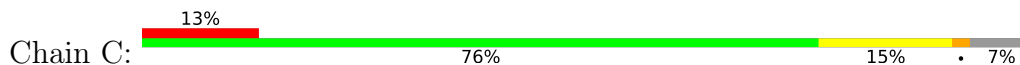
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

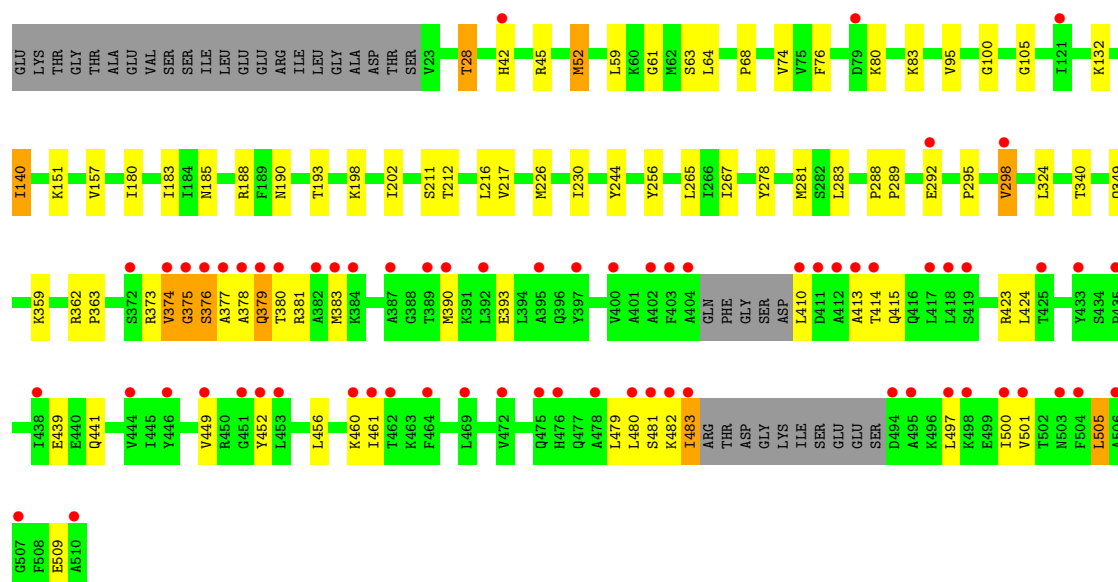


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

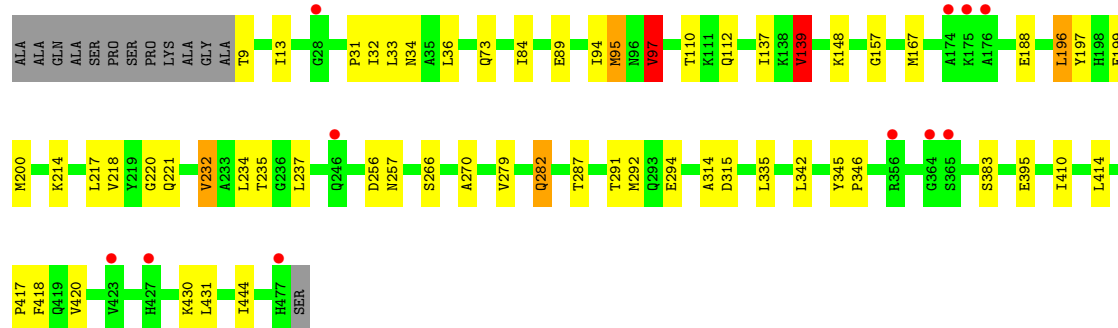
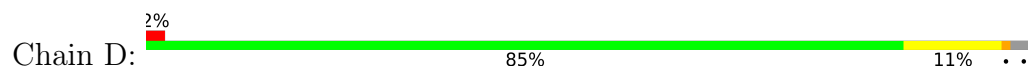


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

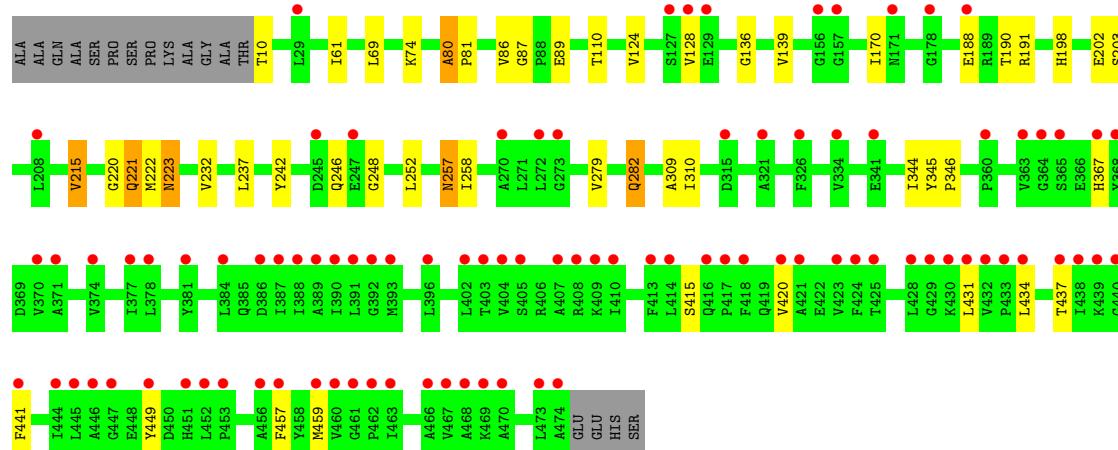
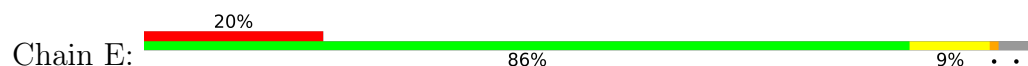




• Molecule 2: ATP SYNTHASE SUBUNIT BETA

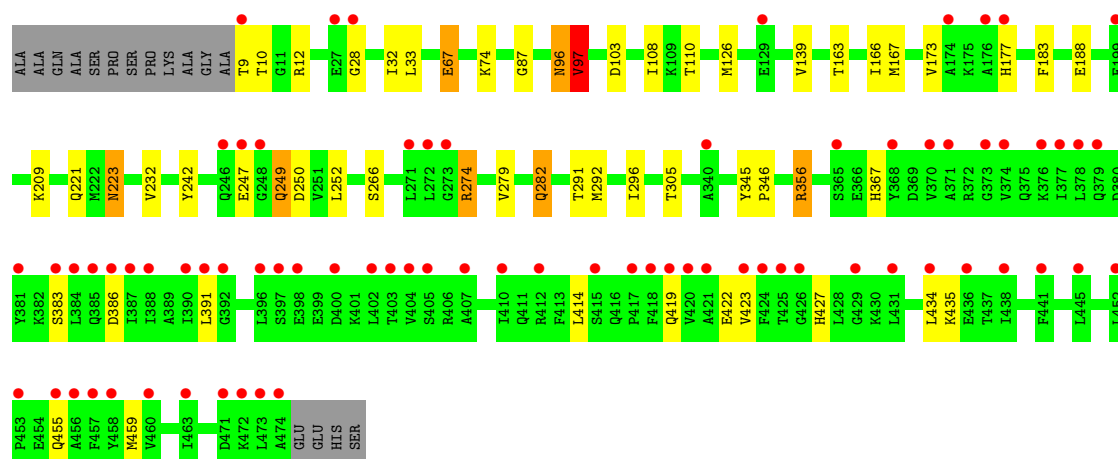


• Molecule 2: ATP SYNTHASE SUBUNIT BETA



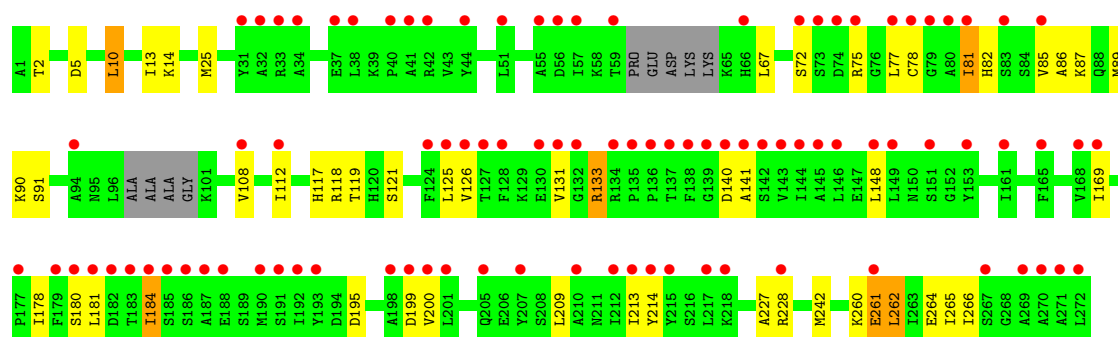
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain F: 



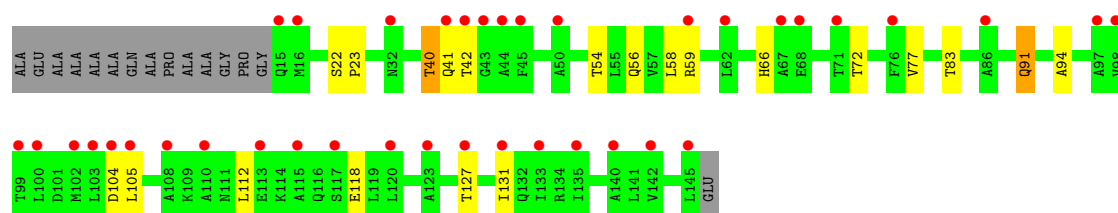
• Molecule 3: ATP SYNTHASE GAMMA CHAIN

Chain G: 



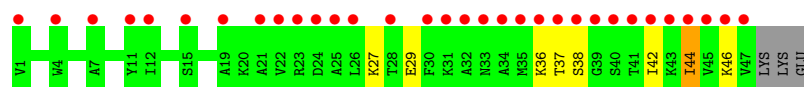
• Molecule 4: ATP SYNTHASE DELTA CHAIN

Chain H: 



• Molecule 5: ATP SYNTHASE EPSILON CHAIN

Chain I: 



• Molecule 6: ATPASE INHIBITOR



4 Data and refinement statistics

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 37.19 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.19-2.10) 98.9 (37.19-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.245 (Not available) , (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)	0.32 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ATP, ADP

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	0.61	2/3766 (0.1%)	0.86	0/5080
1	B	0.60	0/3704	0.88	2/4995 (0.0%)
1	C	0.66	2/3655 (0.1%)	0.88	4/4930 (0.1%)
2	D	0.63	0/3616	0.87	3/4906 (0.1%)
2	E	0.55	0/3580	0.82	1/4857 (0.0%)
2	F	0.62	0/3587	0.84	2/4867 (0.0%)
3	G	0.51	0/2077	0.85	0/2787
4	H	0.49	0/982	0.83	0/1337
5	I	0.49	0/374	0.82	1/501 (0.2%)
6	J	0.57	1/343 (0.3%)	1.01	3/453 (0.7%)
All	All	0.60	5/25684 (0.0%)	0.86	16/34713 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	482	LYS	C-N	12.27	1.50	1.33
1	C	373	ARG	C-N	8.16	1.44	1.33
1	A	490	SER	CB-OG	6.37	1.54	1.42
1	A	137	ILE	CA-CB	6.12	1.57	1.54
6	J	23	GLY	C-N	-5.75	1.26	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	97	VAL	CB-CA-C	-10.77	97.94	112.04
2	F	97	VAL	CB-CA-C	-8.92	100.35	112.04
6	J	18	ALA	O-C-N	-7.84	111.64	122.46
2	D	139	VAL	CB-CA-C	-7.74	102.06	111.97
1	C	379	GLN	N-CA-C	-7.63	102.78	112.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3715	0	3812	45	0
1	B	3656	0	3763	37	0
1	C	3607	0	3717	59	0
2	D	3558	0	3605	46	0
2	E	3523	0	3580	34	0
2	F	3530	0	3586	57	0
3	G	2054	0	2122	44	0
4	H	970	0	972	10	0
5	I	369	0	395	7	0
6	J	339	0	333	5	0
7	A	31	0	12	2	0
7	B	31	0	12	0	0
7	C	31	0	12	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
9	D	27	0	12	0	0
9	F	27	0	12	0	0
10	E	5	0	0	0	0
11	A	286	0	0	4	0
11	B	294	0	0	4	0
11	C	296	0	0	7	0
11	D	367	0	0	3	0
11	E	216	0	0	1	0
11	F	316	0	0	10	0
11	G	112	0	0	3	0
11	H	27	0	0	0	0
11	I	6	0	0	0	0
11	J	20	0	0	0	0
All	All	27418	0	25945	318	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 6.

The worst 5 of 318 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)
2:F:166:ILE:HG23	2:F:167:MET:HE2	1.24	1.14
1:C:52:MET:HE3	1:C:95:VAL:HG22	1.29	1.08
2:D:167:MET:HE1	2:D:196:LEU:HD13	1.35	1.08
1:C:211:SER:HB3	2:F:126:MET:HE2	1.37	1.02
2:F:126:MET:HE3	11:F:2122:HOH:O	1.60	1.02

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	485/510 (95%)	472 (97%)	13 (3%)	0	100	100
1	B	475/510 (93%)	459 (97%)	15 (3%)	1 (0%)	43	44
1	C	467/510 (92%)	447 (96%)	16 (3%)	4 (1%)	14	10
2	D	467/482 (97%)	451 (97%)	16 (3%)	0	100	100
2	E	463/482 (96%)	448 (97%)	14 (3%)	1 (0%)	43	44
2	F	464/482 (96%)	452 (97%)	10 (2%)	2 (0%)	30	28
3	G	257/272 (94%)	244 (95%)	11 (4%)	2 (1%)	16	12
4	H	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
5	I	45/50 (90%)	42 (93%)	2 (4%)	1 (2%)	5	2
6	J	41/66 (62%)	40 (98%)	1 (2%)	0	100	100
All	All	3293/3510 (94%)	3177 (96%)	105 (3%)	11 (0%)	36	36

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	374	VAL
1	B	194	ASP
2	F	247	GLU
5	I	29	GLU
3	G	148	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	328/413 (79%)	311 (95%)	17 (5%)	21	20
1	C	381/413 (92%)	361 (95%)	20 (5%)	21	20
2	D	379/386 (98%)	364 (96%)	15 (4%)	28	29
2	E	375/386 (97%)	364 (97%)	11 (3%)	37	42
2	F	376/386 (97%)	362 (96%)	14 (4%)	30	33
3	G	225/230 (98%)	211 (94%)	14 (6%)	16	14
4	H	104/109 (95%)	97 (93%)	7 (7%)	15	12
5	I	38/41 (93%)	36 (95%)	2 (5%)	20	19
6	J	30/50 (60%)	28 (93%)	2 (7%)	15	12
All	All	2236/2414 (93%)	2134 (95%)	102 (5%)	24	25

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	221	GLN
2	F	282	GLN
5	I	46	LYS
2	E	237	LEU
2	F	96	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	249	GLN
3	G	120	HIS
2	F	282	GLN
2	F	379	GLN
4	H	85	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 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	$\# Z > 2$
7	ATP	C	1511	8	32,33,33	1.44	5 (15%)	48,52,52	1.85	10 (20%)
9	ADP	F	1475	8	28,29,29	1.39	3 (10%)	43,45,45	1.83	9 (20%)
7	ATP	A	1511	8	32,33,33	1.41	5 (15%)	48,52,52	1.92	10 (20%)
10	PO4	E	1475	-	4,4,4	0.95	0	6,6,6	0.48	0
9	ADP	D	1478	8	28,29,29	1.51	5 (17%)	43,45,45	1.93	7 (16%)
7	ATP	B	1511	8	32,33,33	1.62	6 (18%)	48,52,52	1.79	9 (18%)

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	C	1511	8	-	3/22/38/38	0/3/3/3
9	ADP	F	1475	8	-	2/16/32/32	0/3/3/3
7	ATP	A	1511	8	-	4/22/38/38	0/3/3/3
9	ADP	D	1478	8	-	2/16/32/32	0/3/3/3
7	ATP	B	1511	8	-	0/22/38/38	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1511	ATP	C5-C4	4.95	1.47	1.39
9	D	1478	ADP	C5-C4	4.95	1.47	1.39
7	A	1511	ATP	C5-C4	4.89	1.47	1.39
9	F	1475	ADP	C5-C4	4.71	1.47	1.39
7	C	1511	ATP	C5-C4	4.61	1.47	1.39

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1511	ATP	C5-C4-N3	-6.30	118.04	126.72
9	D	1478	ADP	C5-C4-N3	-6.30	118.04	126.72
7	B	1511	ATP	C5-C4-N3	-5.90	118.60	126.72
7	C	1511	ATP	C5-C4-N3	-5.71	118.85	126.72
9	F	1475	ADP	C5-C4-N3	-5.66	118.92	126.72

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

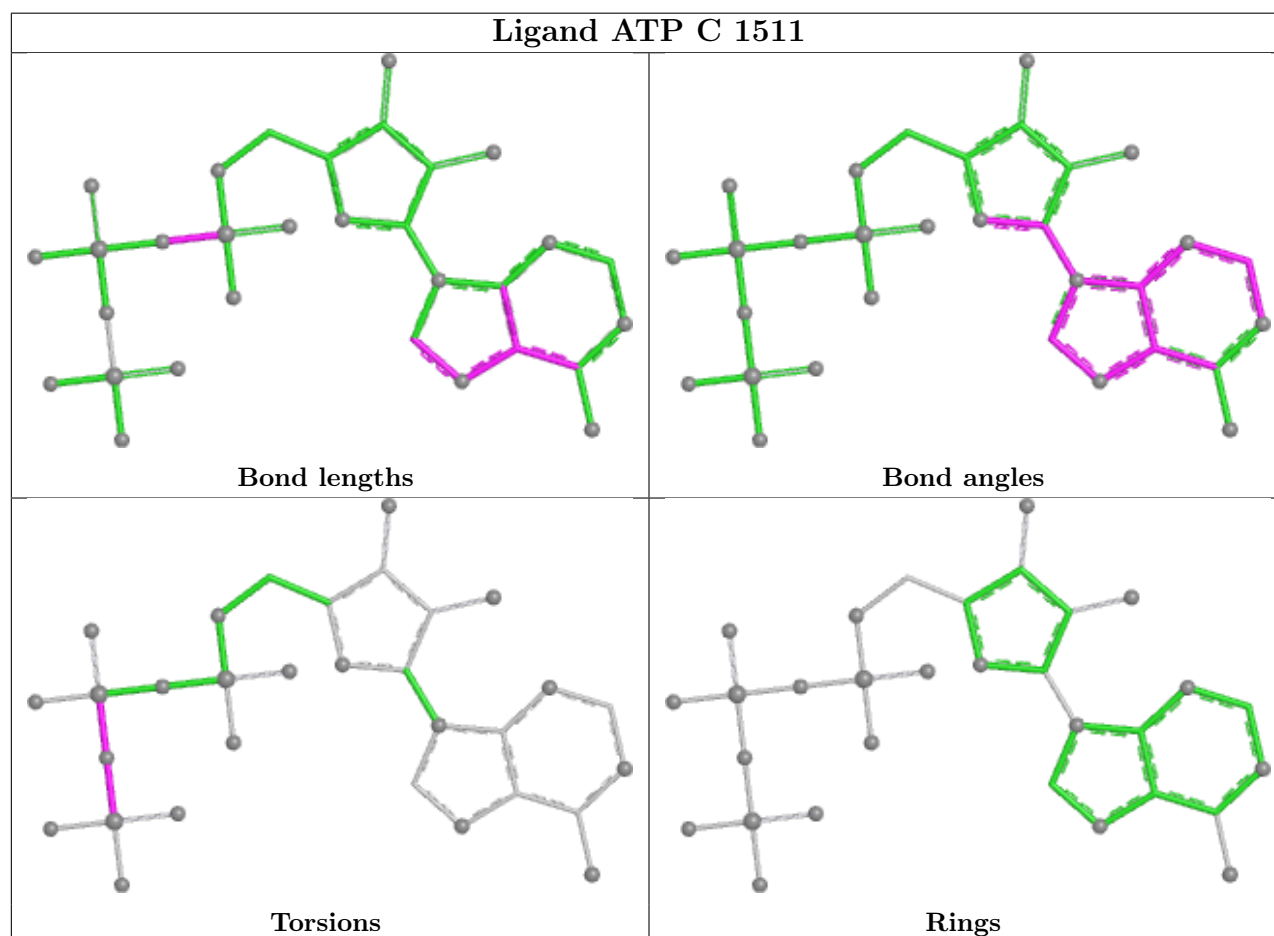
Mol	Chain	Res	Type	Atoms
7	A	1511	ATP	PB-O3B-PG-O2G
7	C	1511	ATP	PB-O3B-PG-O2G
9	D	1478	ADP	PA-O3A-PB-O2B
9	F	1475	ADP	PA-O3A-PB-O2B
9	F	1475	ADP	PA-O3A-PB-O1B

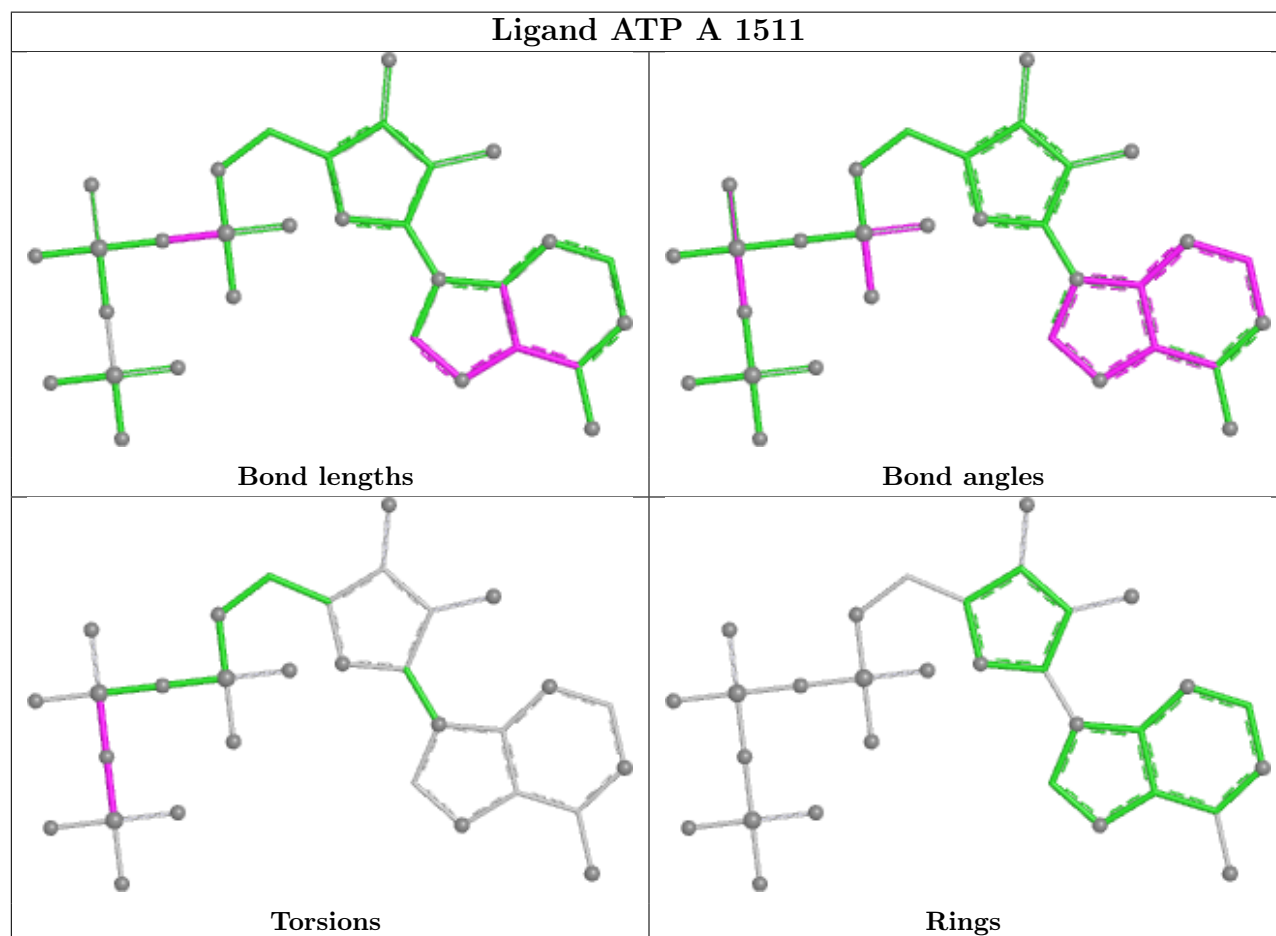
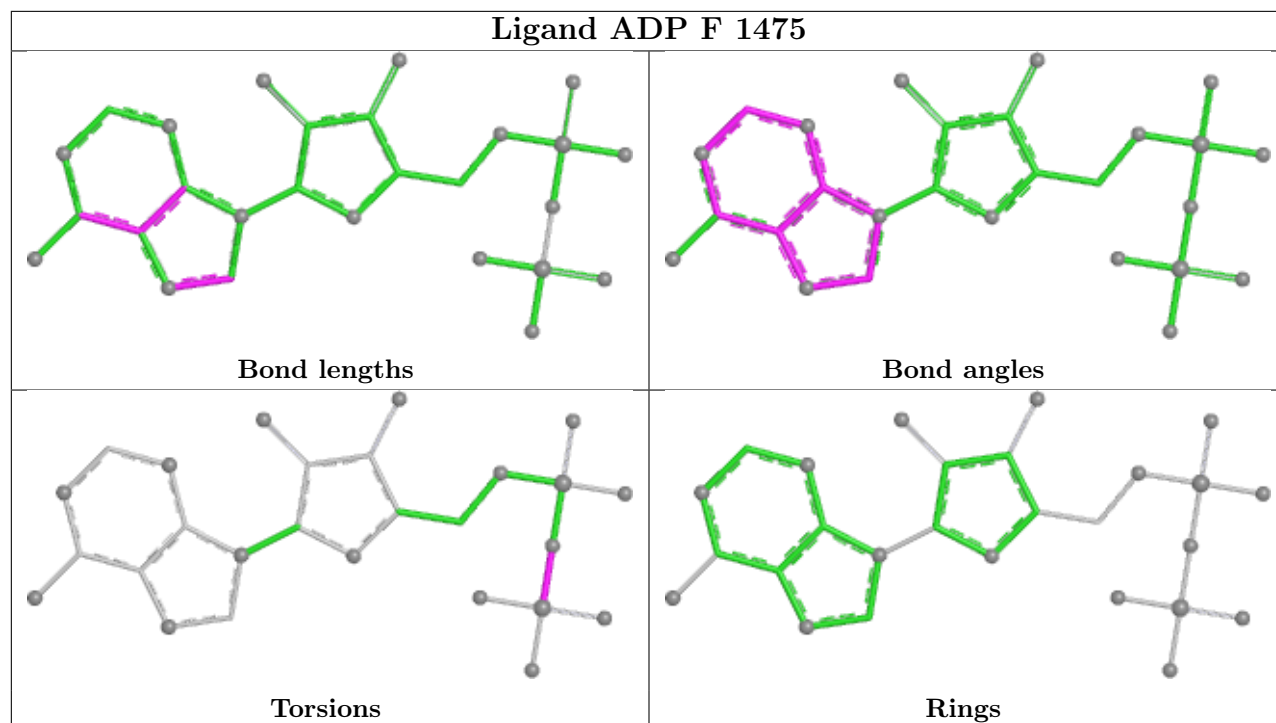
There are no ring outliers.

1 monomer is involved in 2 short contacts:

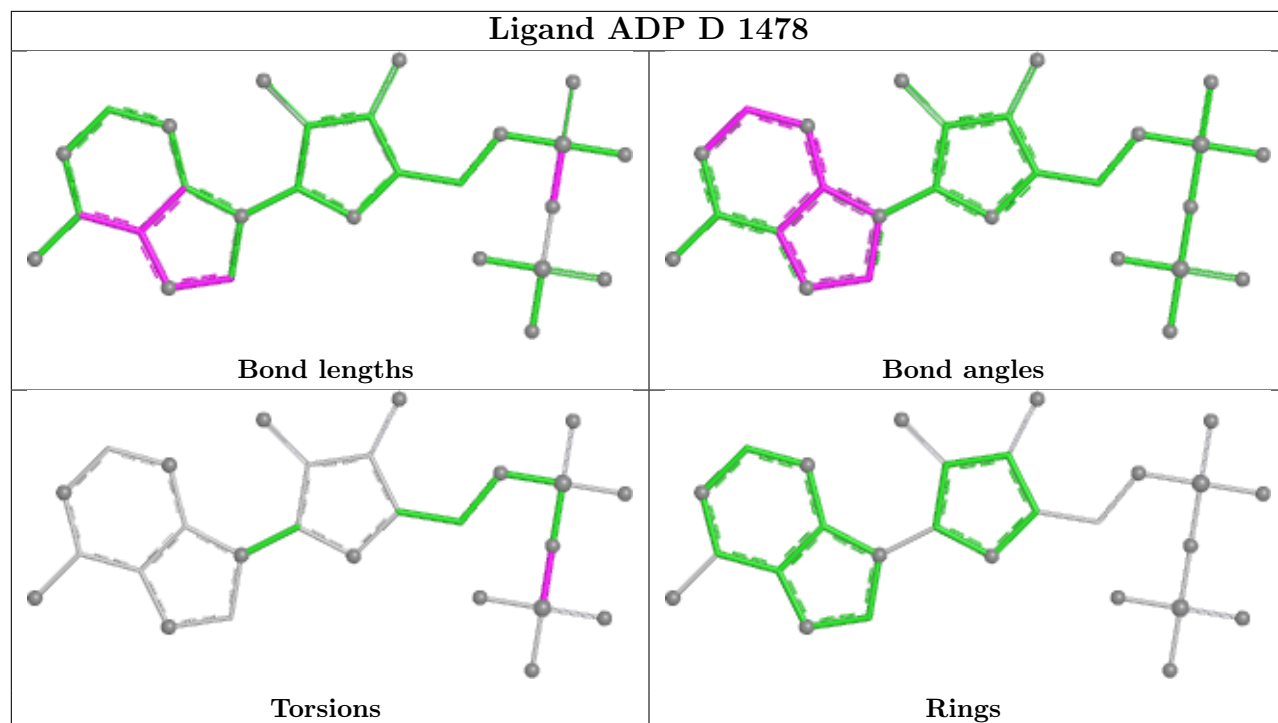
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1511	ATP	2	0

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

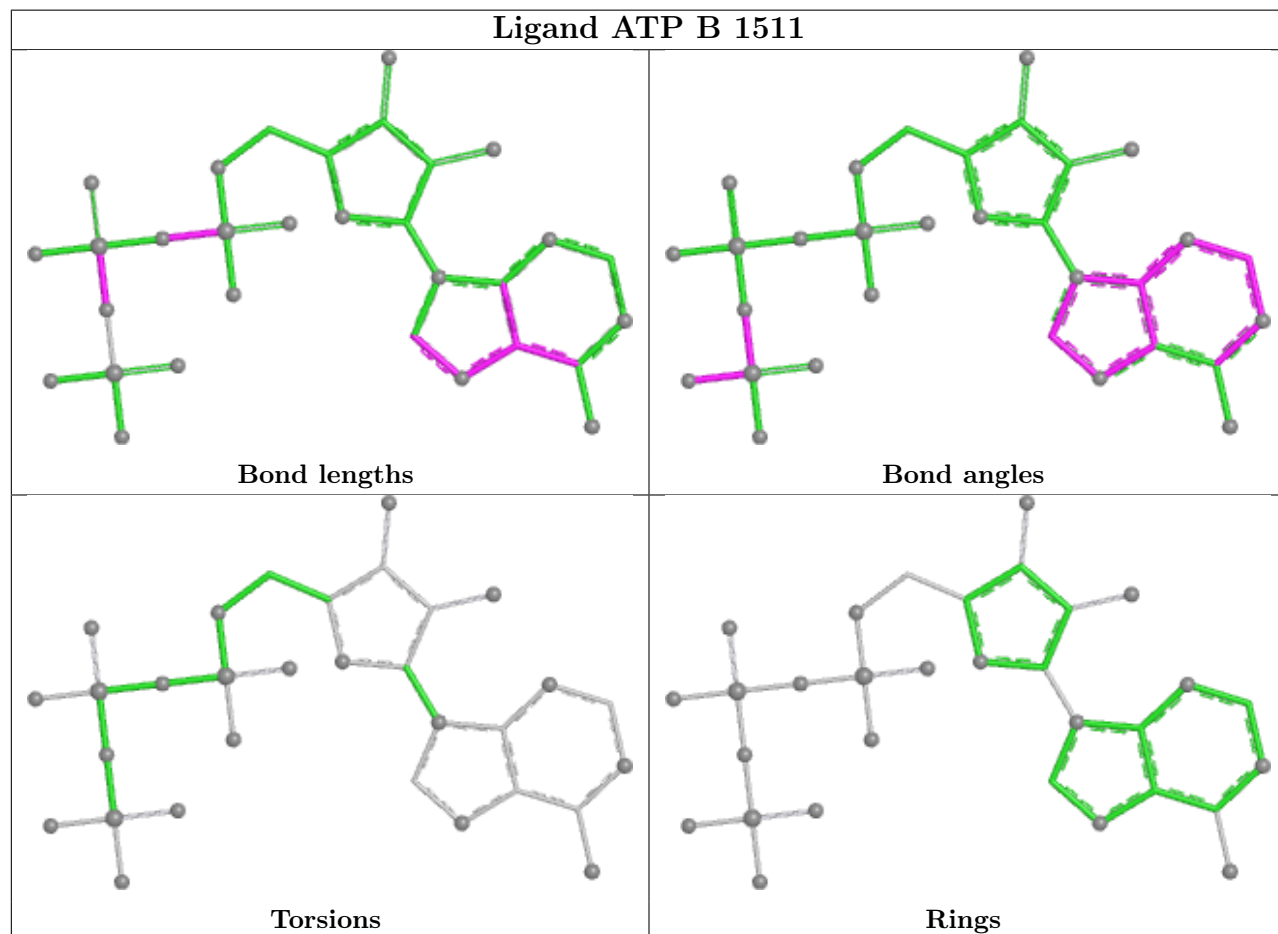




Ligand ADP D 1478



Ligand ATP B 1511



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 [i](#)

6.1 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%)	0.70	46 (9%)	14 14	22, 34, 60, 86	0
1	B	479/510 (93%)	0.92	87 (18%)	3 3	21, 33, 70, 82	0
1	C	473/510 (92%)	0.85	68 (14%)	6 6	22, 32, 65, 87	0
2	D	469/482 (97%)	0.36	11 (2%)	61 64	21, 30, 47, 65	0
2	E	465/482 (96%)	1.13	94 (20%)	3 3	23, 40, 84, 89	0
2	F	466/482 (96%)	0.87	75 (16%)	4 5	22, 32, 58, 77	0
3	G	263/272 (96%)	1.67	94 (35%)	1 1	26, 53, 83, 93	0
4	H	131/146 (89%)	1.64	38 (29%)	1 1	36, 54, 75, 76	0
5	I	47/50 (94%)	2.79	32 (68%)	0 0	46, 60, 105, 108	0
6	J	43/66 (65%)	0.54	3 (6%)	22 24	12, 24, 56, 65	0
All	All	3323/3510 (94%)	0.93	548 (16%)	4 4	12, 35, 74, 108	0

The worst 5 of 548 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	377	ALA	6.9
1	C	374	VAL	6.3
5	I	45	VAL	6.2
1	A	406	PHE	5.9
2	E	388	ILE	5.9

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

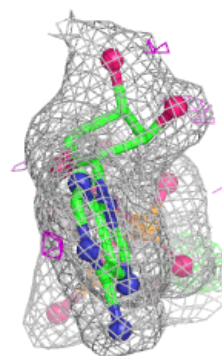
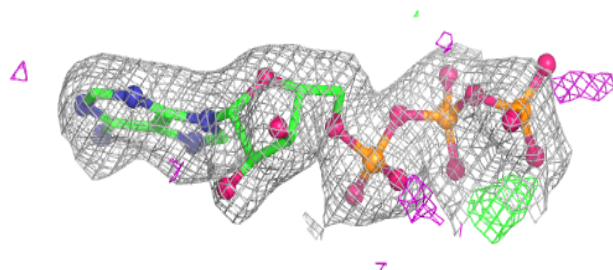
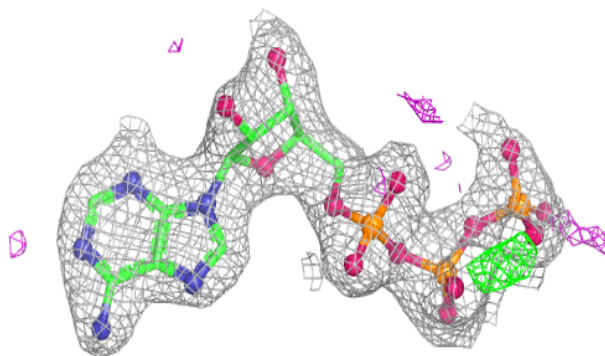
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	PO4	E	1475	5/5	0.72	0.11	88,90,90,90	0
8	MG	F	1476	1/1	0.77	0.12	27,27,27,27	0
8	MG	A	1512	1/1	0.85	0.13	27,27,27,27	0
8	MG	C	1512	1/1	0.89	0.07	29,29,29,29	0
8	MG	B	1512	1/1	0.91	0.12	27,27,27,27	0
8	MG	D	1479	1/1	0.93	0.07	24,24,24,24	0
7	ATP	A	1511	31/31	0.95	0.08	23,28,38,40	4
7	ATP	B	1511	31/31	0.96	0.07	23,34,37,44	0
9	ADP	F	1475	27/27	0.96	0.07	27,32,37,41	0
7	ATP	C	1511	31/31	0.96	0.07	25,30,37,39	4
9	ADP	D	1478	27/27	0.98	0.06	22,29,33,36	0

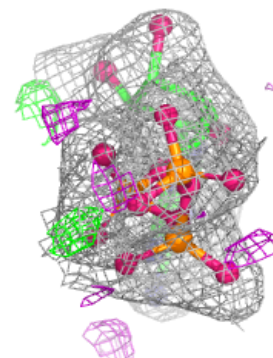
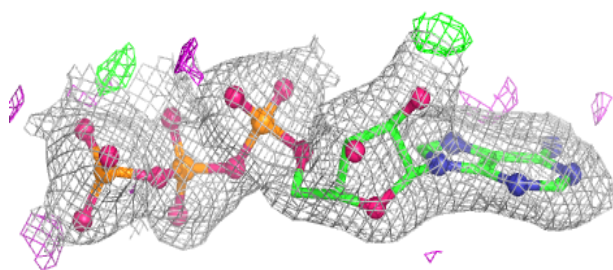
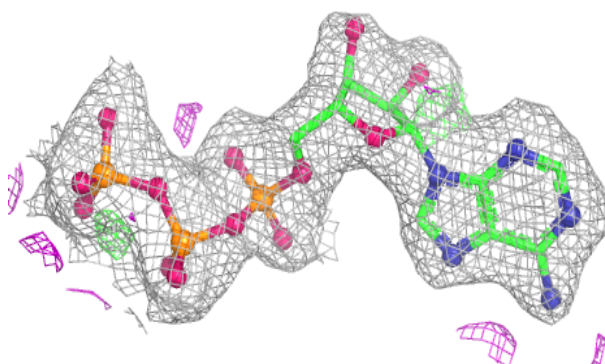
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 1511:

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

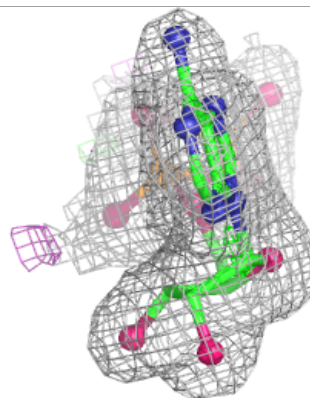
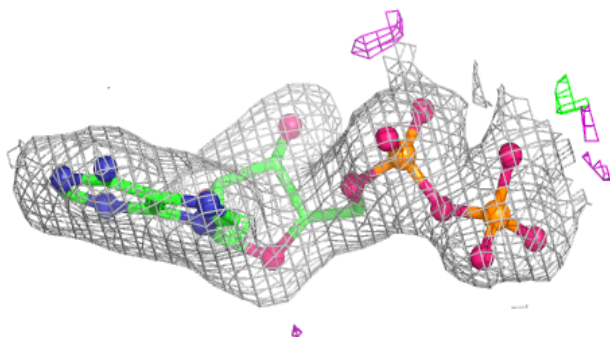
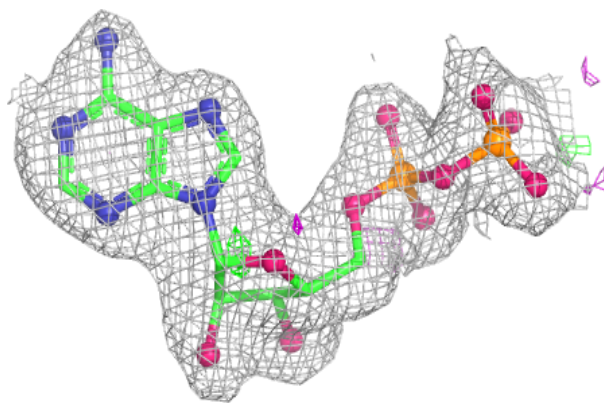
**Electron density around ATP B 1511:**

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

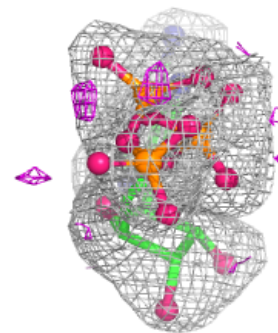
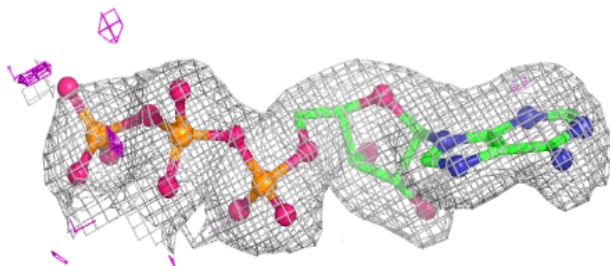
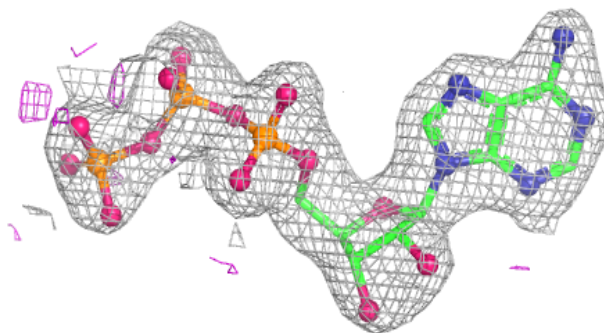


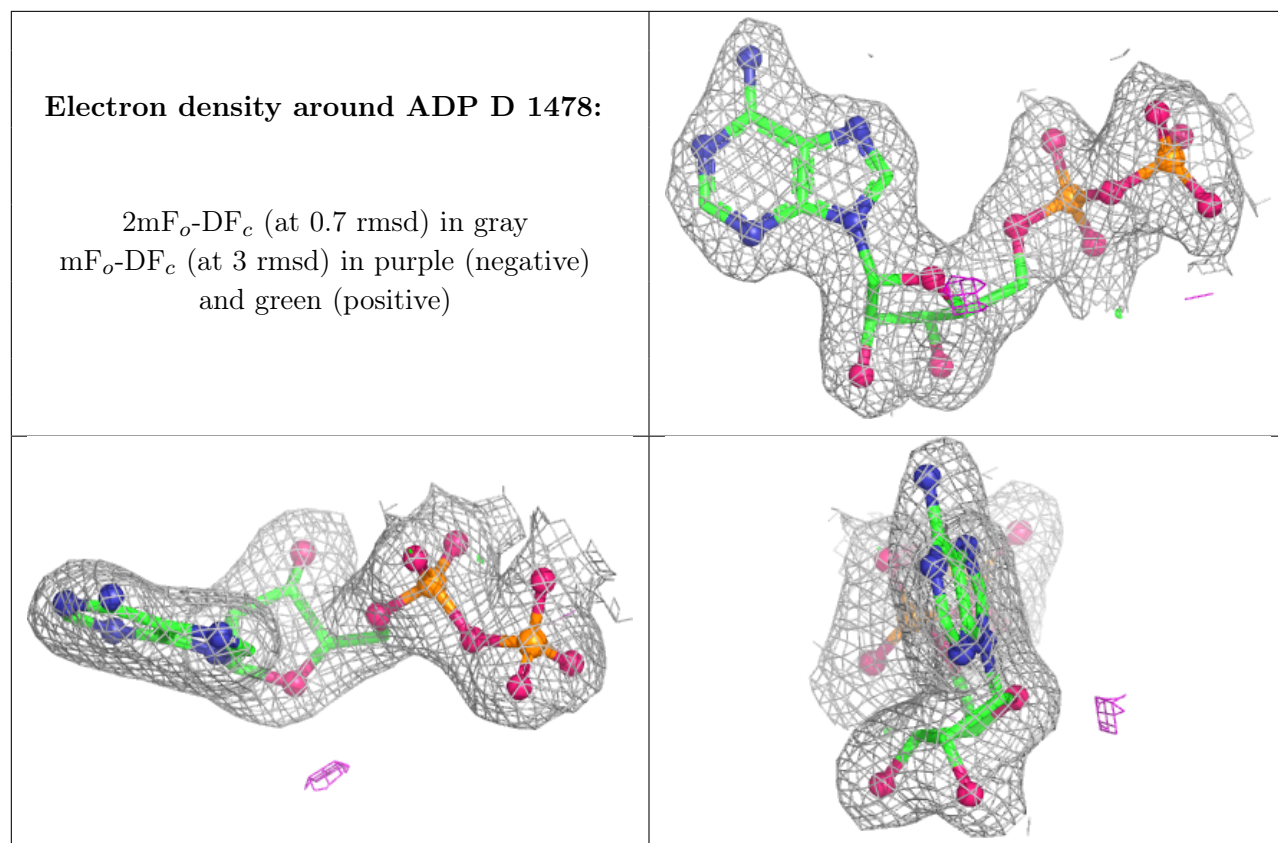
Electron density around ADP F 1475:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.