



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 6, 2023 – 09:13 pm GMT

PDB ID : 1H8H  
Title : Bovine mitochondrial F1-ATPase crystallised in the presence of 5mm AMPPNP  
Authors : Braig, K.; Menz, R.I.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2001-02-06  
Resolution : 2.90 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](mailto: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>.

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

MolProbity : 4.02b-467  
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

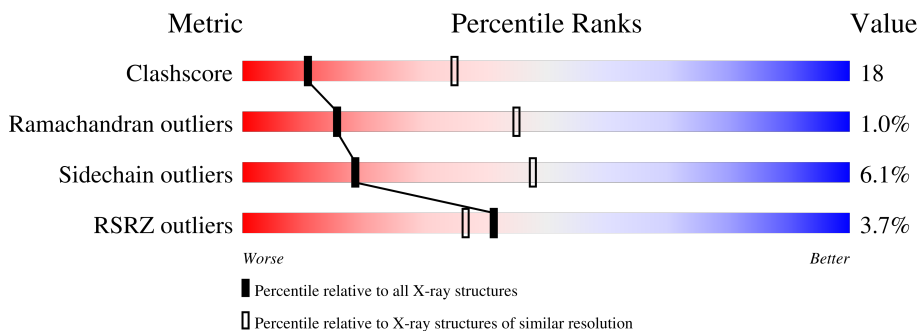
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	 2% 58% 33% 5% 5%
1	B	510	 2% 53% 37% 6% 6%
1	C	510	 % 58% 34% 6% 6%
2	D	482	 2% 60% 34% 6% 6%
2	E	482	 6% 53% 39% 6% 6%
2	F	482	 % 63% 29% 6% 6%

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Mol	Chain	Length	Quality of chain
3	G	272	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (12%), a green segment (26%), a yellow segment (15%), and a grey segment (55%). The percentages are labeled below the bar. A small black dot is located at the end of the yellow segment.</p>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 22941 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 BOVINE MITOCHONDRIAL F1-ATPASE.

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	492	3748	2360	661	715	12	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	engineered mutation	UNP P19483
B	481	GLY	SER	engineered mutation	UNP P19483
C	481	GLY	SER	engineered mutation	UNP P19483

- Molecule 2 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	467	3539	2243	601	684	11	0	0	0
2	E	466	3530	2238	600	681	11	0	0	0
2	F	466	3530	2238	600	681	11	0	0	0

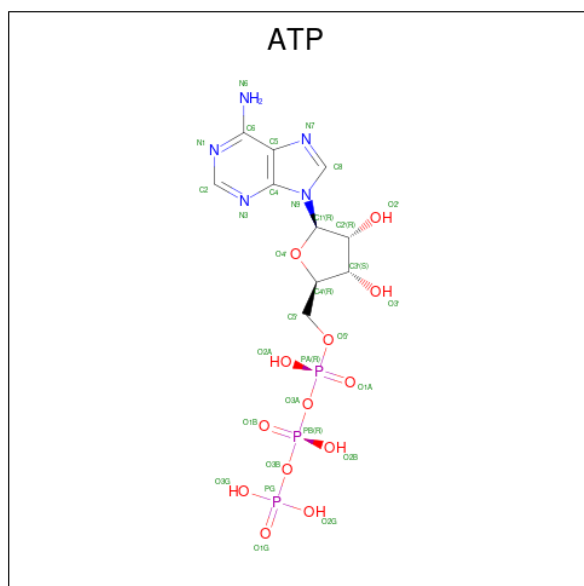
- Molecule 3 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	122	945	591	171	176	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	43	VAL	ILE	engineered mutation	UNP P05631

- Molecule 4 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		
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

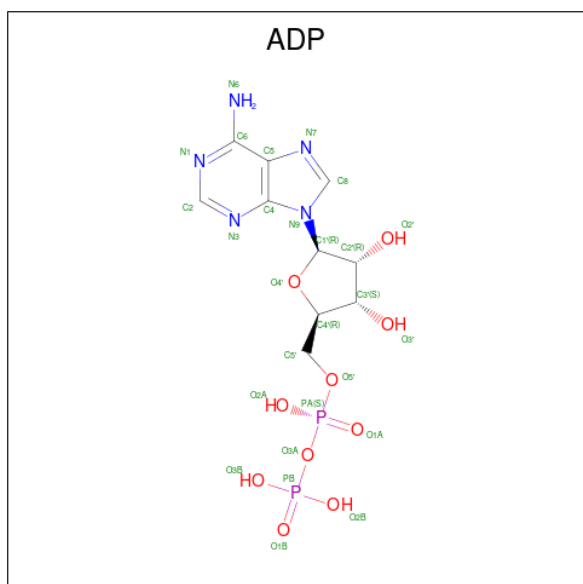
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

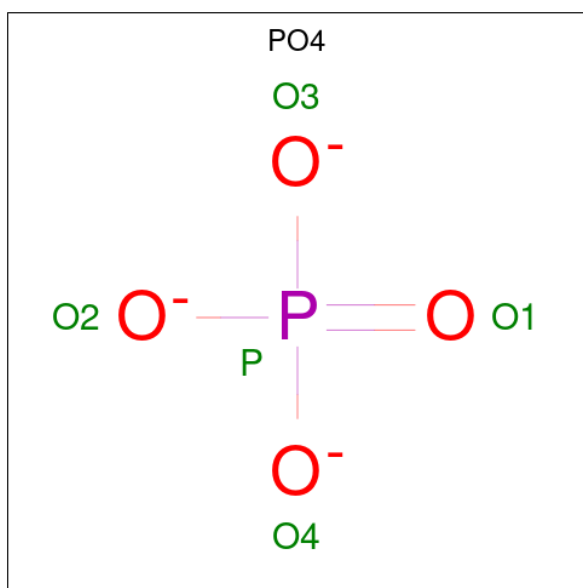


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

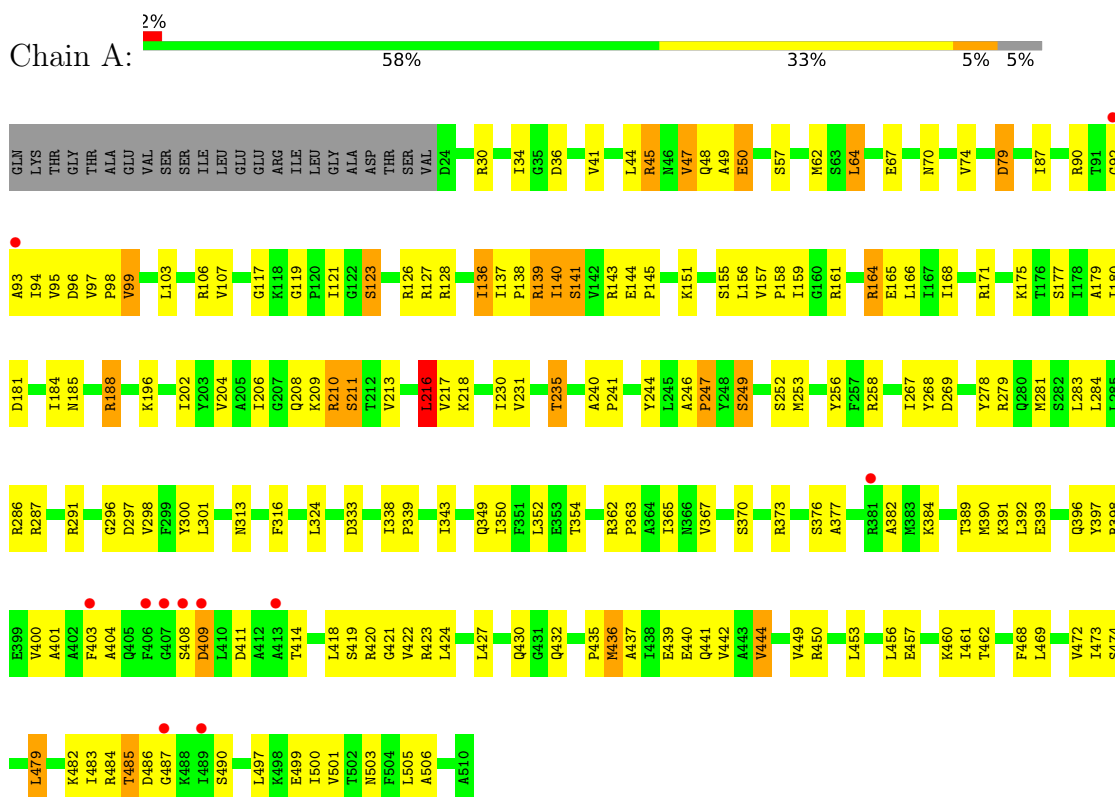
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	24	Total	O	0	0
			24	24		
9	B	26	Total	O	0	0
			26	26		
9	C	14	Total	O	0	0
			14	14		
9	D	15	Total	O	0	0
			15	15		
9	E	13	Total	O	0	0
			13	13		
9	F	17	Total	O	0	0
			17	17		
9	G	2	Total	O	0	0
			2	2		

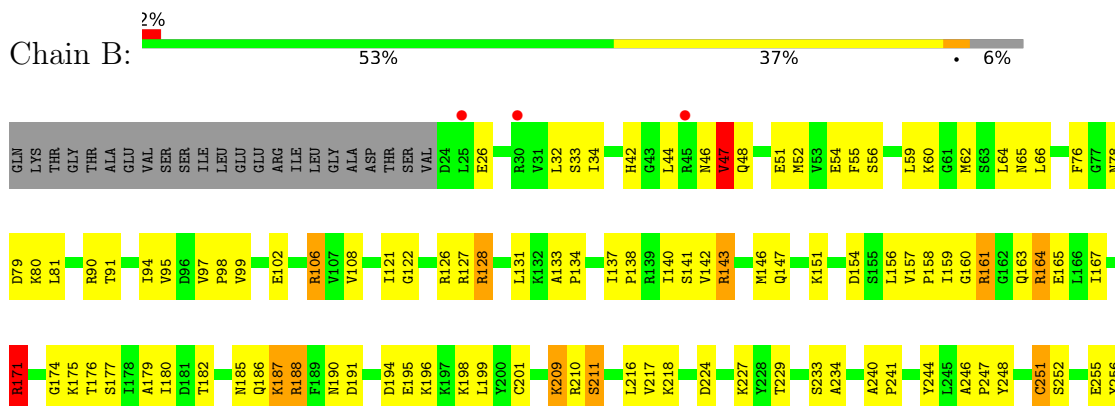
### 3 Residue-property plots [i](#)

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.

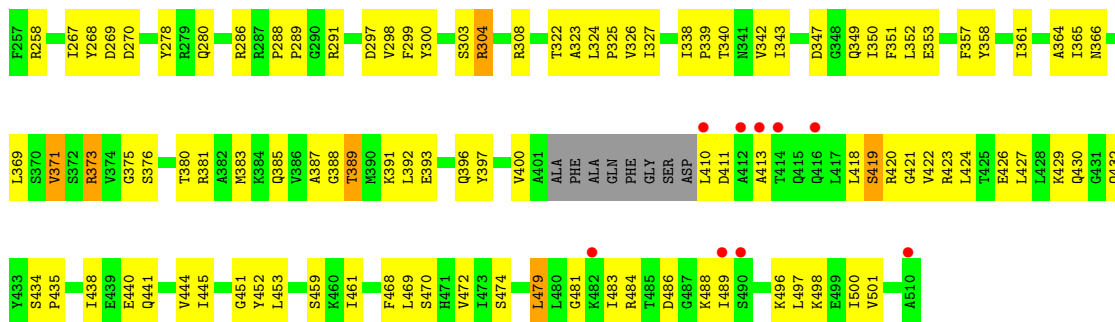
#### • Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE



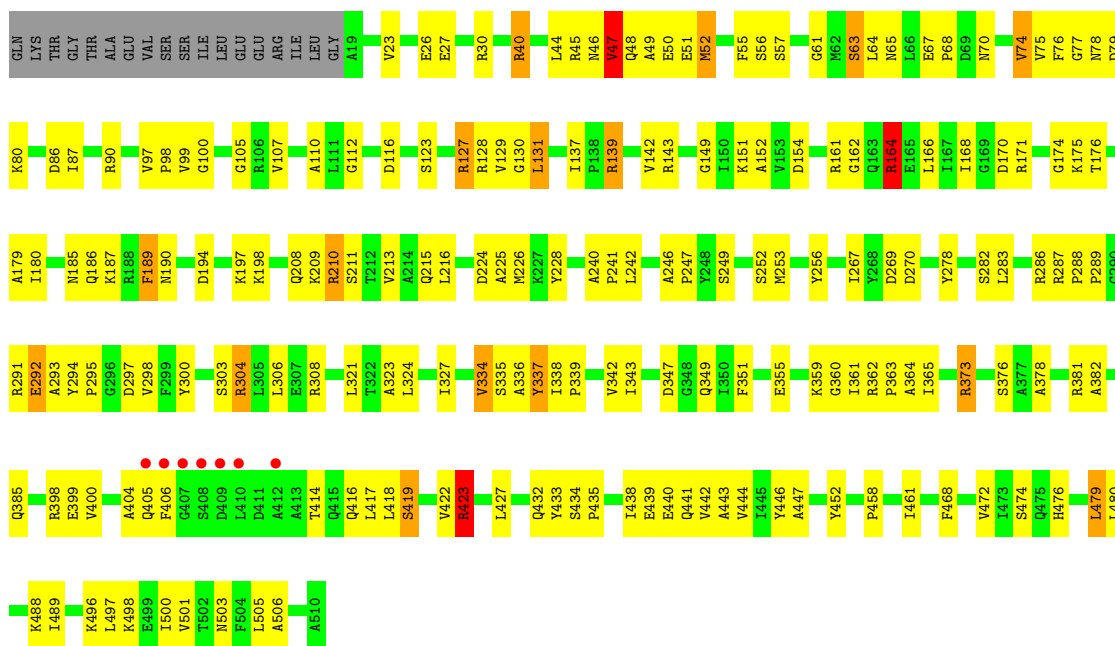
#### • Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE



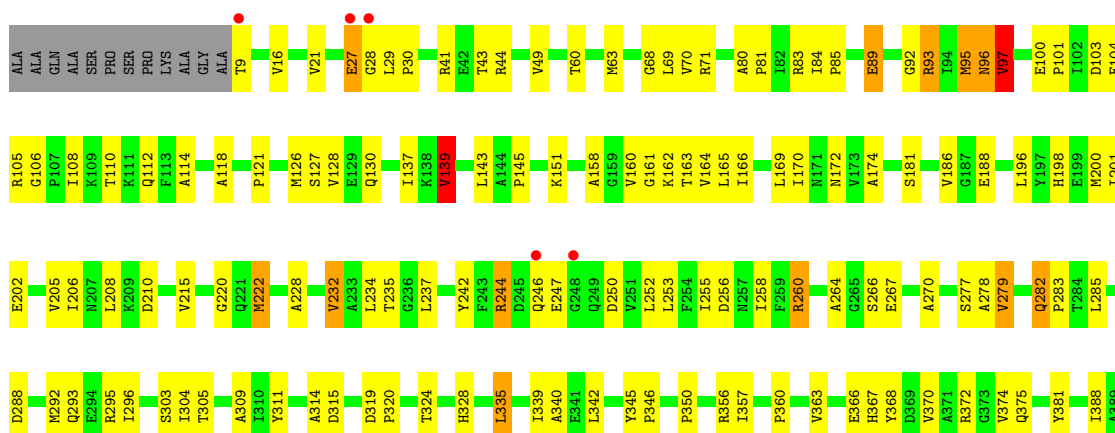


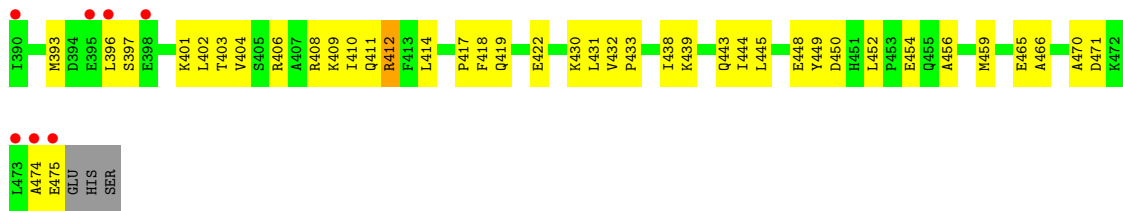


● Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

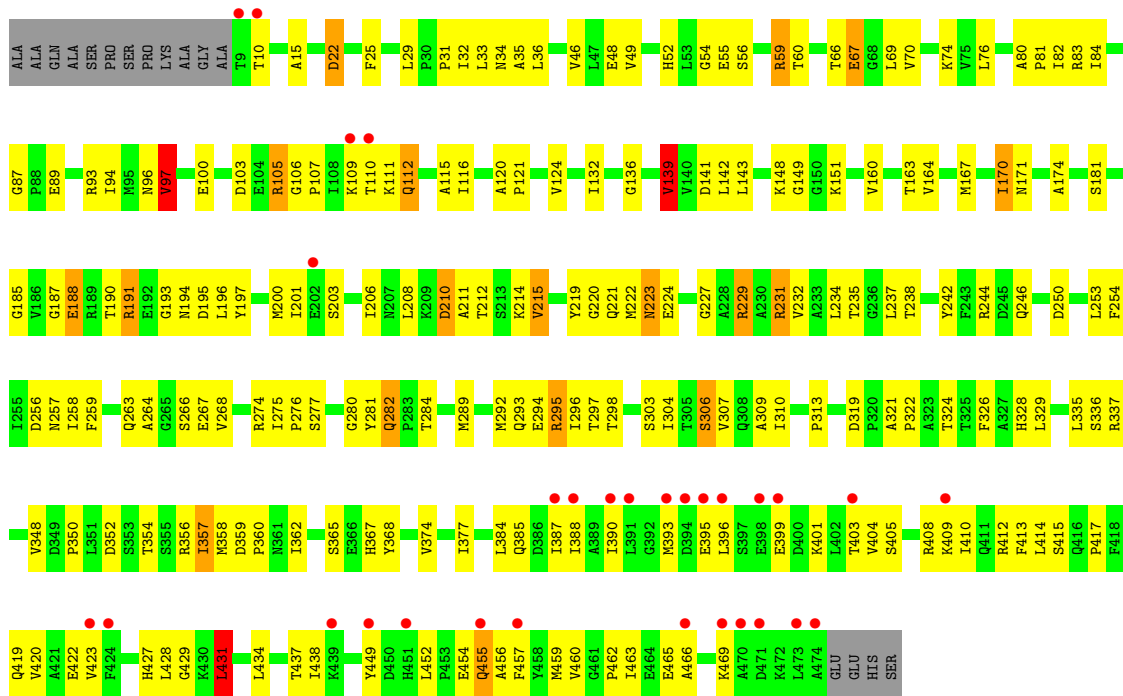


● Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

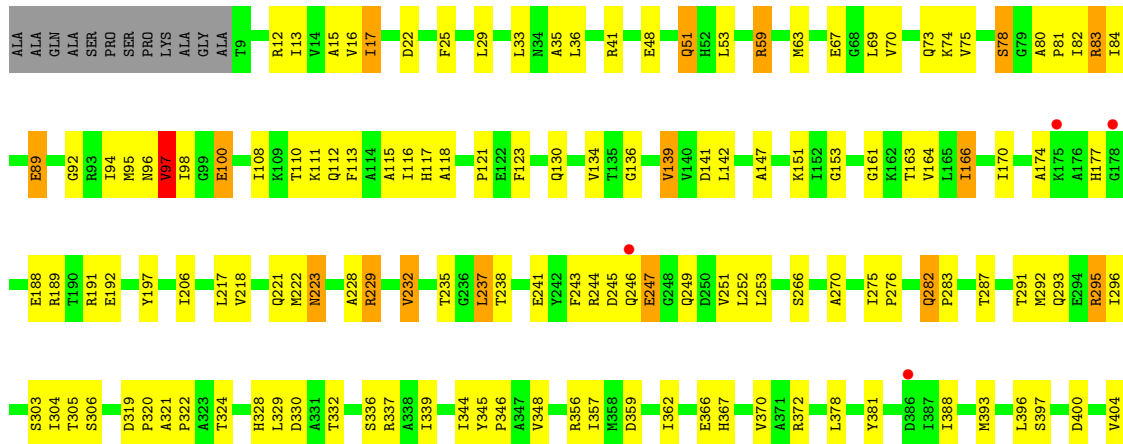




• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	280.00Å 107.00Å 139.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 37.27 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-2.90) 96.5 (37.27-2.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.37 (at 2.90Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.236 , 0.292 0.211 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtrriage
Anisotropy	0.465	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 71.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	22941	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, ADP, PO4, 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	0.54	0/3766	1.23	23/5080 (0.5%)
1	B	0.55	0/3704	1.20	20/4995 (0.4%)
1	C	0.57	0/3799	1.25	21/5126 (0.4%)
2	D	0.56	0/3596	1.23	17/4879 (0.3%)
2	E	0.50	0/3587	1.12	19/4867 (0.4%)
2	F	0.57	0/3587	1.23	21/4867 (0.4%)
3	G	0.44	0/949	0.93	1/1266 (0.1%)
All	All	0.54	0/22988	1.20	122/31080 (0.4%)

There are no bond length outliers.

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	93	ARG	NE-CZ-NH2	-12.76	113.92	120.30
2	D	260	ARG	NE-CZ-NH2	12.66	126.63	120.30
2	D	93	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	C	373	ARG	CD-NE-CZ	11.85	140.18	123.60
1	C	139	ARG	NE-CZ-NH1	-11.79	114.40	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3715	0	3814	134	0
1	B	3656	0	3765	158	0
1	C	3748	0	3844	151	0
2	D	3539	0	3592	127	0
2	E	3530	0	3587	160	0
2	F	3530	0	3587	127	0
3	G	945	0	1019	43	0
4	A	31	0	12	2	0
4	B	31	0	12	2	0
4	C	31	0	12	5	0
4	F	31	0	12	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	B	6	0	8	3	0
7	D	27	0	12	2	0
8	E	5	0	0	1	0
9	A	24	0	0	2	0
9	B	26	0	0	6	0
9	C	14	0	0	0	0
9	D	15	0	0	0	0
9	E	13	0	0	3	0
9	F	17	0	0	3	0
9	G	2	0	0	0	0
All	All	22941	0	23276	845	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 18.

The worst 5 of 845 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:B:351:PHE:HE2	1:B:353:GLU:HG2	1.26	1.01
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.43	1.00
2:F:12:ARG:HE	2:F:74:LYS:HE2	1.27	1.00
1:C:294:TYR:HB3	1:C:298:VAL:HG21	1.48	0.94
2:F:282:GLN:H	2:F:282:GLN:HE21	1.00	0.92

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%)	438 (90%)	38 (8%)	9 (2%)	8	28
1	B	475/510 (93%)	428 (90%)	44 (9%)	3 (1%)	25	58
1	C	490/510 (96%)	446 (91%)	42 (9%)	2 (0%)	34	66
2	D	465/482 (96%)	419 (90%)	43 (9%)	3 (1%)	25	58
2	E	464/482 (96%)	408 (88%)	50 (11%)	6 (1%)	12	37
2	F	464/482 (96%)	427 (92%)	35 (8%)	2 (0%)	34	66
3	G	116/272 (43%)	103 (89%)	9 (8%)	4 (3%)	3	15
All	All	2959/3248 (91%)	2669 (90%)	261 (9%)	29 (1%)	15	45

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	409	ASP
1	C	337	TYR
3	G	210	ALA
1	A	93	ALA
1	A	404	ALA

### 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	393/412 (95%)	360 (92%)	33 (8%)	11	31
1	B	388/412 (94%)	364 (94%)	24 (6%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	397/412 (96%)	372 (94%)	25 (6%)	18	46
2	D	377/386 (98%)	358 (95%)	19 (5%)	24	57
2	E	376/386 (97%)	353 (94%)	23 (6%)	18	48
2	F	376/386 (97%)	358 (95%)	18 (5%)	25	58
3	G	102/230 (44%)	97 (95%)	5 (5%)	25	57
All	All	2409/2624 (92%)	2262 (94%)	147 (6%)	18	48

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	266	SER
3	G	77	LEU
2	E	336	SER
2	F	97	VAL
1	B	376	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	34	ASN
2	F	443	GLN
2	E	249	GLN
2	F	223	ASN
2	E	246	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	ATP	F	600	5	26,33,33	0.99	2 (7%)	31,52,52	1.53	4 (12%)
4	ATP	B	600	5	26,33,33	1.11	2 (7%)	31,52,52	1.48	3 (9%)
4	ATP	A	600	5	26,33,33	1.20	4 (15%)	31,52,52	1.88	8 (25%)
8	PO4	E	602	-	4,4,4	0.62	0	6,6,6	0.32	0
7	ADP	D	600	5	24,29,29	1.00	1 (4%)	29,45,45	1.17	4 (13%)
4	ATP	C	600	5	26,33,33	0.98	2 (7%)	31,52,52	1.55	6 (19%)
6	GOL	B	701	-	5,5,5	0.74	0	5,5,5	0.92	0

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	ATP	F	600	5	-	0/18/38/38	0/3/3/3
4	ATP	B	600	5	-	0/18/38/38	0/3/3/3
4	ATP	A	600	5	-	1/18/38/38	0/3/3/3
7	ADP	D	600	5	-	0/12/32/32	0/3/3/3
4	ATP	C	600	5	-	0/18/38/38	0/3/3/3
6	GOL	B	701	-	-	3/4/4/4	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	ATP	C2-N1	2.83	1.39	1.33
4	A	600	ATP	PG-O3G	-2.65	1.44	1.54
4	B	600	ATP	C2-N1	2.45	1.38	1.33
4	B	600	ATP	PG-O3G	-2.45	1.45	1.54
4	A	600	ATP	O3'-C3'	2.40	1.48	1.43

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	ATP	O3'-C3'-C4'	-4.80	97.17	111.05
4	B	600	ATP	PB-O3B-PG	-4.14	118.63	132.83
4	F	600	ATP	PB-O3B-PG	-4.12	118.70	132.83
4	F	600	ATP	C5-C6-N6	4.11	126.60	120.35
4	F	600	ATP	PA-O3A-PB	-3.91	119.41	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

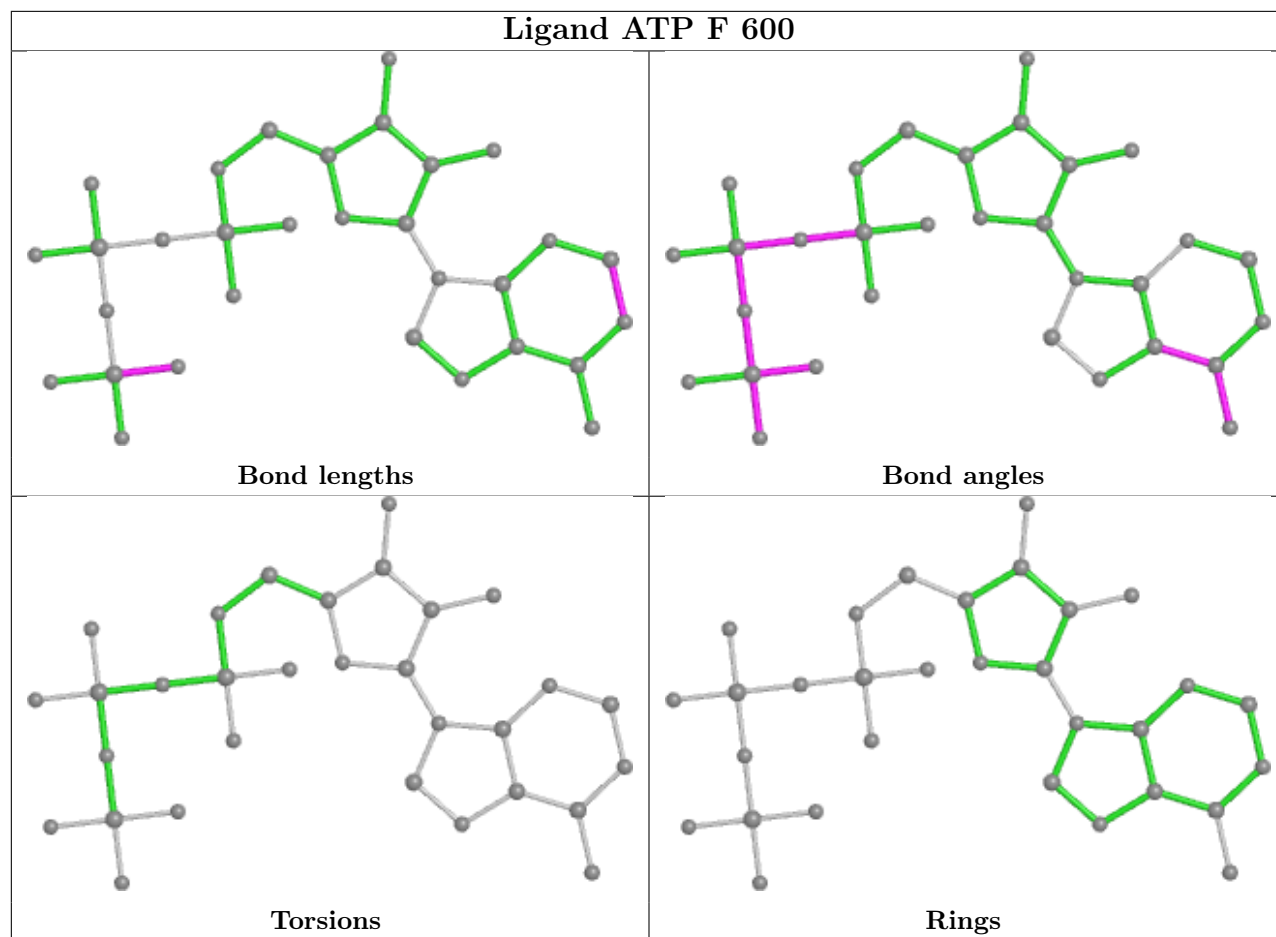
Mol	Chain	Res	Type	Atoms
6	B	701	GOL	C1-C2-C3-O3
6	B	701	GOL	O2-C2-C3-O3
4	A	600	ATP	O4'-C4'-C5'-O5'
6	B	701	GOL	O1-C1-C2-O2

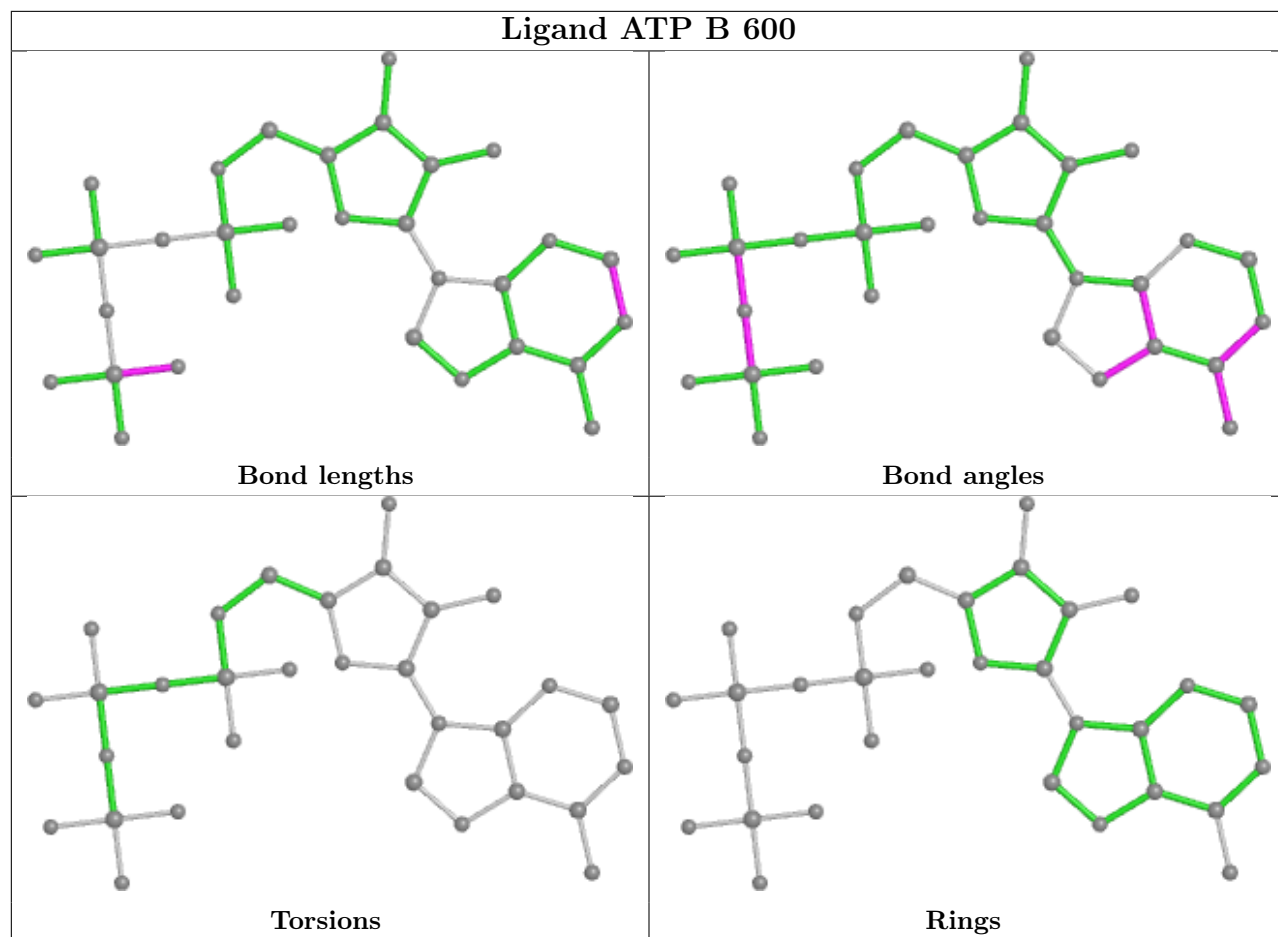
There are no ring outliers.

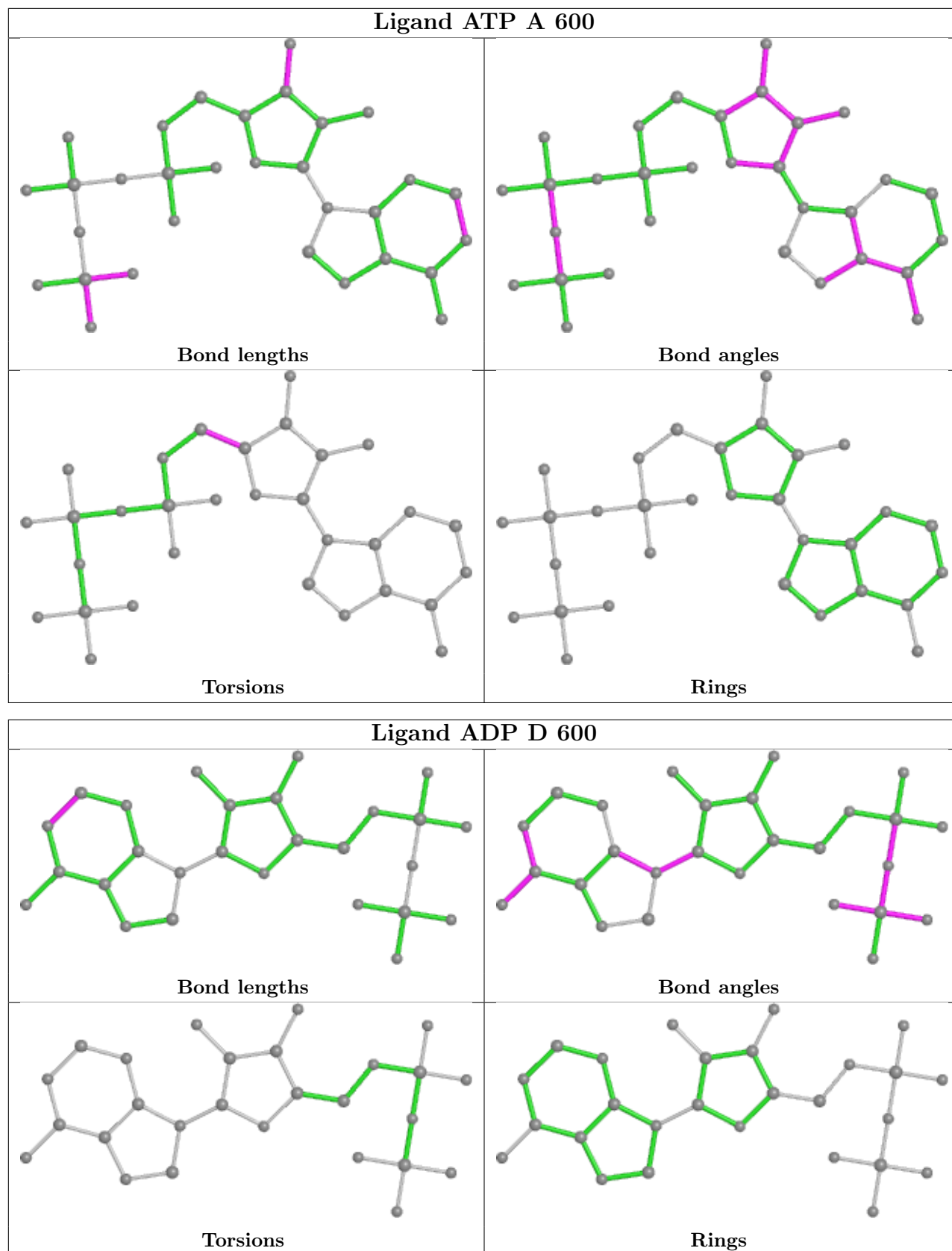
7 monomers are involved in 16 short contacts:

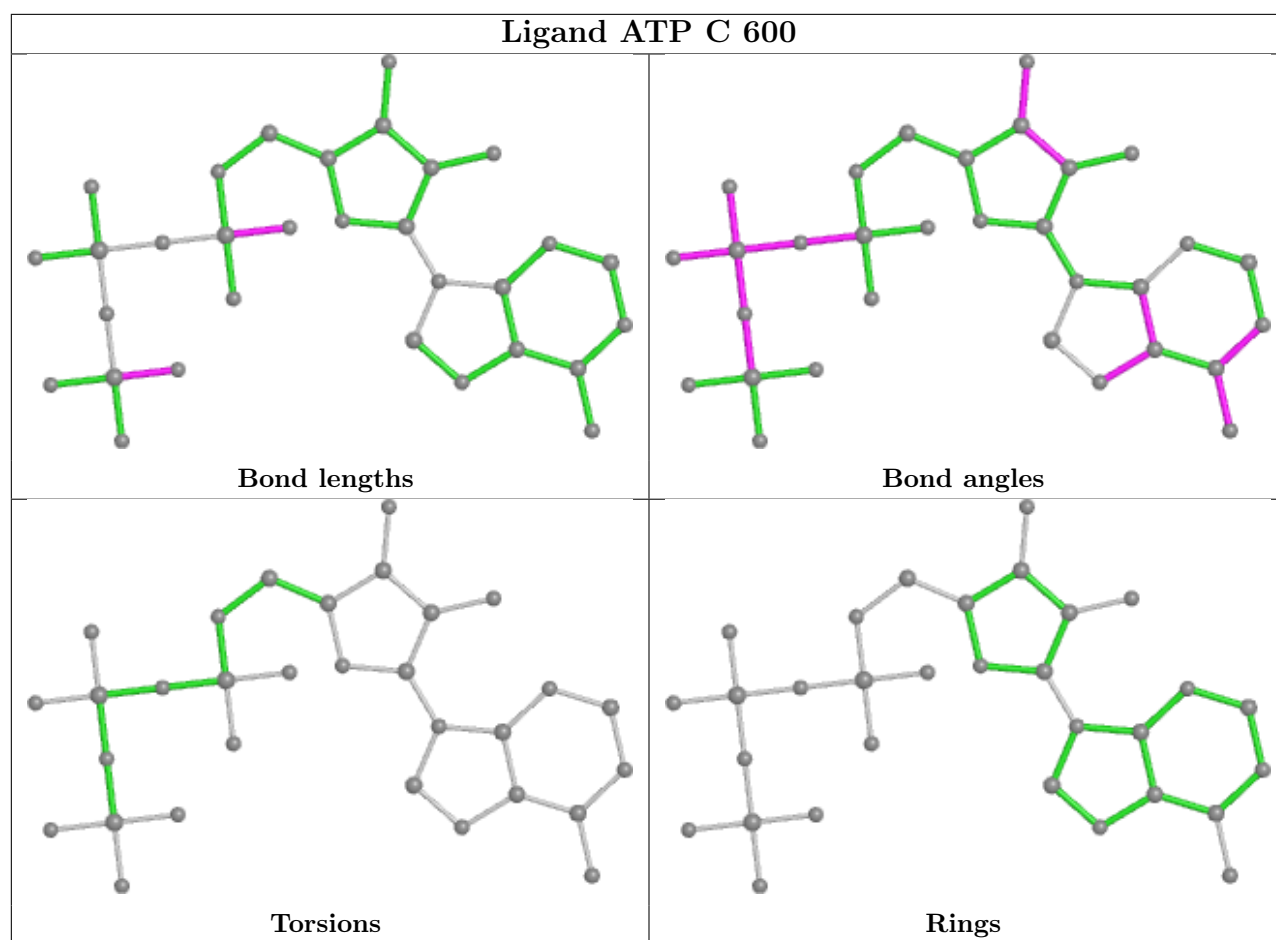
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	600	ATP	1	0
4	B	600	ATP	2	0
4	A	600	ATP	2	0
8	E	602	PO4	1	0
7	D	600	ADP	2	0
4	C	600	ATP	5	0
6	B	701	GOL	3	0

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.









## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	487/510 (95%)	-0.24	11 (2%) 60 58	17, 41, 77, 101	0
1	B	479/510 (93%)	-0.18	12 (2%) 57 55	15, 37, 89, 102	0
1	C	492/510 (96%)	-0.38	7 (1%) 75 75	15, 34, 65, 106	0
2	D	467/482 (96%)	-0.15	12 (2%) 56 52	17, 37, 77, 105	0
2	E	466/482 (96%)	0.11	30 (6%) 19 15	13, 49, 100, 114	0
2	F	466/482 (96%)	-0.31	5 (1%) 80 80	14, 36, 73, 94	0
3	G	122/272 (44%)	1.18	34 (27%) 0 0	17, 70, 100, 104	0
All	All	2979/3248 (91%)	-0.14	111 (3%) 41 37	13, 40, 87, 114	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	390	ILE	6.9
1	C	408	SER	6.5
3	G	209	LEU	6.4
3	G	86	ALA	5.7
2	E	395	GLU	5.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

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<sup>th</sup> 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.

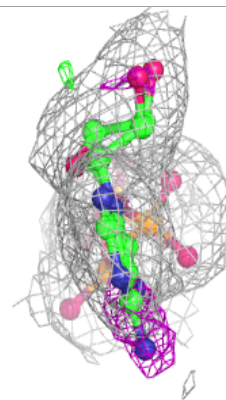
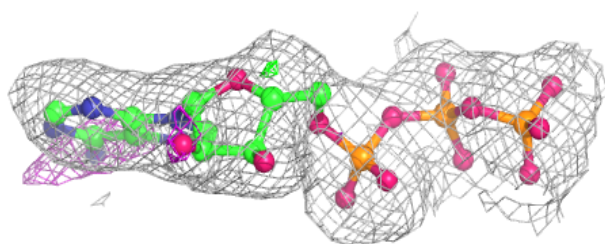
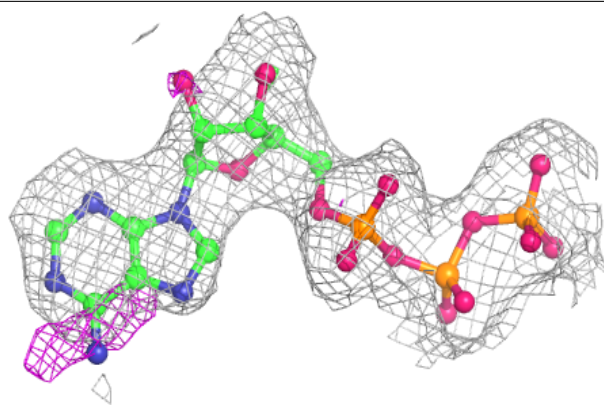
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	F	601	1/1	0.86	0.42	34,34,34,34	0
5	MG	D	601	1/1	0.87	0.52	38,38,38,38	0
5	MG	C	601	1/1	0.89	0.20	23,23,23,23	0
5	MG	A	601	1/1	0.90	0.22	30,30,30,30	0
8	PO4	E	602	5/5	0.93	0.15	80,80,81,81	0
4	ATP	B	600	31/31	0.94	0.16	21,28,32,38	0
4	ATP	A	600	31/31	0.95	0.16	13,25,31,38	0
5	MG	B	601	1/1	0.95	0.21	29,29,29,29	0
6	GOL	B	701	6/6	0.95	0.22	39,40,41,43	0
4	ATP	C	600	31/31	0.95	0.14	3,19,25,29	0
7	ADP	D	600	27/27	0.97	0.12	8,19,26,28	0
4	ATP	F	600	31/31	0.97	0.13	4,21,27,30	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.

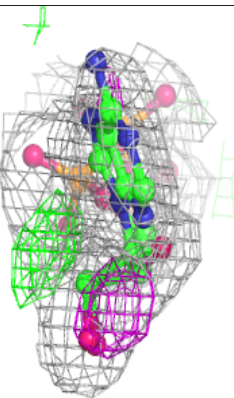
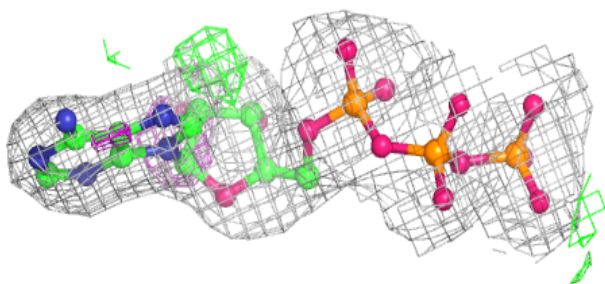
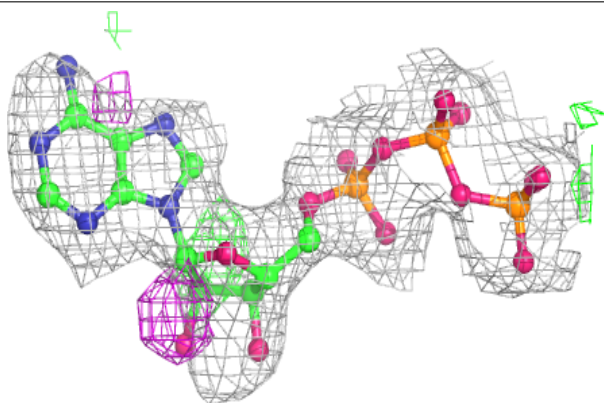


**Electron density around ATP B 600:**

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

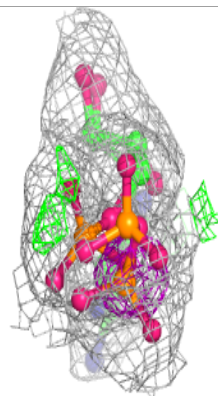
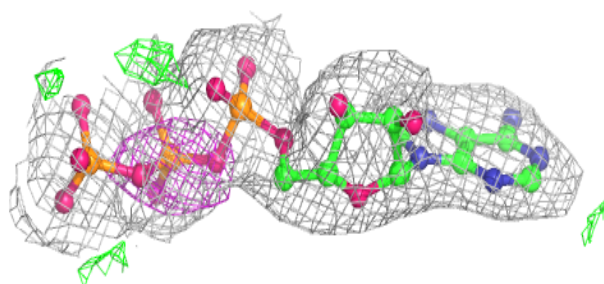
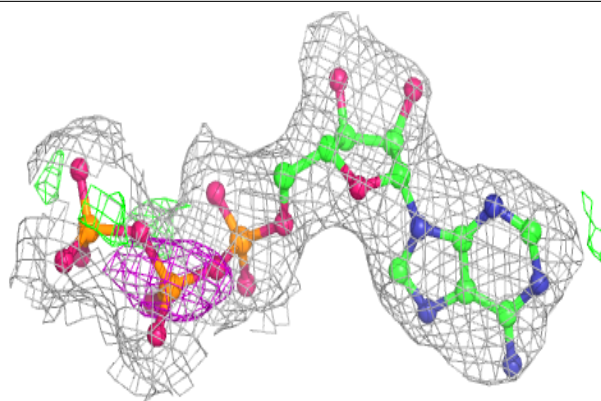
**Electron density around ATP A 600:**

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

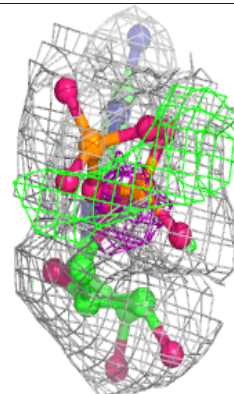
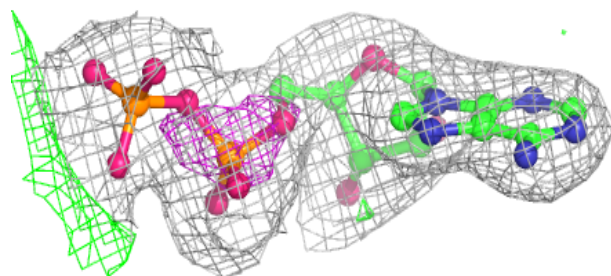
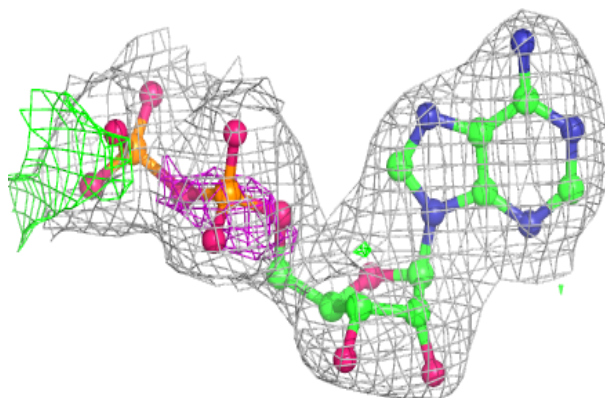


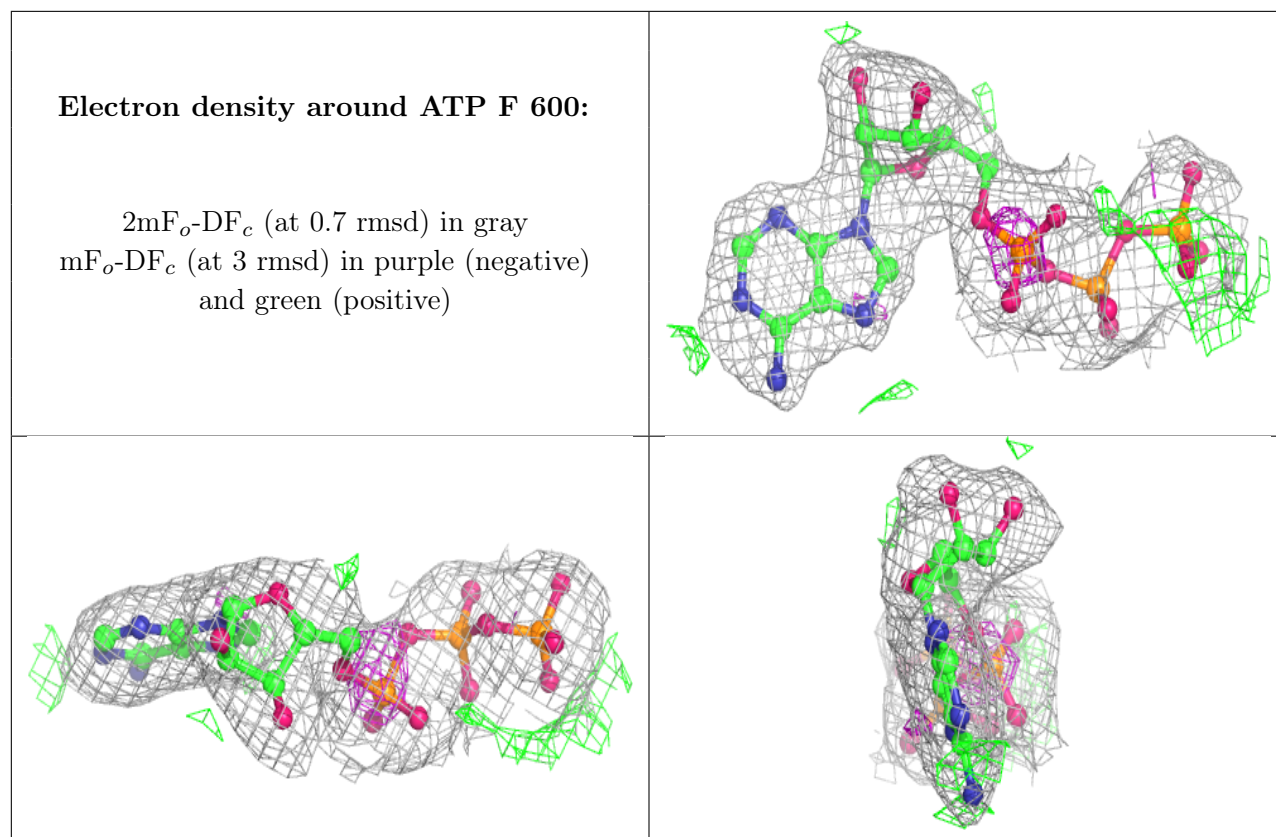
**Electron density around ATP C 600:**

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

**Electron density around ADP D 600:**

$2mF_o-DF_c$  (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.