



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 02:38 am BST

PDB ID : 1E1R
Title : BOVINE MITOCHONDRIAL F1-ATPASE INHIBITED BY MG2+ADP
AND ALUMINIUM FLUORIDE
Authors : Braig, K.; Menz, R.I.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2000-05-10
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

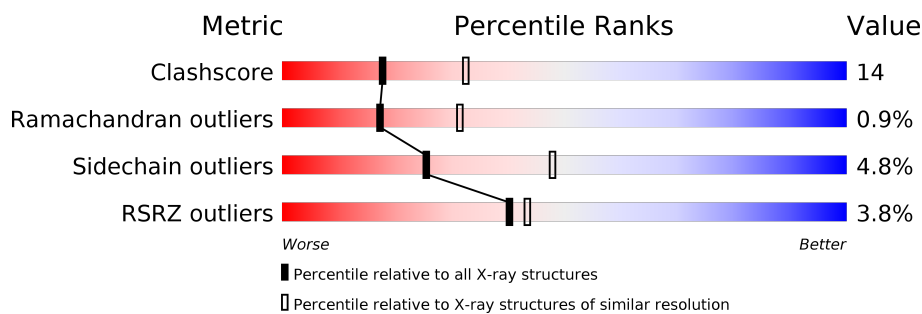
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>2%</div> <div>63%</div> <div>30%</div> <div>5%</div> </div>
1	B	510	<div> <div>5%</div> <div>59%</div> <div>31%</div> <div>6%</div> </div>
1	C	510	<div> <div>2%</div> <div>67%</div> <div>26%</div> <div>.</div> </div>
2	D	482	<div> <div>%</div> <div>67%</div> <div>26%</div> <div>.</div> </div>
2	E	482	<div> <div>6%</div> <div>61%</div> <div>33%</div> <div>.</div> </div>
2	F	482	<div> <div>2%</div> <div>72%</div> <div>22%</div> <div>.</div> </div>
3	G	272	<div> <div>8%</div> <div>32%</div> <div>12%</div> <div>55%</div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 23688 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
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	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

There are 3 discrepancies between the modelled and reference sequences:

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

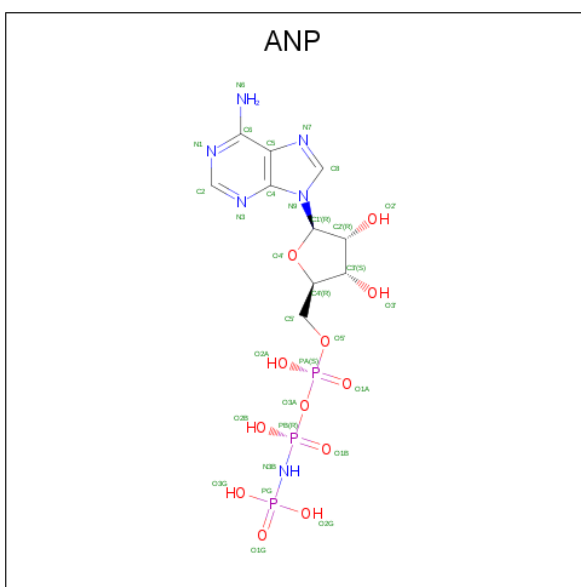
- Molecule 2 is a protein called BOVINE MITOCHONDRIAL F1-ATPASE.

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

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

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

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

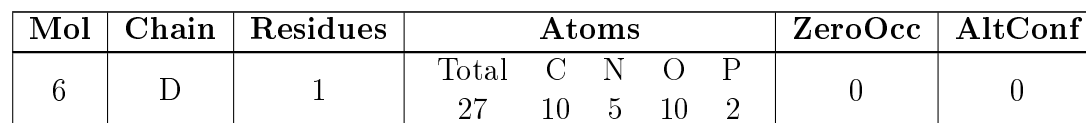


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

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

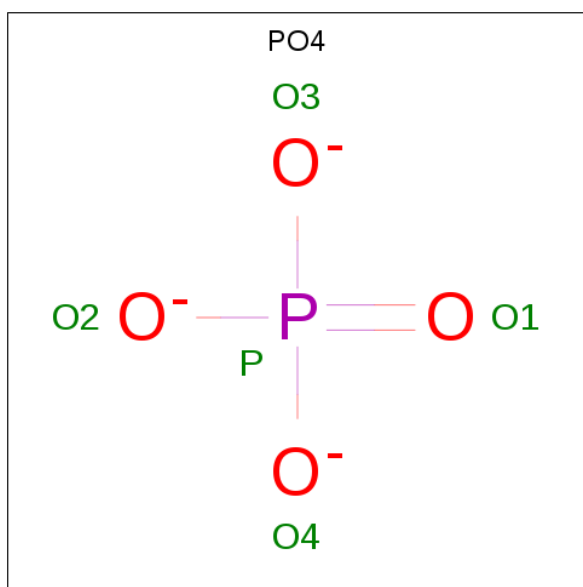
- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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- Diagram illustrating the Lewis structure of AlF_3 (Aluminum Fluoride). The central Aluminum atom (Al) is bonded to three Fluorine atoms (F). The Aluminum atom is labeled "AL" and the Fluorine atoms are labeled "F1", "F2", and "F3". The bonds are shown as lines, with one bond to F1 and two bonds to F2 and F3.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total 4	Al 1	F 3	0	0

- 



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

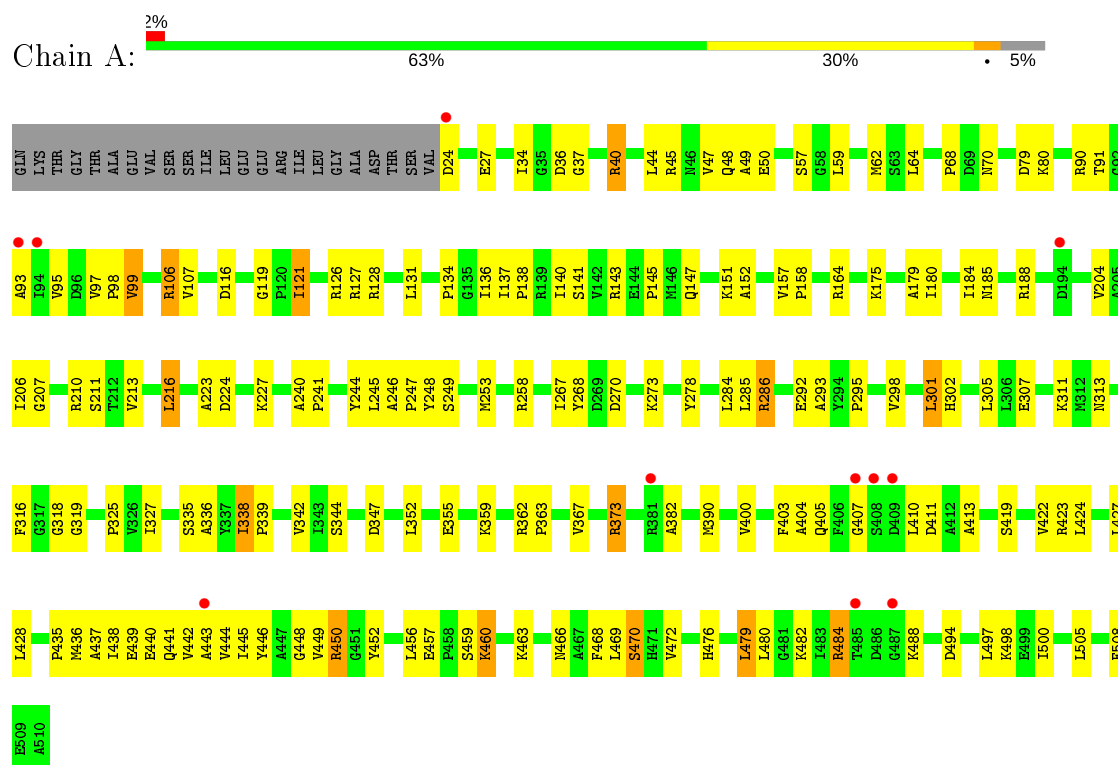
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	144	Total	O	0	0
			144	144		
9	B	126	Total	O	0	0
			126	126		
9	C	171	Total	O	0	0
			171	171		
9	D	145	Total	O	0	0
			145	145		
9	E	105	Total	O	0	0
			105	105		
9	F	148	Total	O	0	0
			148	148		
9	G	21	Total	O	0	0
			21	21		

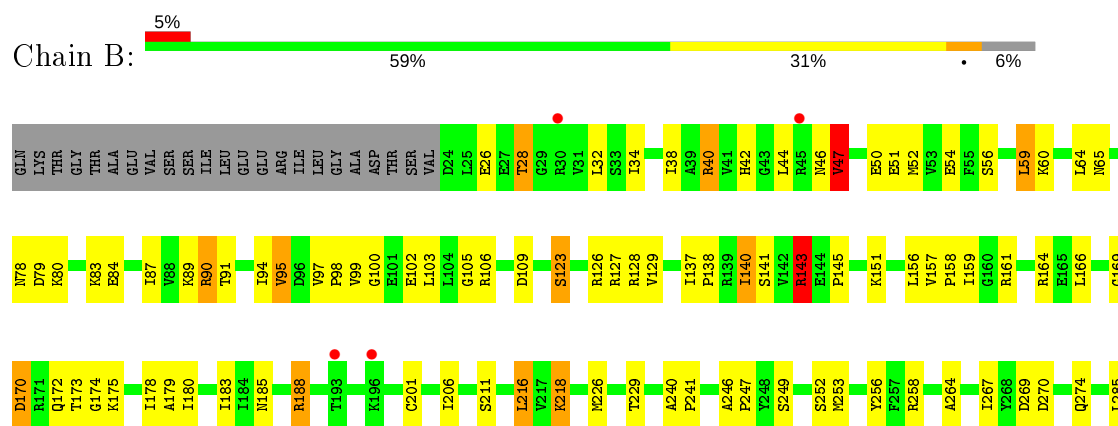
3 Residue-property plots [i](#)

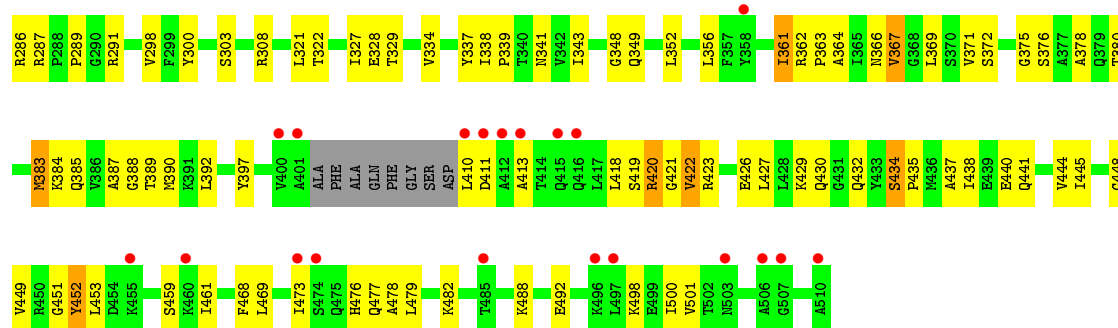
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

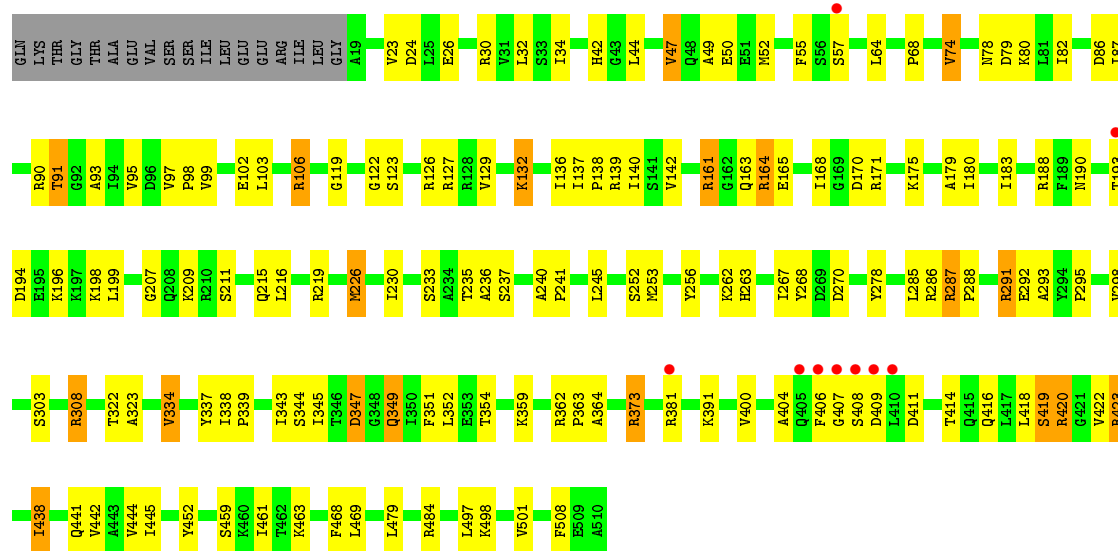


• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

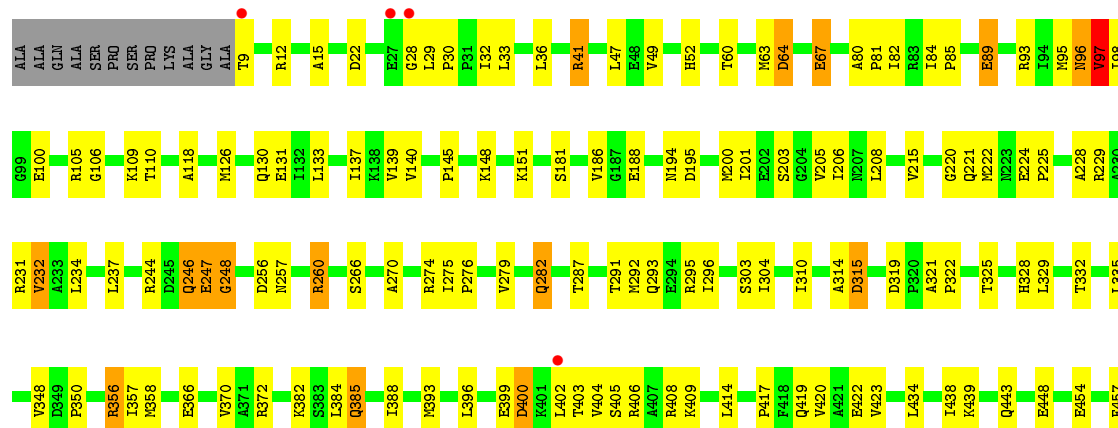


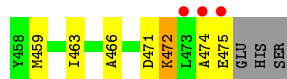


• Molecule 1: BOVINE MITOCHONDRIAL F1-ATPASE

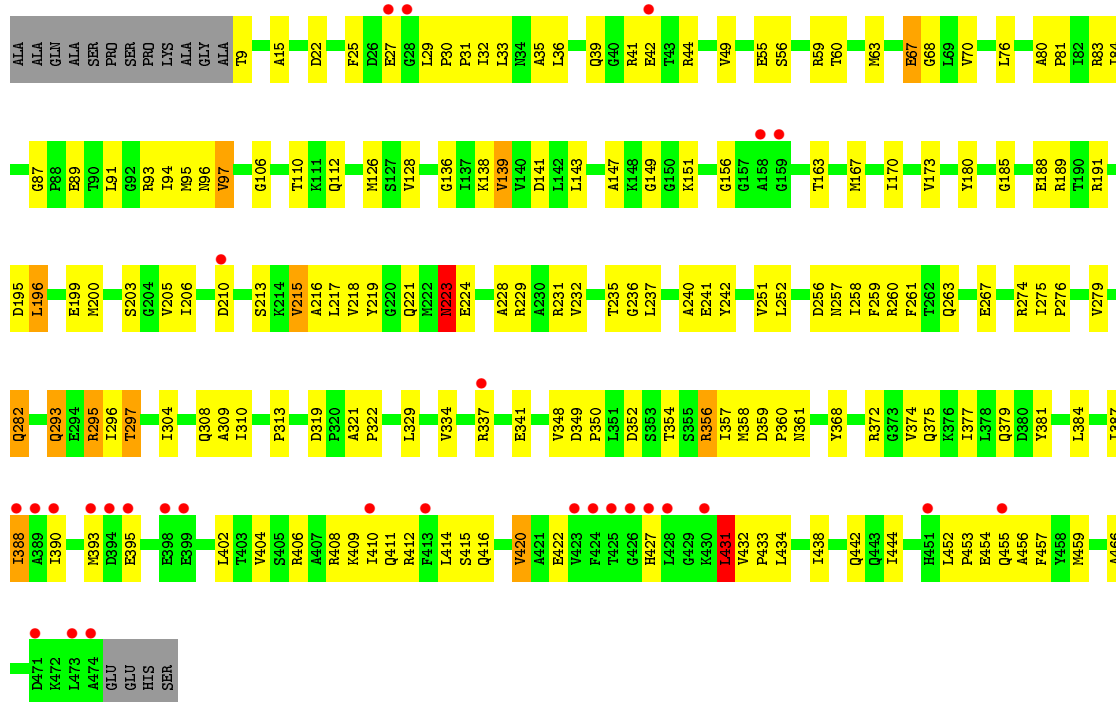


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

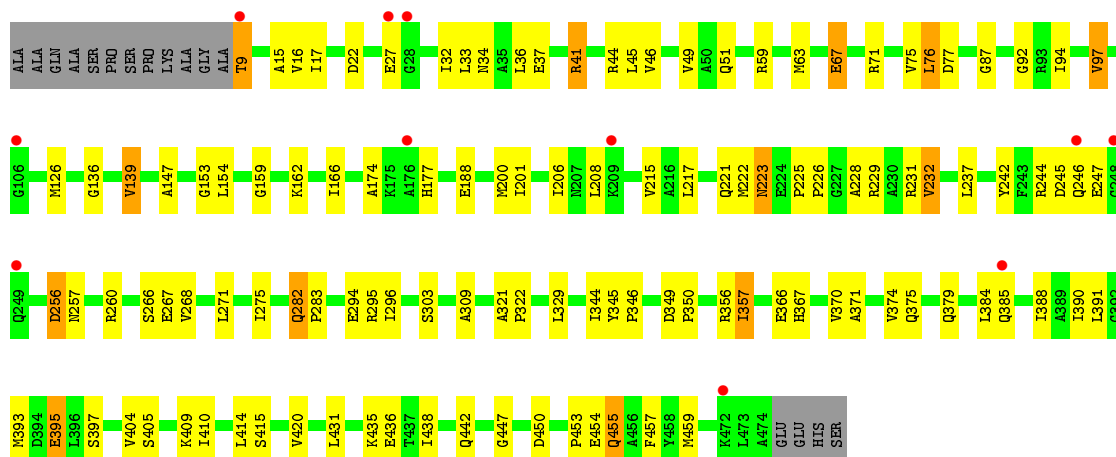




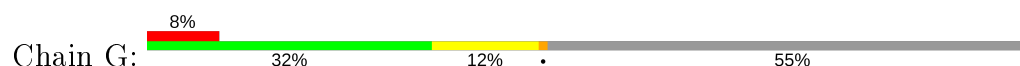
• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE

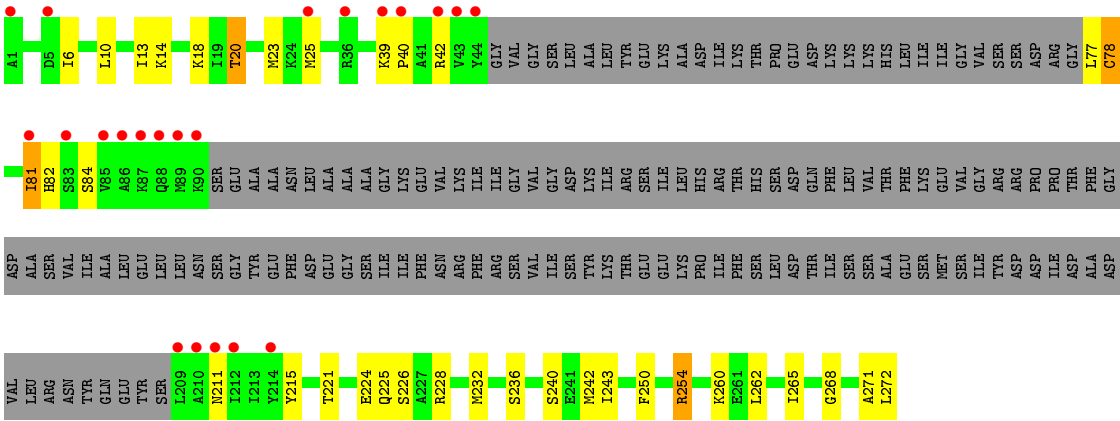


• Molecule 2: BOVINE MITOCHONDRIAL F1-ATPASE



• Molecule 3: BOVINE MITOCHONDRIAL F1-ATPASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	278.60Å 106.70Å 137.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-2.50) 95.4 (19.99-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.282 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23688	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: MG, ANP, PO4, ADP, AF3

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	0.51	0/3766	1.05	12/5080 (0.2%)
1	B	0.52	0/3704	1.09	19/4995 (0.4%)
1	C	0.56	0/3799	1.17	22/5126 (0.4%)
2	D	0.56	0/3596	1.13	17/4879 (0.3%)
2	E	0.51	0/3587	1.10	19/4867 (0.4%)
2	F	0.53	0/3587	1.09	13/4867 (0.3%)
3	G	0.46	0/949	1.01	3/1266 (0.2%)
All	All	0.53	0/22988	1.10	105/31080 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

There are no bond length outliers.

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	254	ARG	CD-NE-CZ	15.19	144.86	123.60
3	G	254	ARG	NE-CZ-NH1	10.28	125.44	120.30
2	D	231	ARG	NE-CZ-NH2	9.88	125.24	120.30
1	C	127	ARG	NE-CZ-NH2	-9.83	115.39	120.30
2	D	229	ARG	NE-CZ-NH2	-9.80	115.40	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	223	ASN	Mainchain

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	3814	124	0
1	B	3656	0	3765	117	0
1	C	3748	0	3844	96	0
2	D	3539	0	3592	92	0
2	E	3530	0	3587	121	0
2	F	3530	0	3586	89	0
3	G	945	0	1019	20	0
4	A	31	0	13	0	0
4	B	31	0	13	4	0
4	C	31	0	13	1	0
4	F	31	0	13	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	D	27	0	12	1	0
7	D	4	0	0	1	0
8	E	5	0	0	0	0
9	A	144	0	0	6	0
9	B	126	0	0	4	0
9	C	171	0	0	4	0
9	D	145	0	0	5	0
9	E	105	0	0	4	0
9	F	148	0	0	5	0
9	G	21	0	0	1	0
All	All	23688	0	23271	626	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 14.

The worst 5 of 626 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:C:91:THR:HG22	1:C:93:ALA:H	1.27	1.00
2:F:282:GLN:H	2:F:282:GLN:HE21	0.99	0.98
2:F:166:ILE:HD11	2:F:309:ALA:HB2	1.41	0.98
3:G:39:LYS:HB2	3:G:40:PRO:HD3	1.50	0.94
2:D:282:GLN:H	2:D:282:GLN:HE21	1.11	0.93

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	449 (93%)	33 (7%)	3 (1%)	25	43
1	B	475/510 (93%)	447 (94%)	25 (5%)	3 (1%)	25	43
1	C	490/510 (96%)	462 (94%)	26 (5%)	2 (0%)	34	54
2	D	465/482 (96%)	432 (93%)	26 (6%)	7 (2%)	10	18
2	E	464/482 (96%)	423 (91%)	35 (8%)	6 (1%)	12	21
2	F	464/482 (96%)	430 (93%)	31 (7%)	3 (1%)	25	43
3	G	116/272 (43%)	110 (95%)	4 (3%)	2 (2%)	9	16
All	All	2959/3248 (91%)	2753 (93%)	180 (6%)	26 (1%)	17	31

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
2	E	388	ILE
1	B	95	VAL
1	B	367	VAL
1	C	409	ASP

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%)	375 (95%)	18 (5%)	27	50
1	B	388/412 (94%)	365 (94%)	23 (6%)	19	37
1	C	397/412 (96%)	372 (94%)	25 (6%)	18	34
2	D	377/386 (98%)	364 (97%)	13 (3%)	37	63
2	E	376/386 (97%)	359 (96%)	17 (4%)	27	51
2	F	376/386 (97%)	364 (97%)	12 (3%)	39	65
3	G	102/230 (44%)	94 (92%)	8 (8%)	12	24
All	All	2409/2624 (92%)	2293 (95%)	116 (5%)	25	48

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	188	ARG
1	C	459	SER
2	F	455	GLN
1	C	209	LYS
1	C	334	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	130	GLN
2	D	385	GLN
2	F	223	ASN
2	D	221	GLN
1	B	172	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 carbohydrates 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	ANP	A	600	5	29,33,33	1.31	3 (10%)	31,52,52	1.22	2 (6%)
6	ADP	D	600	5,7	24,29,29	1.07	2 (8%)	29,45,45	1.13	2 (6%)
4	ANP	B	600	5	29,33,33	1.41	4 (13%)	31,52,52	1.42	2 (6%)
4	ANP	C	600	5	29,33,33	1.35	4 (13%)	31,52,52	1.45	3 (9%)
4	ANP	F	600	5	29,33,33	1.33	3 (10%)	31,52,52	1.23	5 (16%)
7	AF3	D	602	9,1,5,6	0,3,3	0.00	-	-		
8	PO4	E	602	-	4,4,4	0.72	0	6,6,6	0.40	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	ANP	C	600	5	-	2/14/38/38	0/3/3/3
4	ANP	B	600	5	-	1/14/38/38	0/3/3/3
4	ANP	A	600	5	-	3/14/38/38	0/3/3/3
6	ADP	D	600	5,7	-	2/12/32/32	0/3/3/3
4	ANP	F	600	5	-	4/14/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	600	ANP	PG-O2G	-4.59	1.44	1.56
4	A	600	ANP	PG-O2G	-4.03	1.45	1.56
4	C	600	ANP	PG-O3G	-3.53	1.47	1.56
4	B	600	ANP	PG-O2G	-3.35	1.47	1.56
4	F	600	ANP	PB-O2B	-3.23	1.48	1.56

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	600	ANP	O1B-PB-N3B	4.85	118.91	111.77
4	A	600	ANP	O1G-PG-N3B	-3.57	106.51	111.77
4	B	600	ANP	C5-C6-N6	3.26	125.31	120.35
4	C	600	ANP	O1G-PG-N3B	-3.20	107.05	111.77
4	A	600	ANP	C5-C6-N6	2.81	124.62	120.35

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	ANP	PB-N3B-PG-O1G
4	A	600	ANP	PG-N3B-PB-O1B
6	D	600	ADP	PA-O3A-PB-O2B
6	D	600	ADP	PA-O3A-PB-O3B
4	B	600	ANP	PG-N3B-PB-O1B

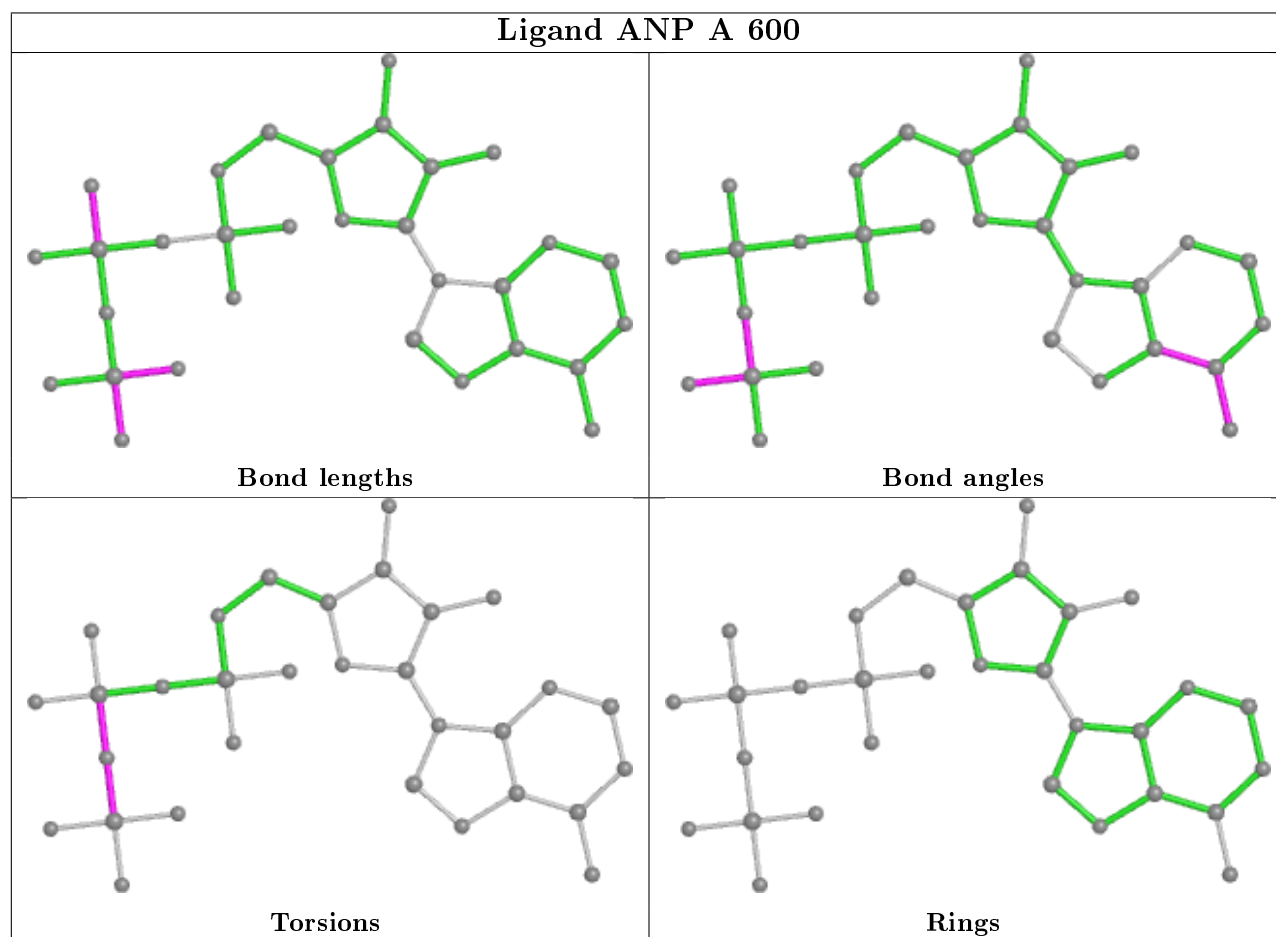
There are no ring outliers.

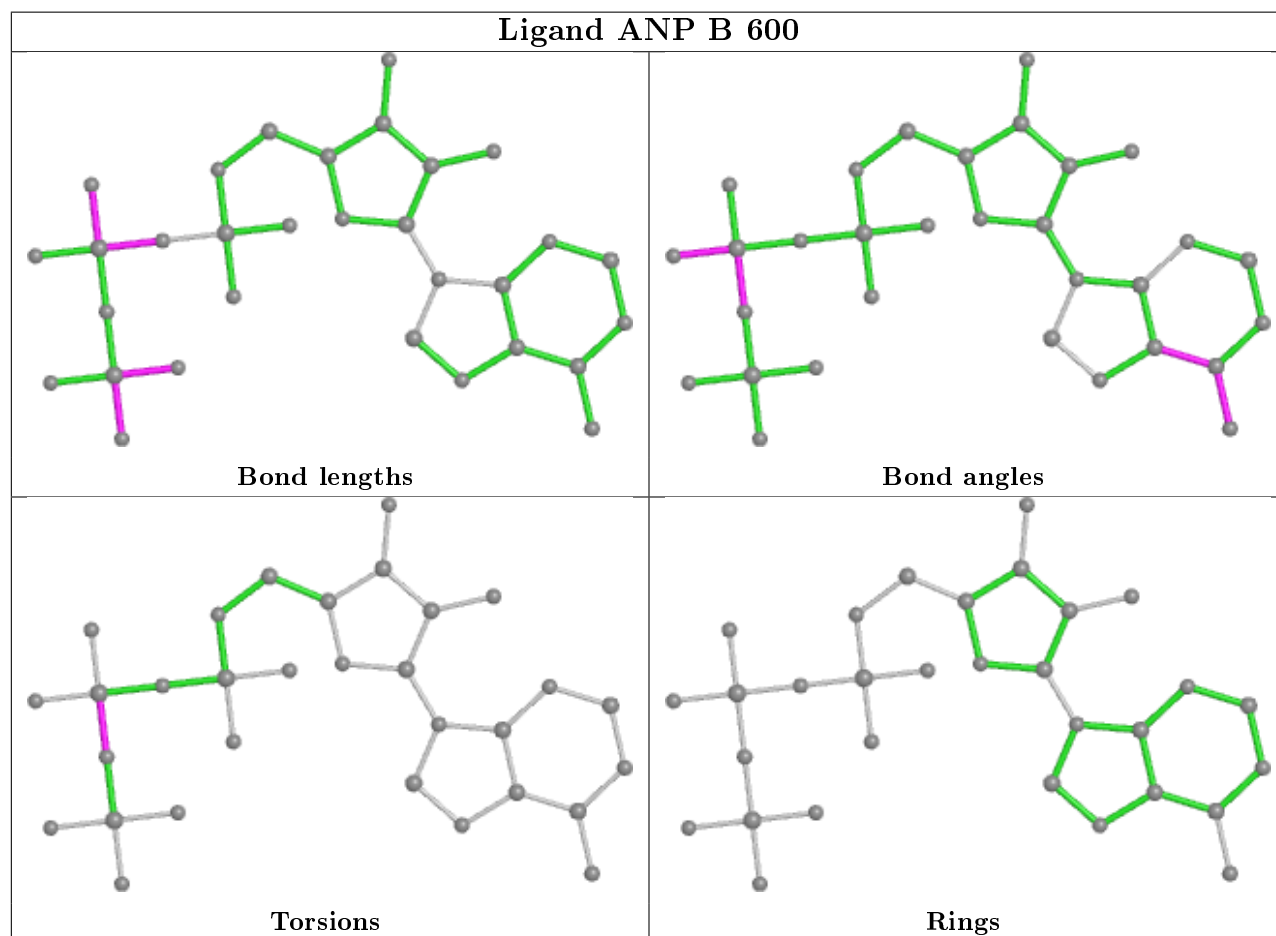
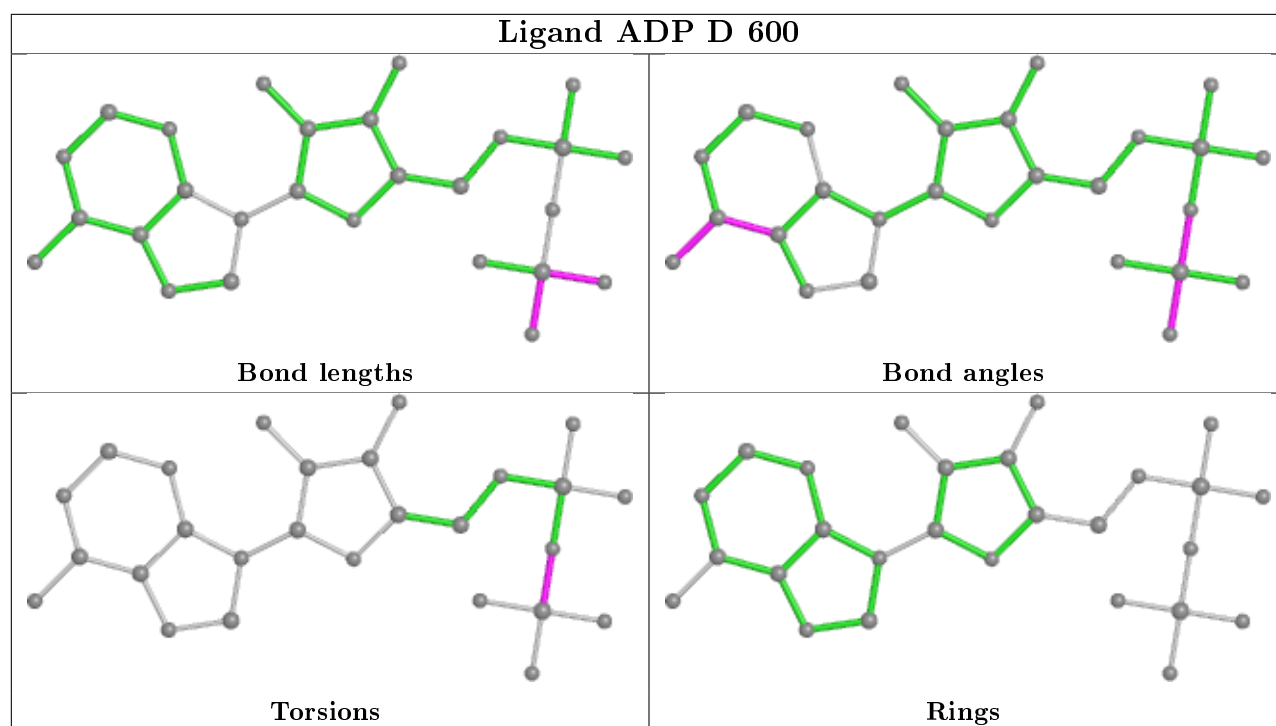
5 monomers are involved in 8 short contacts:

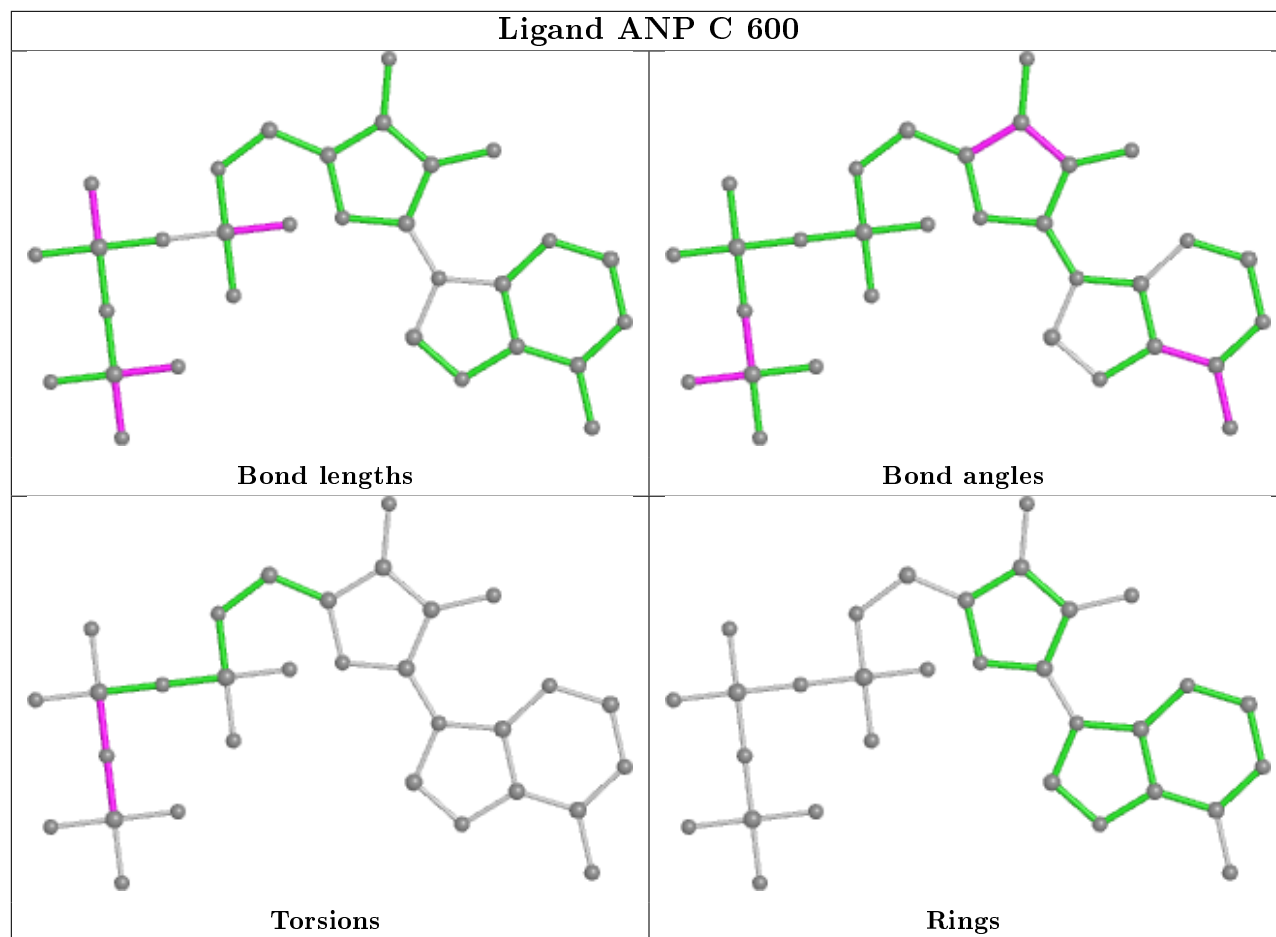
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	600	ADP	1	0
4	B	600	ANP	4	0
4	C	600	ANP	1	0
4	F	600	ANP	1	0
7	D	602	AF3	1	0

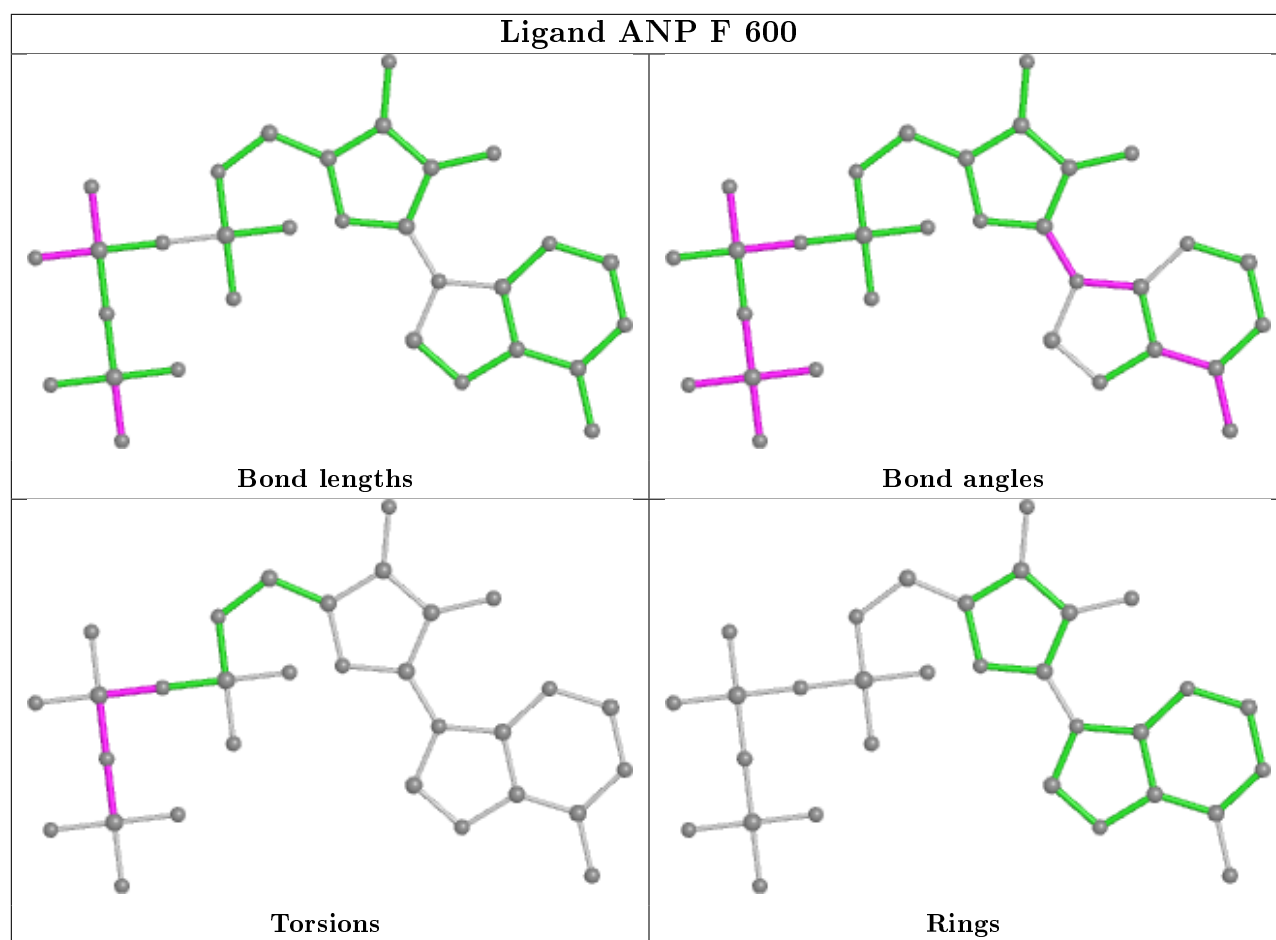
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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%)	-0.23	11 (2%) 60 63	26, 46, 76, 110	0
1	B	479/510 (93%)	-0.10	24 (5%) 28 30	25, 43, 97, 110	0
1	C	492/510 (96%)	-0.39	9 (1%) 68 71	24, 38, 65, 106	0
2	D	467/482 (96%)	-0.37	7 (1%) 73 75	24, 40, 73, 103	0
2	E	466/482 (96%)	0.11	29 (6%) 20 21	26, 51, 102, 119	0
2	F	466/482 (96%)	-0.33	11 (2%) 59 62	24, 41, 72, 90	0
3	G	122/272 (44%)	0.70	22 (18%) 1 1	29, 68, 108, 111	0
All	All	2979/3248 (91%)	-0.18	113 (3%) 40 43	24, 44, 88, 119	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	389	ALA	9.5
2	E	390	ILE	7.9
1	C	408	SER	6.2
3	G	209	LEU	5.9
2	E	28	GLY	5.8

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 carbohydrates in this entry.

6.4 Ligands

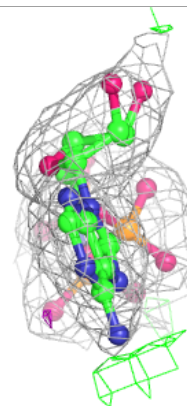
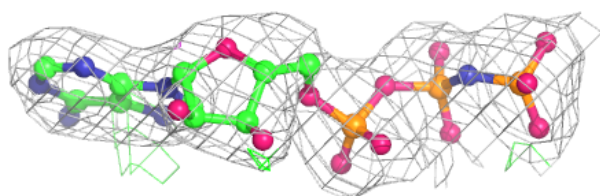
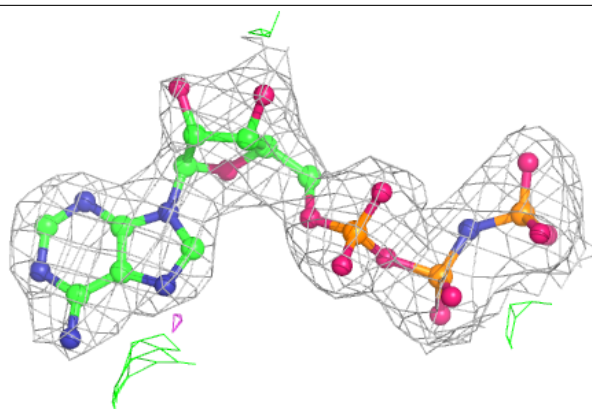
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PO4	E	602	5/5	0.78	0.24	86,87,87,87	0
5	MG	B	601	1/1	0.82	0.08	37,37,37,37	0
5	MG	A	601	1/1	0.82	0.12	41,41,41,41	0
7	AF3	D	602	4/4	0.93	0.17	41,41,43,45	0
5	MG	F	601	1/1	0.94	0.17	32,32,32,32	0
5	MG	D	601	1/1	0.98	0.15	33,33,33,33	0
4	ANP	B	600	31/31	0.98	0.10	32,47,51,54	0
4	ANP	C	600	31/31	0.98	0.10	29,37,41,45	0
4	ANP	F	600	31/31	0.98	0.10	34,38,45,45	0
4	ANP	A	600	31/31	0.98	0.08	29,36,40,42	0
5	MG	C	601	1/1	0.98	0.06	28,28,28,28	0
6	ADP	D	600	27/27	0.99	0.09	28,33,35,36	0

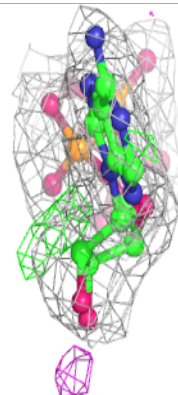
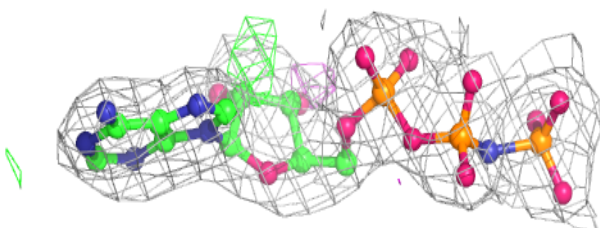
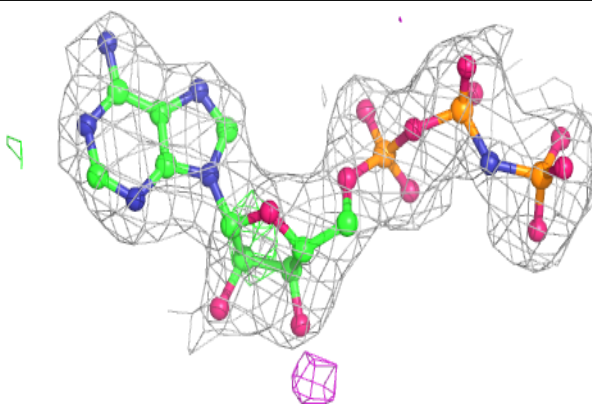
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP 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)

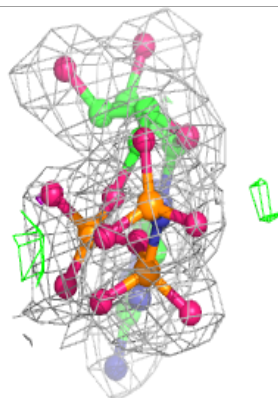
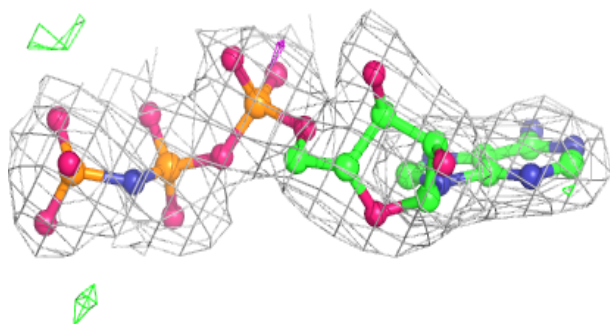
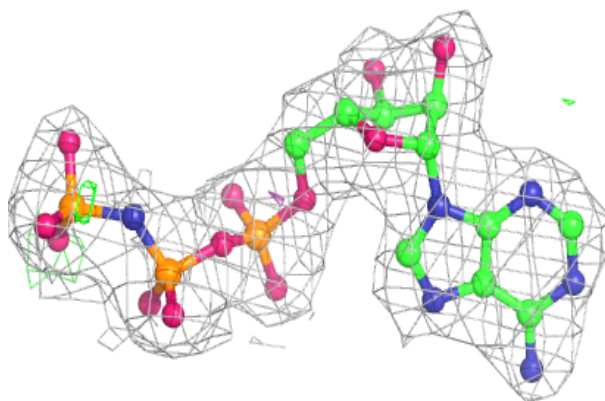
**Electron density around ANP C 600:**

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

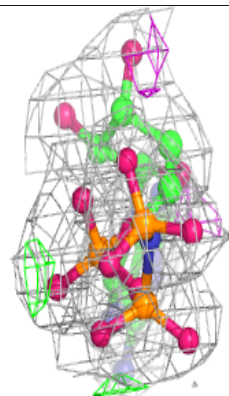
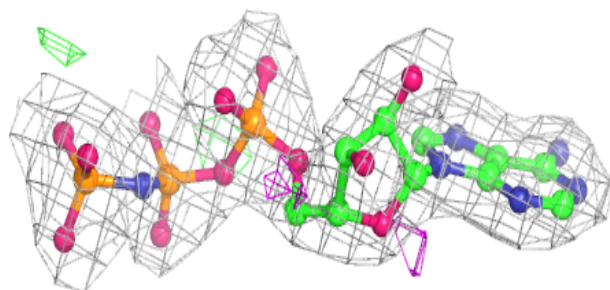
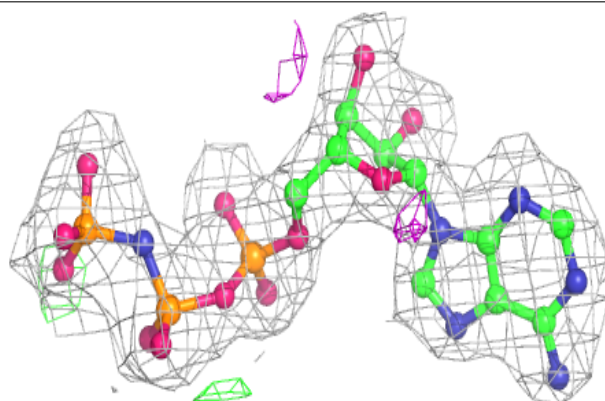


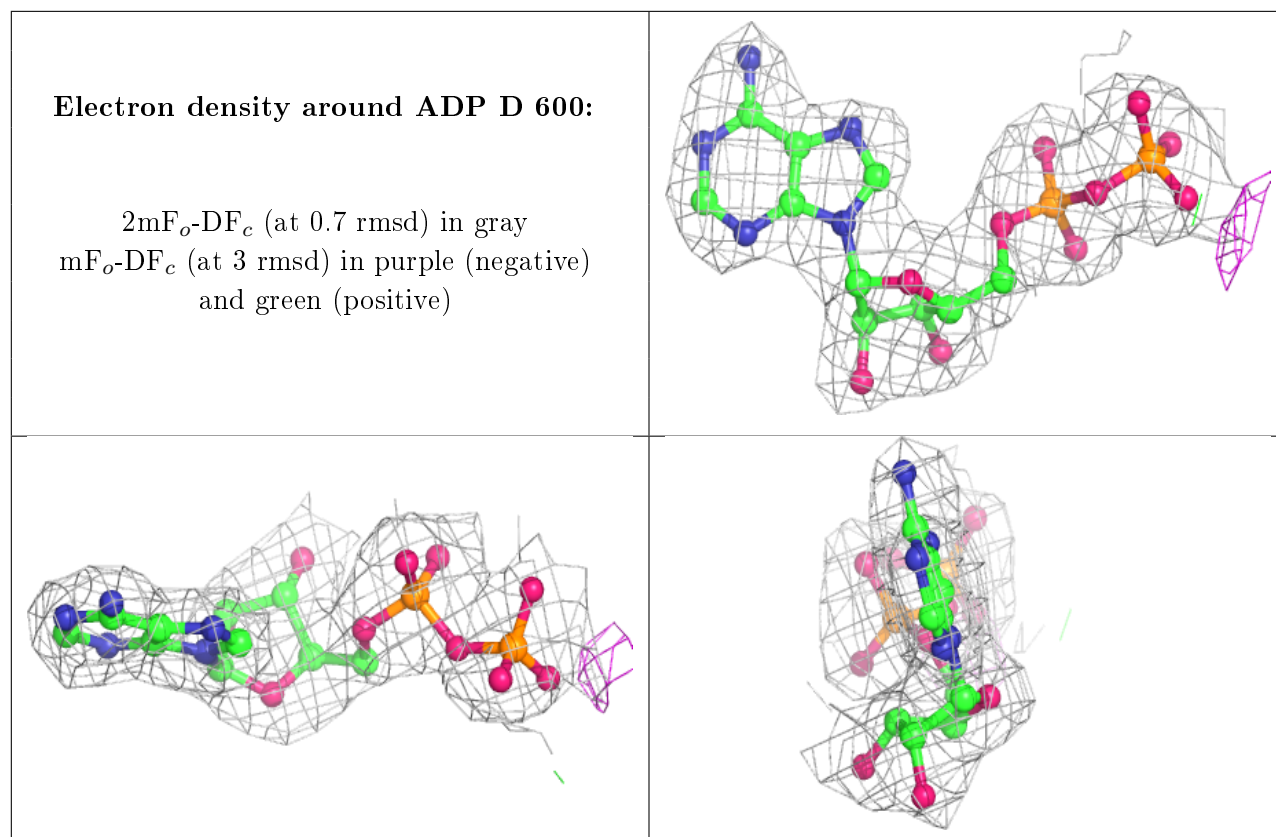
Electron density around ANP F 600:

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

**Electron density around ANP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.